Cause-Effect Structures Behaving like Reaction System

Ludwik Czaja
Vistula University
University of Warsaw

1. Informal exposition of cause-effect (c-e) structures

2. Sketch of formalism

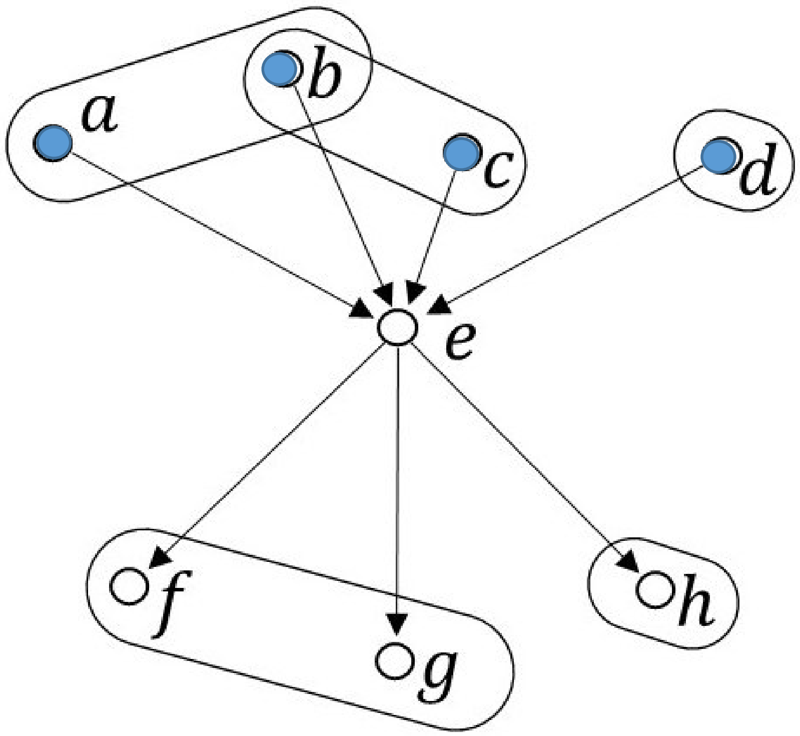
3. Examples

4. Basic notions of c-e structures

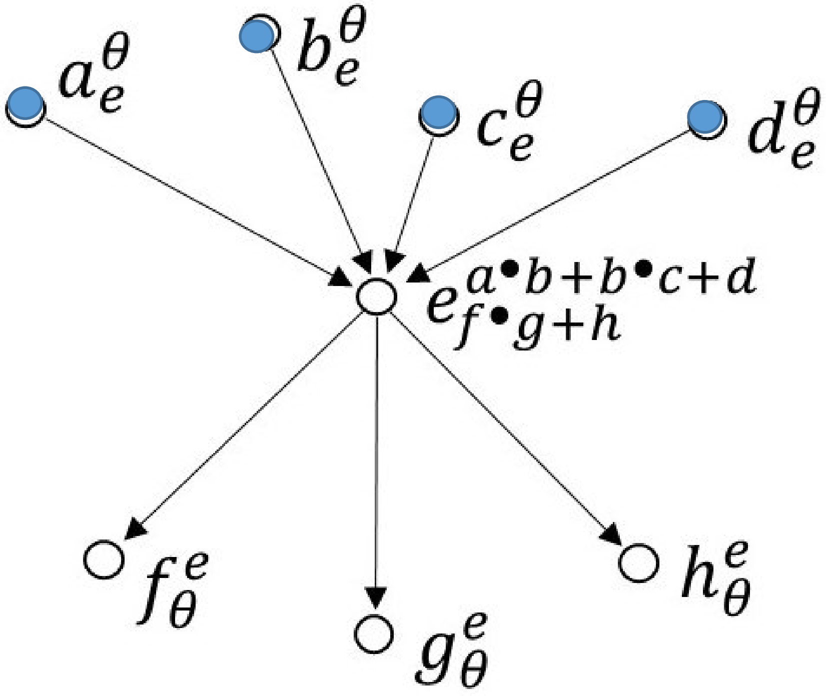
5. Basic notions of reaction systems

6. Examples

Informal presentation of of cause-effect structures



Graphic representation
with grouping of nodes



Upper (entry - causes) and lower (exit - effects) formal polynomials annotaing nodes and determining movement of signals: „•” – simultaneous, „+” – nondeterministic. Hence: arrows redundant – for visualization only!

