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Standard

ISO/IEC 14888-4

**Information security — Digital
signatures with appendix —**

Part 4:
Stateful hash-based mechanisms

*Sécurité de l'information — Signatures digitales avec
appendice —*

Partie 4: Mécanismes basés sur le hachage dynamique

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Foreword

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The procedures used to develop this document and those intended for its further maintenance are described in the ISO/IEC Directives, Part 1. In particular, the different approval criteria needed for the different types of document should be noted. This document was drafted in accordance with the editorial rules of the ISO/IEC Directives, Part 2 (see www.iso.org/directives or www.iec.ch/members_experts/refdocs).

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This document was prepared by Joint Technical Committee ISO/IEC JTC 1, *Information technology*, Subcommittee SC 27, *Information security, cybersecurity and privacy protection*.

A list of all parts in the ISO/IEC 14888 series can be found on the ISO and IEC websites.

Any feedback or questions on this document should be directed to the user's national standards body. A complete listing of these bodies can be found at www.iso.org/members.html and www.iec.ch/national-committees.

Introduction

Digital signatures with appendix are designed to offer integrity, authentication and non-repudiation. ISO/IEC 14888-2 specifies the class of digital signature mechanisms in which the security is based on the difficulty of integer factorization. ISO/IEC 14888-3 specifies the class in which the security is based on computing discrete logarithms. Unfortunately, if and when a large-scale general purpose quantum computer becomes available, all of these techniques will no longer be secure for practical key sizes.^[1]

This document specifies a class of digital signatures whose security depends only on the security of the underlying hash function. At the time of publication of this document, standardized hash functions are believed to be secure even against attacks using large scale quantum computers. Hence, the schemes specified in this document do not suffer from the same problems as the schemes specified in ISO/IEC 14888-2 and ISO/IEC 14888-3.

The hash-based signature (HBS) schemes specified in this document are stateful schemes, whereby the private key is part of the state of the scheme. This means that at every signature generation, state information held by the signer must be updated, as otherwise the security of the scheme is compromised. Therefore, when deploying any of the schemes specified in this document, it is expected that robust state-management practices are implemented to ensure that state information is correctly updated.

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Information security — Digital signatures with appendix —

Part 4: Stateful hash-based mechanisms

1 Scope

This document specifies stateful digital signature mechanisms with appendix, where the level of security is determined by the security properties of the underlying hash function.

This document also provides requirements for implementing basic state management, which is needed for the secure deployment of the stateful schemes described in this document.

2 Normative references

There are no normative references in this document.

3 Terms and definitions

For the purposes of this document, the following terms and definitions apply.

ISO and IEC maintain terminology databases for use in standardization at the following addresses:

- ISO Online browsing platform: available at <https://www.iso.org/obp>
- IEC Electropedia: available at <https://www.electropedia.org/>

3.1 authentication path

list of hash values that show that a specific node belongs to a *Merkle tree* (3.5)

3.2 balanced binary tree

ordered tree in which each node has exactly two other nodes that are directly subordinate

3.3 binary tree

ordered tree in which each node has at most two other nodes that are directly subordinate

[SOURCE: ISO/IEC-2382:2015, 2121636, modified — notes to entry have been removed.]

3.4 L-tree

unbalanced *binary tree* (3.3) used to compress the Winternitz+ One-Time Signature Scheme (WOTS+) public keys in the eXtended Merkle Signature Scheme (XMSS)

3.5 Merkle tree

balanced binary tree (3.2), where each node of the tree corresponds to the hash of the labels of the child nodes

3.6 one-time signature

digital signature scheme where the security is limited to signing a single message for a given key pair

3.7

**state
state information**

information regarding key usage stored with an eXtended Merkle Signature Scheme (XMSS) or Leighton-Micali signature scheme (LMS) private key

3.8

state management

processes by which the *state* (3.7) is updated with each signature

Note 1 to entry: This is a crucial part of any stateful hash-based signature, as incorrect state information can lead to signature forgeries.

