InfoChem Standardization Rules for Structures

V 4.21

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1 Structure Checking

1.1 Reading Structure

1.1.1 Checking for Molecule Size

If the structure from input contains more than 999 atoms and/or 1050 bonds, this structure will not be processed and an error message will be issued:

"ERROR: TOO MANY ATOMS, STRUCTURE SKIPPED"
"ERROR: TOO MANY BONDS, STRUCTURE SKIPPED"

1.2 Structural Checks

1.2.1 Checking and Replacing Alias Groups

When reading structures from SD or RD files, alias groups will be replaced with structural fragments read from an alias definition file if possible. If that file cannot be found a message will be issued:

"WARNING: ALIAS DEFINITION FILE NOT AVAILABLE"

If an alias group is detected, a warning will be issued:

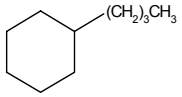
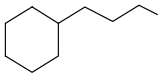
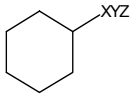
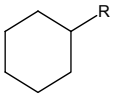
"WARNING: ALIAS ATOM DETECTED: *alias text*"

If an alias group is replaced by a structural fragment, a warning will be issued:

"WARNING: ALIAS ATOM REPLACED: *alias text* --> STRUCTURE "

If no structural fragment is available it will be checked whether the alias text corresponds to a chemical element symbol. In that case the alias atom will be replaced by the chemical element, in all other cases it is replaced by a R-atom and a warning will be issued:

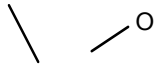
"WARNING: UNKNOWN ALIAS DETECTED: *alias text*"
"WARNING: ALIAS ATOM REPLACED: *alias text* --> R-GROUP"

Example	Original representation	Standardized representation	Message Text
			"WARNING: ALIAS ATOM DETECTED: (CH2)3CH3" "WARNING: ALIAS ATOM REPLACED: (CH2)3CH3 → STRUCTURE"
			"WARNING:ALIAS ATOM DETECTED:XYZ" "WARNING: UNKNOWN ALIAS DETECTED: XYZ" "WARNING: ALIAS ATOM REPLACED: XYZ → R-GROUP" "WARNING: QUERY OR ILLEGAL ATOMS DETECTED, structure will be only checked partially"

1.2.2 Check for Multi Component Structures

A message will be created if the input structure consists of more than one component.

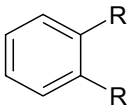
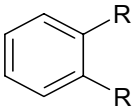
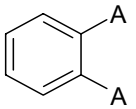
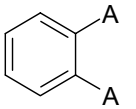
"INFO: multi component structure in input"

Example	Original representation	Standardized representation	Message Text
			"INFO: multi component structure in input"

1.2.3 Check for Query or Generic Structures

A message will be created if the structure contains query features or is of type generic.

"WARNING: QUERY OR ILLEGAL ATOMS DETECTED,
structure will be checked only partially"

Example	Original representation	Standardized representation	Message Text
			"WARNING: QUERY OR ILLEGAL ATOMS DETECTED, structure will be checked only partially"
			"WARNING: QUERY OR ILLEGAL ATOMS DETECTED, structure will be checked only partially"

1.2.4 Check and Correction of Molecular Charge

All atoms with valence zero, transition metal atoms without charge and atoms in an unusual valence state bearing no charge or radical electrons will be assigned reversibly a charge determined by application of the “octet rule”.

Some special cases apply:

- Elements of the first main group of the periodic table of the elements:

  All atoms with valence zero will be assigned irreversibly charge = +1, except Hydrogen which will be assigned reversibly +1 or –1 if a transition metal atom is present.

  "WARNING: MISSING CHARGE AT UNCONNECTED ATOM (H, Li, Na, K etc.)"
  "WARNING: ATOM CHARGES MODIFIED"

- Elements of the second main group of the periodic table of the elements:

  All atoms with valence zero will be assigned irreversibly charge = +2

  "WARNING: MISSING CHARGE AT UNCONNECTED ATOM (Be, Mg, Ca, Sr etc.)"
  "WARNING: ATOM CHARGES MODIFIED"

- Elements of the third main group of the periodic table of the elements:

  All atoms with valence zero will be assigned irreversibly charge = +3.