Two other representations:

Set (of names) of nodes with superscript/subscript formal polynomials:

$$U = \{a_e^\theta, b_e^\theta, c_e^\theta, d_e^\theta, e_{f\bullet g+h}^{a\bullet b+b\bullet c+d}, f_\theta^e, g_\theta^e, h_\theta^e\}$$

Arrow expression:

$$(a\rightarrow e)\bullet(b\rightarrow e)+(b\rightarrow e)\bullet(c\rightarrow e)+(d\rightarrow e)+(e\rightarrow f)\bullet(e\rightarrow g)+(e\rightarrow h)$$

which may be reduced to:

$$(b\rightarrow e)\bullet[(a\rightarrow e)+(c\rightarrow e)]+(d\rightarrow e)+(e\rightarrow f)\bullet(e\rightarrow g)+(e\rightarrow h)$$

Thus: c-e structures may be combined by „addition" (+) and „multiplication" (•) - respective algebra, called a ***quasi-semiring.***

Thus: c-e structures may be compared: $U \leq V$ iff $V = U+V$

U is a ***substructure*** of V. „$\leq$" is a partial order.

A crucial notion for semantics may be defined:

A ***firing component*** of a c-e structure U is its substructure Q such that every node of Q with annotating polynomials are without „+" (thus monomials) and if one of them is θ then the other is not θ.

Firing components of from the former example c-e structure

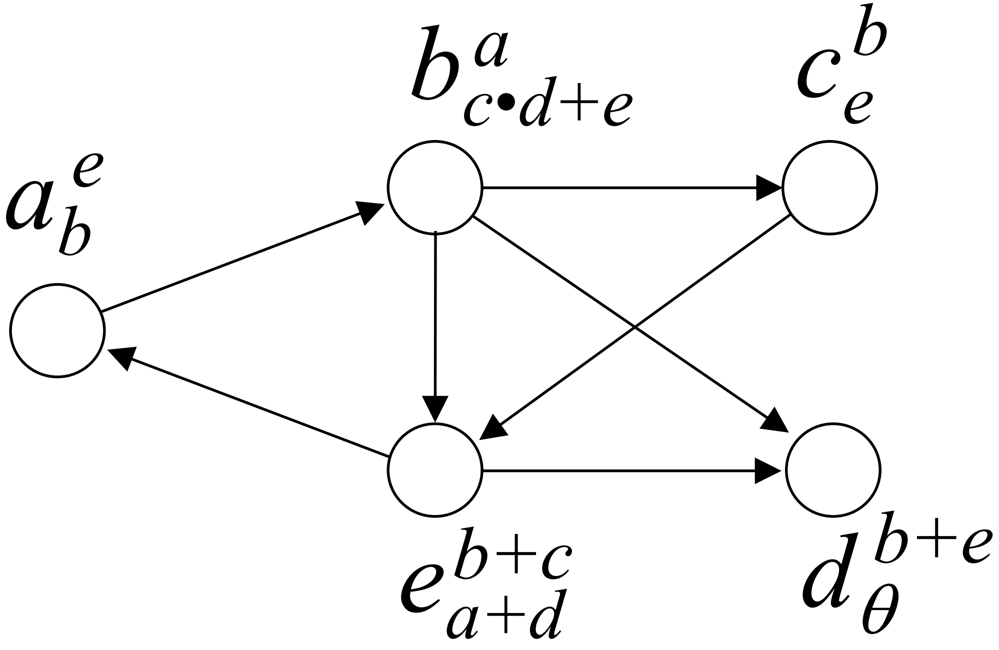
$$U = \{a_e^\theta, b_e^\theta, c_e^\theta, d_e^\theta, e_{f\bullet g+h}^{a\bullet b+b\bullet c+d}, f_\theta^e, g_\theta^e, h_\theta^e\}$$

are:

$$\{a_e^\theta, b_e^\theta, e_\theta^{a\bullet b}\} \quad \{b_e^\theta, c_e^\theta, e_\theta^{b\bullet \mathrm{c}}\} \quad \{d_e^\theta, e_\theta^d\}$$

$$\{e_{f\bullet g}^\theta, g_\theta^e \quad f_\theta^e\} \quad \{e_h^\theta, h_\theta^e\}$$