3.9

Winternitz parameter

parameter in the Winternitz *one-time signature* (3.6) scheme, which allows a trade-off between signature size and computation time

4 Symbols and abbreviated terms

4.1 Symbols

$0x00$	the hexadecimal representation of the 0 byte
$a b$	concatenation of the bit sequences a and b in the order specified
$a * b$	multiplication of a and b
$a \& b$	bitwise logical AND of two bit strings a and b
$a \text{ XOR } b$	bitwise logical EXCLUSIVE OR of two bit strings a and b
$a \text{ mod } b$	the remainder when a is divided by b
$a \ll x$	the result of left-shifting a bit-string a by x positions (e.g. $0x08 \ll 1 = 0x10$)
$a \gg x$	the result of right-shifting a bit-string a by x positions (e.g. $0x08 \gg 1 = 0x04$)
$\text{ceil}(x)$	the least integer greater than or equal to x
d	the number of layers of sub-trees in XMSS-MT
$\text{floor}(x)$	the greatest integer less than or equal to x
h	total height of the Merkle tree (or hyper tree for XMSS-MT and HSS) NOTE 1 h is the parameter which controls the maximum number of signatures, which are given by 2^h .
$\text{lb}(x)$	the base 2 logarithm of x
n	the length in bytes of one element of the private key, public key or signature, and the length of the message representative
m	the arbitrary length message to be signed in XMSS, XMSS-MT, LM-OTS, LMS, and HSS
M'	the message representative signed in XMSS and XMSS-MT
$\text{toByte}(x,y)$	computation of the y -byte string containing the binary representation of x in big-endian byte order

w	the Winternitz parameter used in the XMSS and XMSS-MT algorithms
	NOTE 2 w controls the trade-off between computation time and signature size. Smaller values of w/W lead to faster computations, while larger values of w lead to smaller signatures.
W	the Winternitz parameter used in the LMS and HSS algorithms. W and w are related as follows: $w = 2^W$.
$x[i]$	the i th element of the array x
$[X]_y$	the result of truncating X to its leftmost y bits, e.g. $[0\text{x}fe]_4 = 0\text{x}f$

4.2 Abbreviated terms

HBS	hash-based signature
HSS	hierarchical signature scheme
LMS	Leighton-Micali signature scheme
OTS	one-time signature
RBG	random bit generator
WOTS+	Winternitz+ One-Time signature scheme
XMSS	eXtended Merkle Signature Scheme
XMSS-MT	eXtended Merkle Signature Scheme Multi Tree

5 XMSS and XMSS-MT

5.1 General

The XMSS scheme is a stateful hash-based signature scheme for which only a limited number of signatures can be created using a particular private key. The security of XMSS is based on the hardness of the Target Collision Resistance (TCR) problem, and XMSS has been proven to be secure in the standard model (see Reference [13]).

The XMSS-MT scheme, a variant of the XMSS scheme, is a stateful hash-based signature scheme that supports a larger number of signatures than XMSS. XMSS-MT inherits all the security properties of XMSS.[14]

The OIDs for these algorithms shall be in accordance with [Annex A](#). Test vectors can be found in [Annex C](#).

5.2 Common building blocks

5.2.1 General

The XMSS and the XMSS-MT schemes are described in a unified way since they employ common building blocks.

5.2.2 Address format

The *ADRS* input has three different address formats (see [Table 1](#)). Each layout is appropriate for a different step of the algorithms:

- the OTS address format is for the hash calls in the one-time signature schemes;
- the L-tree address format is for hashes used in the L-trees;

— the hash tree address format is for the Merkle-tree construction.

An L-tree is an unbalanced binary hash tree used to compute the leaves of the main XMSS binary hash tree.

Each *ADRS* address format consists of six 32-bit fields and one 64-bit field. The fields are encoded as unsigned integers. The *layerAddress* field refers to the layer in a multi-tree construction (0 if not using multi-trees). The *treeAddress* refers to the position (from left to right) of a tree in a multi-tree construction (0 if not using multi-trees). The *field* type differentiates the three *ADRS* layouts: 0 for OTS, 1 for L-tree and 2 for Hash tree. The field *keyAndMask* is used to distinguish if the hash call intends to generate a key (0) or a bitmask (1) for an OTS address. In the case of the L-tree and Hash tree address, *keyAndMask* is: (0) to generate a key, (1) to generate the most significant *n* bytes of the *2n*-byte bitmask and (2) to generate the least significant *n* bytes of the *2n*-byte bitmask.