  "WARNING: MISSING CHARGE AT UNCONNECTED ATOM (B, Al, Ga etc.)"
  "WARNING: ATOM CHARGES MODIFIED"

  All atoms with valence IV will be assigned irreversibly charge = -1

  "WARNING: MISSING CHARGE AT ATOM WITH VALENCE 4 (B, Al, Ga etc.)"
  "WARNING: ATOM CHARGES MODIFIED"

- Elements of the fourth main group of the periodic table of the elements:

  Carbon with valence II will be assigned irreversibly two radicals and charge = 0 (carbene).

  "WARNING: VALENCE 2 AT C-ATOM "

  Carbon atoms with more than 4 bonds will be reported.

  "WARNING: EXCEEDED VALENCE AT C-ATOM "

  Charged, 4-bonded Carbon atoms will be reported

  "WARNING: CHARGED C-ATOM WITH VALENCE 4"

- Elements of the fifth main group of the periodic table of the elements:

  Nitrogen with valence zero will be assigned reversibly charge = –3,

  "WARNING: MISSING CHARGE AT UNCONNECTED N-ATOM "
  "WARNING: ATOM CHARGES MODIFIED"

  Nitrogen with valence I will be assigned irreversibly two radicals and a charge = 0 (nitrene).

  "WARNING: VALENCE 1 AT N-ATOM "

  Nitrogen with valence IV will be assigned irreversibly charge = +1, all other elements will be assigned reversibly charge = +1.

  "WARNING: MISSING CHARGE AT ATOM WITH VALENCE 4 (N, P, As etc.)"
  "WARNING: ATOM CHARGES MODIFIED"

  All atoms with valence V will be assigned irreversibly charge = 0.

- Elements of the sixth main group of the periodic table of the elements:

  Oxygen with valence zero will be assigned irreversibly charge = -2

  "WARNING: MISSING CHARGE AT UNCONNECTED O-ATOM "
  "WARNING: ATOM CHARGES MODIFIED"

  Oxygen with valence I will be assigned irreversibly charge = -1

  "WARNING: MISSING CHARGE AT 1-BONDED O-ATOM "
  "WARNING: ATOM CHARGES MODIFIED"

  Oxygen with valence III will be assigned irreversibly charge = +1

  "WARNING: MISSING CHARGE AT 3-BONDED O-ATOM "
  "WARNING: ATOM CHARGES MODIFIED"

  All other elements with valence IV will be assigned irreversibly charge = 0,

  with valence V will be assigned reversibly charge = -1,

  "WARNING: MISSING CHARGE AT 5-BONDED ATOM (O, S, Se etc.)"
  "WARNING: ATOM CHARGES MODIFIED"

  and with valence VI will be assigned reversibly charge = 0.

- Elements of the seventh main group of the periodic table of the elements:

  All atoms with valence zero will be assigned irreversibly charge = -1

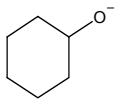
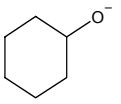
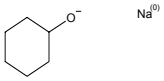
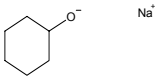
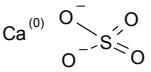
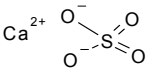
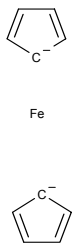
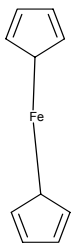
  "WARNING: MISSING CHARGE AT UNCONNECTED HALOGEN-ATOM "
  "WARNING: ATOM CHARGES MODIFIED"

  with valence VII will be assigned reversibly charge = 0.

Using these assigned charges the overall charge of the structure is calculated. If the overall charge equals zero, then reversibly assigned charges are accepted. If the overall charge does not equal zero, reversibly assigned charges will partly be removed.