Table 1 — XMSS address formats

OTS address	L-tree address	Hash tree address
+-----+ layerAddress (32 bits) +-----+	+-----+ layerAddress (32 bits) +-----+	+-----+ layerAddress (32 bits) +-----+
+-----+ treeAddress (64 bits) +-----+	+-----+ treeAddress (64 bits) +-----+	+-----+ treeAddress (64 bits) +-----+
+-----+ type = 0 (32 bits) +-----+	+-----+ type = 1 (32 bits) +-----+	+-----+ type = 2 (32 bits) +-----+
+-----+ OTSAddress (32 bits) +-----+	+-----+ ltreeAddress (32 bits) +-----+	+-----+ padding = 0 (32 bits) +-----+
+-----+ chainAddress (32 bits) +-----+	+-----+ treeHeight (32 bits) +-----+	+-----+ treeHeight (32 bits) +-----+
+-----+ hashAddress (32 bits) +-----+	+-----+ treeIndex (32 bits) +-----+	+-----+ treeIndex (32 bits) +-----+
+-----+ keyAndMask (32 bits) +-----+	+-----+ keyAndMask (32 bits) +-----+	+-----+ keyAndMask (32 bits) +-----+

NOTE Each XMSS Address in this table is 32-bytes.

The field *OTSAddress* encodes the index of the OTS key pair within the tree, the *chainAddress* encodes the chain index and finally the *hashAddress* encodes the hash function call index within the chain.

In the L-tree address layout, the *ltreeAddress* field encodes the index of the leaf computed with this L-tree. The *treeHeight* encodes the height of the node used as input for the next computation inside the L-tree. The *treeIndex* encodes the index of the node at that height, inside the L-tree.

In the tree hash address format, the *padding* field is always 0. The *treeHeight* encodes the height of the tree node being used for the next computation, followed by the *treeIndex* which is the node index at that height. For the L-tree address layout, the *keyAndMask* field can be: 0 (key), 1 (first bitmask), and 2 (second bitmask).

5.2.3 Required cryptographic functions

5.2.3.1 General

The XMSS scheme uses the following cryptographic primitives:

- Keyed Hash-Function $F(KEY, M)$, where *KEY* is an *n*-byte key, *M* is an *n*-byte message and the output is *n* bytes.
- Keyed Hash-Function $H(KEY, M)$, where *KEY* is an *n*-byte key, *M* is a *2n*-byte message and the output is *n* bytes.
- Keyed Hash-Function $H_msg(KEY, M)$, where *KEY* is a *3n*-byte key, *M* is an arbitrary length message and the output is *n* bytes.
- Pseudo-Random Function $PRF(KEY, M)$, where *KEY* is an *n*-byte key, *M* is a 32-byte message and the output is *n* bytes.

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- Pseudo-Random Function $\text{PRF}_{\text{Keygen}}(\text{KEY}, M)$, where KEY is an n -byte key, M is a 32-byte message and the output is n bytes. This function is optional and only used if WOTS+ private keys are generated pseudo-randomly.
- Pseudo-Random Function $\text{PRF}_{\text{Keygen_MT}}(\text{KEY}, M)$, where KEY is an n -byte key, M is a 32-byte message and the output is n bytes. This function is only used in XMSS_keygen if called from XMSS_MT_keygen.
- A non-deterministic random number generator RBG that provides at least a security level of $8n$ bits.

These functions shall be implemented with SHA2-256 (Dedicated Hash-Function 4 defined in ISO/IEC 10118-3), SHAKE256 (see ISO/IEC 10118-3:2018, C.2) as described below (see [Annex B](#) for further considerations on these instantiations).

5.2.3.2 Functions Based on SHA2-256

When using SHA2-256 as the underlying hash function and $n=32$, the following constructions shall be used.

- $F(\text{KEY}, M)$: SHA2-256(toByte(0, 32) || KEY || M)
- $H(\text{KEY}, M)$: SHA2-256(toByte(1, 32) || KEY || M)
- $H_{\text{msg}}(\text{KEY}, M)$: SHA2-256(toByte(2, 32) || KEY || M)
- $\text{PRF}(\text{KEY}, M)$: SHA2-256(toByte(3, 32) || KEY || M)
- $\text{PRF}_{\text{Keygen}}(\text{KEY}, M)$: SHA2-256(toByte(4, 32) || KEY || M)
- $\text{PRF}_{\text{Keygen_MT}}(\text{KEY}, M)$: SHA2-256(toByte(5, 32) || KEY || M)

When using SHA2-256 as the underlying hash function and $n=24$, the following constructions shall be used.

- $F(\text{KEY}, M)$: SHA2-256/192(toByte(0, 4) || KEY || M)
- $H(\text{KEY}, M)$: SHA2-256/192(toByte(1, 4) || KEY || M)
- $H_{\text{msg}}(\text{KEY}, M)$: SHA2-256/192(toByte(2, 4) || KEY || M)
- $\text{PRF}(\text{KEY}, M)$: SHA2-256/192(toByte(3, 4) || KEY || M)
- $\text{PRF}_{\text{Keygen}}(\text{KEY}, M)$: SHA2-256/192(toByte(4, 4) || KEY || M)
- $\text{PRF}_{\text{Keygen_MT}}(\text{KEY}, M)$: SHA2-256/192(toByte(5, 4) || KEY || M)

5.2.3.3 Functions Based on SHAKE

When using SHAKE256 and $n=32$, the following constructions shall be used.

- $F(\text{KEY}, M)$: SHAKE256(toByte(0, 32) || KEY || M , 256)
- $H(\text{KEY}, M)$: SHAKE256(toByte(1, 32) || KEY || M , 256)
- $H_{\text{msg}}(\text{KEY}, M)$: SHAKE256(toByte(2, 32) || KEY || M , 256)
- $\text{PRF}(\text{KEY}, M)$: SHAKE256(toByte(3, 32) || KEY || M , 256)
- $\text{PRF}_{\text{Keygen}}(\text{KEY}, M)$: SHAKE256(toByte(4, 32) || KEY || M , 256)
- $\text{PRF}_{\text{Keygen_MT}}(\text{KEY}, M)$: SHAKE256(toByte(5, 32) || KEY || M , 256)

When using SHAKE256 and $n=24$, the following constructions shall be used.

- $F(\text{KEY}, M)$: SHAKE256(toByte(0, 4) || KEY || M , 192)
- $H(\text{KEY}, M)$: SHAKE256(toByte(1, 4) || KEY || M , 192)

- $H_msg(KEY, M)$: SHAKE256(toByte(2, 4) || KEY || M , 192)
- $PRF(KEY, M)$: SHAKE256(toByte(3, 4) || KEY || M , 192)
- $PRF_{Keygen}(KEY, M)$: SHAKE256(toByte(4, 4) || KEY || M , 192)
- $PRF_{Keygen_MT}(KEY, M)$: SHAKE256(toByte(5, 4) || KEY || M , 192)

5.2.4 Auxiliary functions

5.2.4.1 General

Both XMSS and XMSS-MT make use of two auxiliary functions, namely the *base_w* function and the chain function. The specifications of these auxiliary functions are given in [5.2.4.2](#) and [5.2.4.3](#).

5.2.4.2 *base_w* auxiliary function

This function is used in the signing and verification process to convert a string of bytes into a sequence of base w integers (i.e. integers between 0 and $w-1$).

Algorithm: $base_w(X, w, out_len)$.

Input: A sequence of bytes $X = X[0], \dots, X[len_x - 1]$ of length len_x , the base w which shall be 4 or 16, and the output length out_len .

Output: A sequence of integers $Q = Q[0], \dots, Q[out_len-1]$ of length out_len from the set $\{0, 1, \dots, w-1\}$

Steps:

- a) Set $in = 0, out = 0, total = 0, bits = 0$.
- b) For i from 0 to $out_len - 1$:
 - 1) If $bits$ is equal to 0 then
 - i) Set $total = X[in]$.
 - ii) Set $in = in + 1$.
 - iii) Set $bits = 8$.
 - 2) Set $bits = bits - \text{lb}(w)$.
 - 3) Set $Q[out] = (total \gg bits) \& (w - 1)$.
 - 4) Set $out = out + 1$.
- c) Return Q .

5.2.4.3 Chain auxiliary function

The chain function is the main building block of the XMSS and XMSS-MT schemes. This is the function used multiple times to produce the public key and signature from the private key material.

Algorithm: $chain(X, i, s, SEED, ADRS)$.

Input: A string X , starting index i , length s of the hash chain to be computed, n -byte value $SEED$, 32-byte value $ADRS$ formatted as an OTS address according to [Table 1](#).

Output: An n -byte value output

Steps:

- a) If s is equal to 0, then return X .
- b) If $(i + s) > w - 1$, then return $NULL$.
- c) Set $tmp = \text{chain}(X, i, s - 1, SEED, ADRS)$.
- d) Set $ADRS.hashAddress = (i + s - 1)$.
- e) Set $ADRS.keyAndMask = 0$.
- f) Set $KEY = \text{PRF}(SEED, ADRS)$.
- g) Set $ADRS.keyAndMask = 1$.
- h) Set $BM = \text{PRF}(SEED, ADRS)$.
- i) Return $F(KEY, tmp \text{ XOR } BM)$.