If the resulting overall charge does not equal zero an information message will be issued:

"INFO: molecule charge not zero"

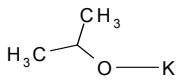
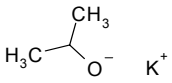
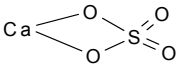
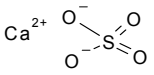
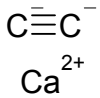
Example	Original representation	Standardized representation	Message Text
			"INFO: molecule charge not zero"
			"INFO: multi component structure in input" "WARNING: MISSING CHARGE AT UNCONNECTED ATOM (H, Li, Na, K etc.)" "WARNING: ATOM CHARGES MODIFIED"
			"INFO: multi component structure in input" "WARNING: MISSING CHARGE AT UNCONNECTED ATOM (Be,Mg,Ca,Sr etc.)" "WARNING: ATOM CHARGES MODIFIED"
			"INFO: multi component structure in input" "WARNING: MISSING CHARGE AT UNCONNECTED ATOM" "WARNING: ATOM CHARGES MODIFIED" "WARNING: IONIC COMPONENTS CONNECTED"

1.3 Representation of Functional Groups

1.3.1 Standardization of Functional Groups

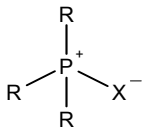
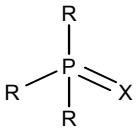
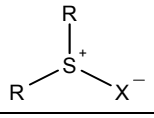
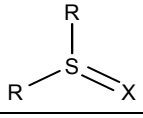
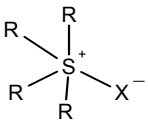
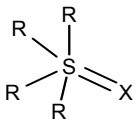
1.3.1.1 MDL Conventions

Structures will be represented using standard MDL conventions. Therefore some covalent structures have to be separated into ionic components.

Example	Original representation	Standardized representation	Message Text
Alkali Alcoholates			"INFO: structure modified" "WARNING: CHARGE SEPARATION CREATED" "WARNING: SIGMA BOND BROKEN" "INFO: multicomponent structure after check"
Complex ions and Q=Q-O^{i-} substructures			"INFO: structure modified" "WARNING: CHARGE SEPARATION CREATED" "WARNING: SIGMA BOND BROKEN" "INFO: multicomponent structure after check"
Carbon to group IIa			"INFO: structure modified" "WARNING: CHARGE SEPARATION CREATED" "WARNING: SIGMA BOND BROKEN" "INFO: multicomponent structure after check"

1.3.1.2 Removing of Charge Separations

Charge separations in “Zwitter ions” will be removed if possible.

Example	Original representation	Standardized representation	Message Text
4-bonded P-Atoms			"INFO: CHARGE SEPARATION DETECTED" "WARNING: CHARGE SEPARATION REMOVED"
3-bonded S-Atoms			"INFO: CHARGE SEPARATION DETECTED" "WARNING: CHARGE SEPARATION REMOVED"
5-bonded S-Atoms			"INFO: CHARGE SEPARATION DETECTED" "WARNING: CHARGE SEPARATION REMOVED"

1.3.1.3 Treatment of Radicals

Atoms with radical electrons are detected and an information message will be issued:

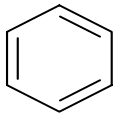
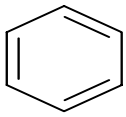
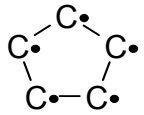
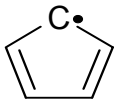
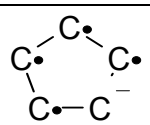
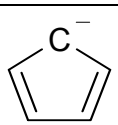
"INFO: free radicals in input"

Radicalic representations of π-systems with an even number of radicals will be converted to normal π-systems with multiple bonds if possible. An information message will be issued:

"INFO: pi-system cleaned"

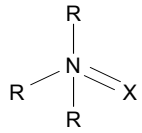
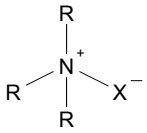
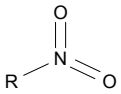
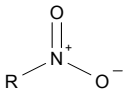
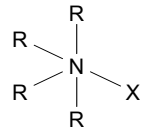
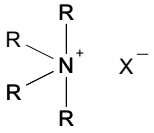
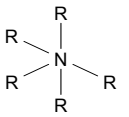
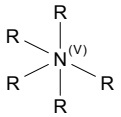
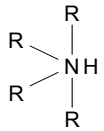
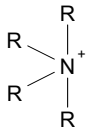
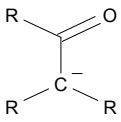
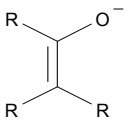
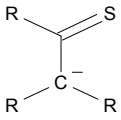
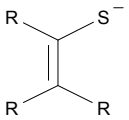
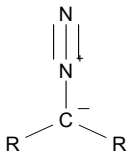
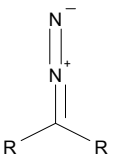
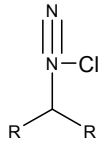
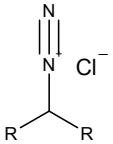
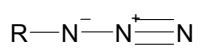
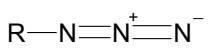
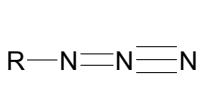
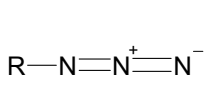
If this cleaning failed an information message will be issued:

"INFO: free radicals after check"

Example	Original representation	Standardized representation	Message Text
			"INFO: free radicals in input" "INFO: pi-system cleaned"
			"INFO: free radicals in input" "INFO: pi-system cleaned" "INFO: free radicals after check"
			"INFO: molecule charge not zero" "INFO: free radicals in input " "INFO: pi-system cleaned"

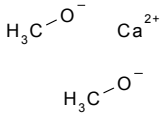
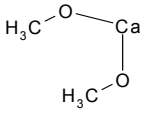
1.3.1.4 Standardization of Functional Groups

Additionally, atoms in an unusual valence state or unusual representations of functional groups will be converted into a standardized representation.

Functional group	Original representation	Standardized representation	Message Text
5-bonded N-Atoms			"INFO: structure modified" "WARNING: CHARGE SEPARATION CREATED"
Nitro group			"INFO: structure modified" "WARNING: CHARGE SEPARATION CREATED"
5-bonded N-Atoms			"INFO: structure modified" "WARNING: CHARGE SEPARATION CREATED" "WARNING: SIGMA BOND BROKEN" "INFO: multicomponent structure after check"
5-bonded N-Atoms			"ERROR: UNCORRECTABLE ATOM"
5-bonded N-Atoms			"WARNING: MISSING CHARGE AT ATOM WITH VALENCE 4 (N, P, As etc.)" "WARNING: ATOM CHARGES MODIFIED" "INFO: molecule charge not zero"
Enolate group			"INFO: molecule charge not zero" "INFO: enolate group cleaned"
thio-enolate group			"INFO: molecule charge not zero" "INFO: thio-enolate group cleaned"
diazo group			"INFO: diazo group cleaned"
Diazonium salt			"INFO: structure modified" "WARNING: CHARGE SEPARATION CREATED" "WARNING: SIGMA BOND BROKEN" "INFO: multicomponent structure after check"
azide			"INFO: azide group cleaned" "WARNING: BAD DRAWN ANGLE AT DOUBLE BOND"
azide			"INFO: structure modified" "WARNING: CHARGE SEPARATION CREATED" "INFO: azide group cleaned" "WARNING: BAD DRAWN ANGLE AT DOUBLE BOND"
Carbon monoxide			"INFO: Carbon Monoxide cleaned"

1.3.1.5 Connecting Unconnected (Ionic) Components

Ionic structures will be connected to covalent structures according to MDL rules.

Example	Original representation	Standardized representation	Message Text
			"INFO: multicomponent structure in input" "WARNING: IONIC COMPONENTS CONNECTED"

1.4 Check for Drawing Errors

1.4.1 Check for Atom/Atom-Overlaps

The structural drawing is checked for atom/atom-overlaps and atom/bond-overlaps, probably indicating drawing errors leading to fragmentations of structures. A warning message will be issued:

"WARNING: ATOM/ATOM-OVERLAPS IN STRUCTURE"
"WARNING: ATOM/BOND-OVERLAPS IN STRUCTURE"

1.4.2 Check for Crossing Bonds

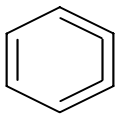
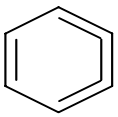
The structural drawing is checked for crossing bonds, probably indicating drawing errors leading to fragmentations of structures. An information message will be issued:

"WARNING: CROSSING BONDS IN STRUCTURE"

1.4.3 Check of Ring Systems

If a ring system contains cumulated multiple bonds a message will be issued:

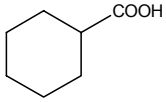
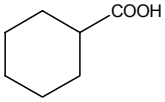
"WARNING: CUMULATED MULTIPLE BONDS IN RINGSYSTEM "

Example	Original representation	Standardized representation	Message Text
			"WARNING: CUMULATED MULTIPLE BONDS IN RINGSYSTEM"

1.4.4 Check for Superatoms

If the structure contains superatoms a message will be issued:

"INFO: Superatom detected "

Example	Original representation	Standardized representation	Message Text
			"INFO: Superatom detected: SUPERATOM "COOH" OF TYPE SUP"

1.4.5 Check of Stereochemistry

Stereocenters with relative configuration will be reported:

"INFO: relative stereocenter(s) detected"

Stereocenters with absolute configuration will be reported:

"INFO: absolute stereocenter(s) detected "

Double bonds with absolute configuration will be reported:

"INFO: absolute configuration at double bond(s) detected "

Stereo-Bonds not starting at a stereocenter will be reported:

"INFO: WRONG STEREOBOND(S) IN INPUT.
NOT STARTING FROM STEREOCENTER "

Stereo-Bonds ending at stereocenter will be reported:

"INFO: WRONG STEREOBOND(S) IN INPUT.
POINTING TO STEREOCENTER "

Double-bonds, connected by a stereo-bond of type 'either' will be reported:

"INFO: AMBIGUOUS CONFIGURATION AT DOUBLE BOND(S)"

Double-bonds with a substituent connected by a bond of type 'either', will be transformed to 'Dble Either'-bonds (crossed lines) and the 'either'-bond will be converted to a regular single bond:

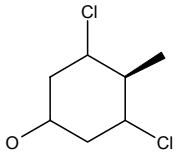
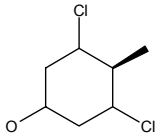
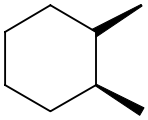
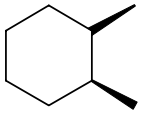
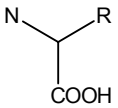
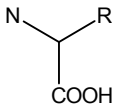
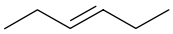
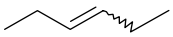
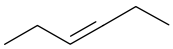
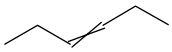
"INFO: double bond with unknown configuration converted "

Stereocenters (except at N-atoms) will be reported, where the configuration has not been specified by assigning up-/down-bonds to the substituents:

"INFO: unspecified stereo center(s)"

Linearly drawn substituents at double-bonds will be reported

"INFO: BAD DRAWN ANGLE AT DOUBLE BOND "

Example	Original representation	Standardized representation	Message Text
			"WARNING: COULD NOT ASSIGN STEREODESCRIPTOR(S)" "WARNING: WRONG STEREOBOND(S) IN INPUT. NOT STARTING FROM STEREOCENTER" "INFO: unspecified stereo center(s)"
			"INFO: relative stereocenter(s) detected WARNING: COULD NOT ASSIGN STEREODESCRIPTOR(S)" "WARNING: WRONG STEREOBOND(S) IN INPUT. NOT STARTING FROM STEREOCENTER" "INFO: unspecified stereo center(s)"
			"WARNING: QUERY OR ILLEGAL ATOMS DETECTED, structure will be checked only partially" "INFO: unspecified stereo center(s)"
			"INFO: absolute configuration at double bond(s) detected"
			"INFO: double bond with unknown configuration converted"
			"WARNING: BAD DRAWN ANGLE AT DOUBLE BOND"

1.5 General Rules for Atom Bonding in Organic Structures

	Group Ia Alkali metals	**Group IIa** Alkali earth metals	**Transition metals** (and lanthanides, actinides)	**Main group elements**	**Oxygen**	**Halogens**
Group Ia Alkali metals	Covalent	Covalent	Covalent	Covalent	Ionic	Ionic
Group IIa Alkali earth metals	Covalent	Covalent	Covalent	Covalent Exception: bonds between IIa and carbanions of alkenes or alkynes are ionic (1.3.1.1)	Covalent Exception: when a negatively-charged Q=Q-O substructure exist draw ionic (1.3.1.1)	Covalent
Transition metals (and lanthanides, actinides)	Covalent	Covalent	Covalent	No general rule defined	Covalent Exception: when a negatively-charged Q=Q-O substructure exist draw ionic (1.3.1.1)	Covalent
Main group elements	Covalent	Covalent Exception: bonds between IIa and carbanions of alkenes or alkynes are ionic (1.3.1.1)	No general rule defined	Covalent	Covalent	Covalent
Oxygen	Ionic	Covalent Exception: when a negatively-charged Q=Q-O substructure exist draw ionic (1.3.1.1)	Covalent Exception: when a negatively-charged Q=Q-O substructure exist draw ionic (1.3.1.1)	Covalent	Covalent	Covalent
Halogens	Ionic	Covalent	Covalent	Covalent	Covalent	Covalent