5.2.5 WOTS+ One-Time Signature Auxiliary Scheme

5.2.5.1 General

Both XMSS and XMSS-MT make use of an underlying one-time signature scheme called WOTS+. A one-time signature scheme has limited applicability because a signing key can only be used to sign a single message. If the same one-time signing key is used twice, the scheme loses its security guarantees (in particular, signature forgery becomes possible). WOTS+ shall not be used outside the context of XMSS and XMSS-MT. [5.2.5.2](#) gives the definition of WOTS+ key generation, signing and verification, which are algorithms used by XMSS/XMSS-MT key generation, signing and verification, respectively.

5.2.5.2 WOTS+ key generation

5.2.5.2.1 General

[5.2.5.2.2](#), [5.2.5.2.3](#) and [5.2.5.2.4](#) describe the key generation process for WOTS+. There are two possible methods to create the private key: 1) generate the private key from a single seed ([5.2.5.2.2](#)), and 2) generate a uniform random private key ([5.2.5.2.3](#)). The main difference is that the method described in [5.2.5.2.2](#) is more memory-efficient as it uses a pseudo-random function to generate all WOTS+ private key elements from a single seed, while the one described in [5.2.5.2.3](#) does not introduce an additional security assumption regarding the pseudo-random function step.

Throughout the document, various other algorithms are required to generate WOTS+ private keys. For those, it is always assumed that the pseudo-random method described in [5.2.5.2.2](#) is used. Trivial changes (omitted for simplicity) to these algorithms are allowed so that the method described in [5.2.5.2.3](#) is used instead, at the cost of storing all WOTS+ private keys. The public key generation given in [5.2.5.2.4](#) is the same for both private key generation methods.

5.2.5.2.2 WOTS+ Private Key (pseudo-random)

This algorithm generates a WOTS+ private key. This method is called by the XMSS and XMSS-MT signatures schemes and makes use of SK_S , which works as a seed for the generation of all WOTS+ private keys. This method also receives an index idx which specifies what WOTS+ private key is required to be generated (among the 2^h possible ones), and the layer L and tree address T to identify the XMSS sub-tree (relevant when using the XMSS-MT variant).

Algorithm: $\text{WOTS+_generate_privkey}(SK_S, SEED, idx, L, T)$.

Input: An n -byte string SK_S , public seed $SEED$, an integer idx , layer L , tree address T .

Output: A sequence of n -byte values sk of length len .

Steps:

- a) Set $ADRS = \text{toByte}(0, 32)$.
- b) Set $ADRS.\text{layerAddress} = L$.
- c) Set $ADRS.\text{treeAddress} = T$.
- d) Set $ADRS.\text{OTSAddress} = \text{idx}$.
- e) Set $ADRS.\text{hashAddress} = 0$.
- f) For i from 0 to $len - 1$:
 - 1) Set $ADRS.\text{chainAddress} = i$.
 - 2) Set $sk[i] = \text{PRF}_{\text{Keygen}}(SK_S, SEED || ADRS)$
- g) Return sk .

5.2.5.2.3 WOTS+ private key (random)

This algorithm generates a WOTS+ private key.

Algorithm: $\text{WOTS+_generate_privkey_random}()$.

Input: None.

Output: A sequence of n -byte values sk of length len .

Steps:

- a) For i from 0 to $len - 1$:
 - 1) Let $sk[i]$ be an n -byte string from the output generation function of an RBG
- b) Return sk .

5.2.5.2.4 WOTS+ public key

This algorithm generates a WOTS+ public key from a private key. It should be noted that the $SEED$ used here is public information that is also made available to the verifier.

Algorithm: $\text{WOTS+_generate_pubkey}(sk, SEED, ADRS)$.

Input: Sequence of n -byte strings sk of length len , n -byte $SEED$, a 32-byte $ADRS$ formatted as an OTS address according to [Table 1](#).

Output: Sequence of n -byte strings pk of length len .

Steps:

- a) For i from 0 to $len - 1$:
 - 1) Set $ADRS.\text{chainAddress} = i$.
 - 2) Set $pk[i] = \text{chain}(sk[i], 0, w - 1, SEED, ADRS)$.
- b) Return pk .