2 List of Program Messages

2.1 Error Messages

ERROR: TOO MANY ATOMS, STRUCTURE SKIPPED	**1.1. Reading structure** **Indicates a limitation of the program.** A record with too many atoms (current maximum allowed value 999) could not be processed by the program. The structure is skipped and replaced by a no structure.
ERROR: TOO MANY BONDS, STRUCTURE SKIPPED	**1.1. Reading structure** **Indicates a limitation of the program.** A record with too many bonds (current maximum allowed value 1050) could not be processed by the program. The structure is skipped and replaced by a no structure.
ERROR: ILLEGAL BOND TYPE	**1.1. Reading structure** **Indicates an input error.**
ERROR: ILLEGAL MASS SPECIFIED	**1.1. Reading structure** **Indicates an input error.**

2.2 Warnings

WARNING: EMPTY STRUCTURE FOUND	**1.1. Reading structure**
WARNING: ISOTOPE MASS OUT OF RANGE	**1.1. Reading structure** **Indicates an input error.**
WARNING: ALIAS DEFINITION FILE NOT AVAILABLE	**1.2.1 Checking for and replacing alias groups**
WARNING: UNEXPECTED QUERY OR ILLEGAL ATOMS DETECTED	**1.2 Structural Checks** Indicates R-Groups or Query-Atoms
WARNING: MISSING CHARGE AT UNCONNECTED ATOM	**1.2.4 Check Charges**
WARNING: MISSING CHARGE AT UNCONNECTED ATOM (H, Li, Na, K etc.)	**1.2.4 Check Charges**
WARNING: MISSING CHARGE AT UNCONNECTED ATOM (Be, Mg, Ca, Sr etc.)	**1.2.4 Check Charges**
WARNING: MISSING CHARGE AT UNCONNECTED ATOM (B, Al, Ga etc.)	**1.2.4 Check Charges**
WARNING: MISSING CHARGE AT ATOM WITH VALENCE 4 (B, Al, Ga etc.)	**1.2.4 Check Charges**

WARNING: MISSING CHARGE AT ATOM WITH VALENCE 4 (N, P, As etc.)	**1.2.4 Check Charges**
WARNING: MISSING CHARGE AT 5-BONDED ATOM (O, S, Se etc.)	**1.2.4 Check Charges**
WARNING: MISSING CHARGE AT UNCONNECTED HALOGEN-ATOM	**1.2.4 Check Charges**
WARNING: MISSING CHARGE AT UNCONNECTED O-ATOM	**1.2.4 Check Charges**
WARNING: MISSING CHARGE AT 1-BONDED O-ATOM	**1.2.4 Check Charges**
WARNING: MISSING CHARGE AT 3-BONDED O-ATOM	**1.2.4 Check Charges**
WARNING: MISSING CHARGE AT UNCONNECTED N-ATOM	**1.2.4 Check Charges**
WARNING: VALENCE 2 AT C-ATOM	**1.2.4 Check Charges**
WARNING: VALENCE 1 AT N-ATOM	**1.2.4 Check Charges**
WARNING: EXCEEDED VALENCE AT C-ATOM	**1.2.4 Check Charges**
WARNING: CHARGED C-ATOM WITH VALENCE 4	**1.2.4 Check Charges**
WARNING: NEGATIVE CHARGE AT METAL ATOM	**1.2.4 Check Charges**
WARNING: CUMULATED MULTIPLE BONDS IN RINGSYSTEM	**1.4.3 Check of Ring Systems**
ERROR: UNCORRECTABLE ATOM	**1.3.1. Standardization of functional groups** **Indicates an input error.** An atom with an illegal valence state could not be corrected.
WARNING: ATOM CHARGES MODIFIED	**1.3. Functional group standardization** **Indicates a structural modification.** While standardizing functional groups, charges at atoms were changed.
WARNING: SIGMA BOND BROKEN INTO IONS	**1.3. Functional group standardization** **Indicates a structural modification.** While standardizing functional groups, a single bond was broken into ions: X-Y --> X^+ + Y^-
WARNING: SIGMA BOND BROKEN	**1.3. Functional group standardization** **Indicates a structural modification.** While standardizing functional groups, a single bond was broken into uncharged fragments: X-Y --> X + Y
WARNING: DISCONNECTED H-ATOM REMOVED	**1.3. Functional group standardization** **Indicates a structural modification.** While standardizing functional groups, a disconnected H-atom has been removed
WARNING: CHARGE SEPARATION CREATED	**1.3. Functional group standardization** **Indicates a structural modification.** While standardizing functional groups, a double bond was replaced by a single bond: X=Y --> X^+-Y^-
WARNING: BOND ORDER REDUCED	**1.3. Functional group standardization** **Indicates a structural modification.** While standardizing functional groups, a double bond was replaced by a single bond: X=Y --> X-Y

WARNING: IONIC COMPONENTS CONNECTED	**1.3. Functional group standardization** **Indicates a structural modification.** Two ionic fragments were connected: $X^+ + Y^- \rightarrow X\text{-}Y$
WARNING: IONIC COMPONENTS RECONNECTED	**1.3. Functional group standardization** **Indicates a structural modification.** Two ionic fragments (previously created) were reconnected: $X^+ + Y^- \rightarrow X\text{-}Y$
WARNING: ERROR CONNECTING COMPONENTS	**1.3. Functional group standardization** **Indicates a structural modification.** Two ionic fragments could not be connected
WARNING: CHARGE SEPARATION REMOVED	**1.3. Functional group standardization** **Indicates a structural modification.** While standardizing functional groups, a single bond was replaced by a double bond: $X^+\text{-}Y^- \rightarrow X{=}Y$
WARNING: CHARGES REMOVED	**1.3. Functional group standardization** **Indicates a structural modification.** While standardizing functional groups, charges were removed
WARNING: ATOM/ATOM-OVERLAPS IN STRUCTURE	**1.4. Check for drawing errors** **Probably indicates a structural fragmentation in input.**
WARNING: ATOM/BOND-OVERLAPS IN STRUCTURE	**1.4. Check for drawing errors** **Probably indicates a structural fragmentation in input.**
WARNING: CROSSING BONDS IN STRUCTURE	**1.4. Check for drawing errors** **Probably indicates a structural fragmentation in input.**
WARNING: PI-CHECK ERROR	**1.3.1.3 Treatment of radicals**

2.3 Information Messages

INFO: Structure modified	
INFO: Structure will be checked only partially	**1.2 Structural Checks** Indicates R-Groups or Query-Atoms
INFO: molecule charge not zero	**1.2.4 Check Charges**
INFO: free radicals in input	**1.3.1.3 Treatment of radicals**
INFO: free radicals after check	**1.3.1.3 Treatment of radicals**
INFO: pi-system cleaned	**1.3.1.3 Treatment of radicals**
INFO: pi-system rearranged	**1.3.1.3 Treatment of radicals**
INFO: atomic coordinates modified	**1.3. Functional group standardization** The structural display was modified.
INFO: enolate group cleaned	**1.3. Functional group standardization** **Indicates a structural modification.**
INFO: thio-enolate group cleaned	**1.3. Functional group standardization** **Indicates a structural modification.**
INFO: fulminate group cleaned	**1.3. Functional group standardization** **Indicates a structural modification.**
INFO: thio-fulminate group cleaned	**1.3. Functional group standardization** **Indicates a structural modification.**
INFO: diazo group cleaned	**1.3. Functional group standardization** **Indicates a structural modification.**
INFO: azide group cleaned	**1.3. Functional group standardization** **Indicates a structural modification.**
INFO: Carbon Monoxide cleaned	**1.3. Functional group standardization** **Indicates a structural modification.**