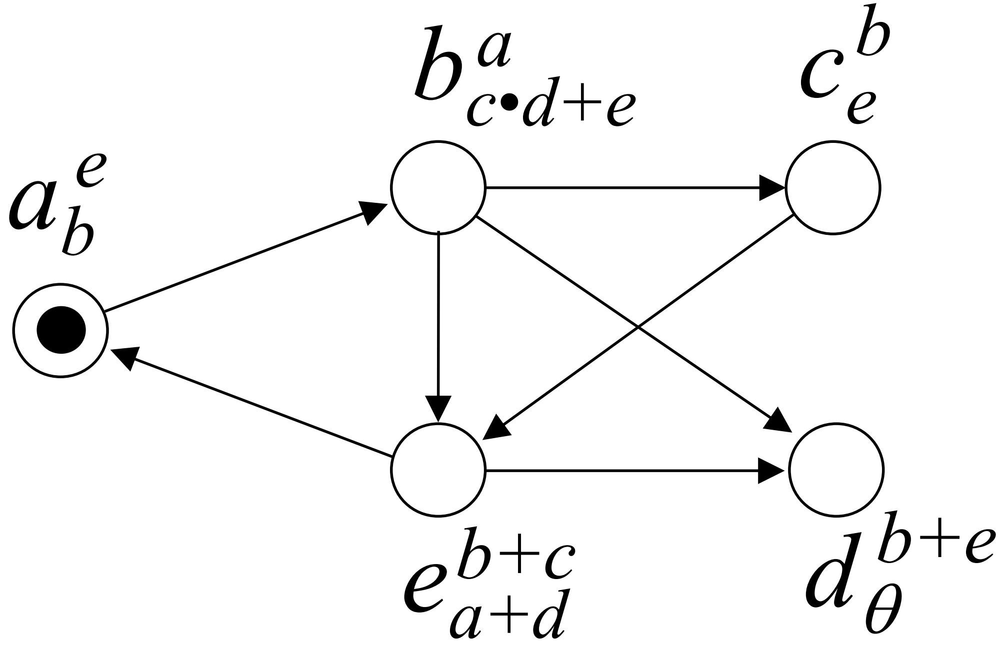
Example:

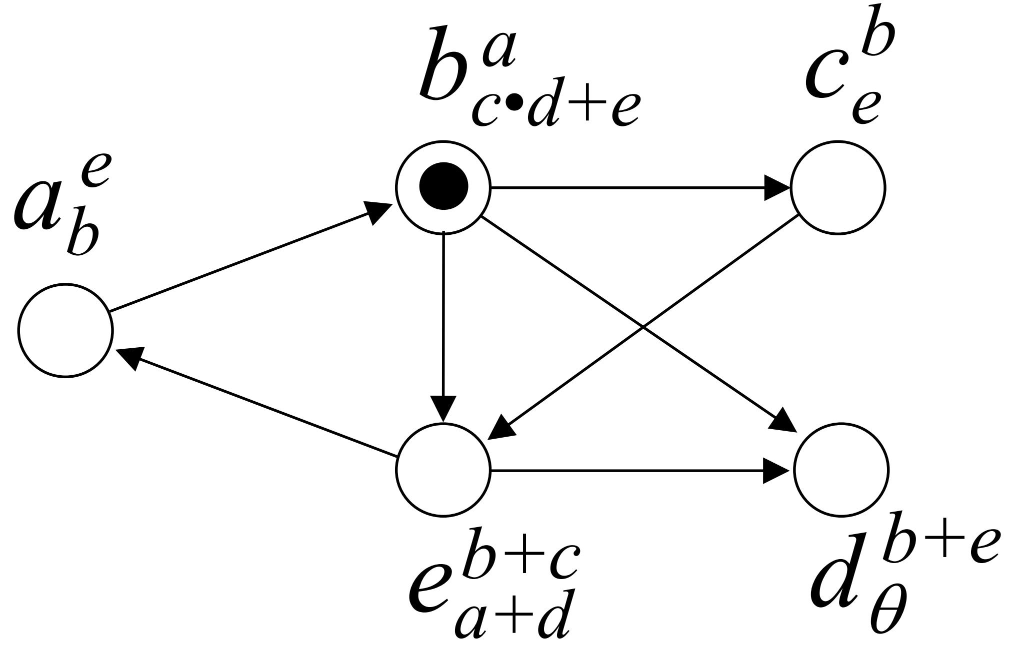


Firing components:

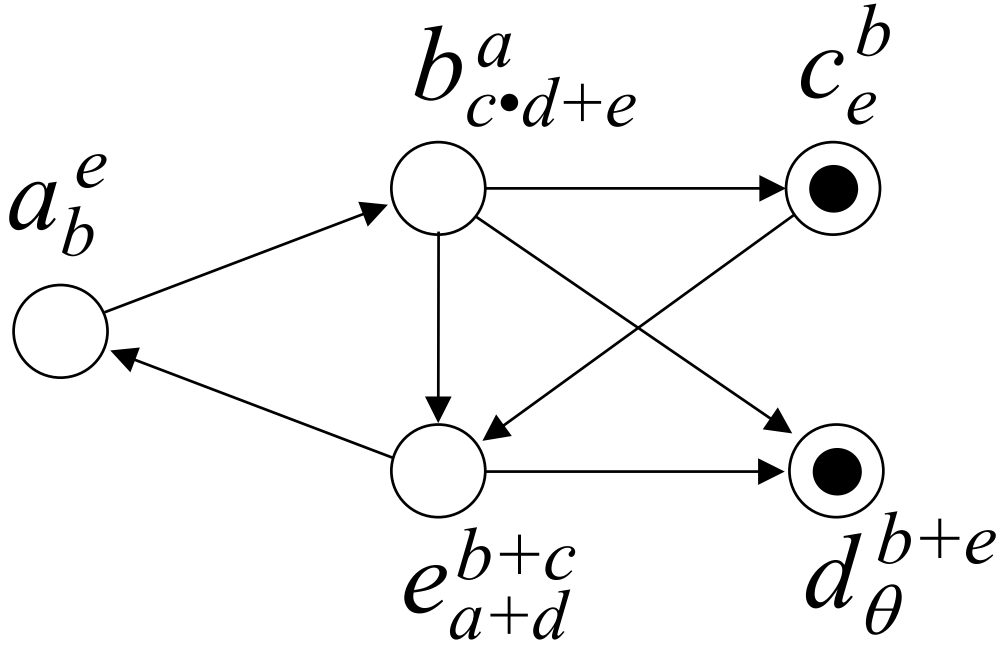
$$\{a_b^\theta, b_\theta^a\} \ \{b^\theta_{c\bullet d}, c_\theta^b, d_\theta^b\} \ \{c_e^\theta, e_\theta^c\} \ \{b_e^\theta, e_\theta^b\} \ \{e_d^\theta, d_\theta^e\} \ \{e_a^\theta, a_\theta^e\}$$

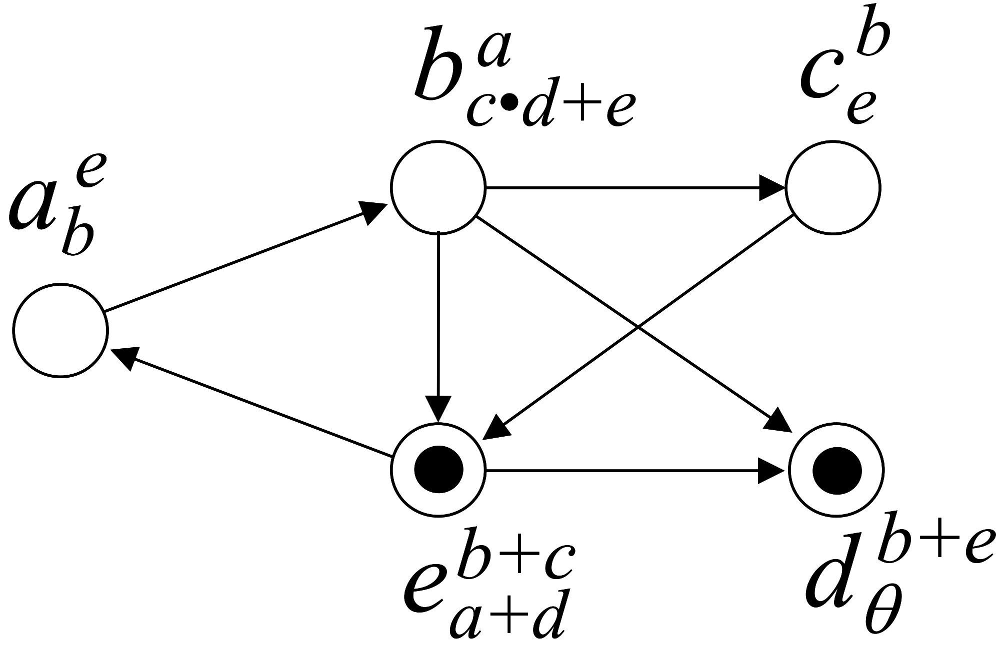
Possible run:

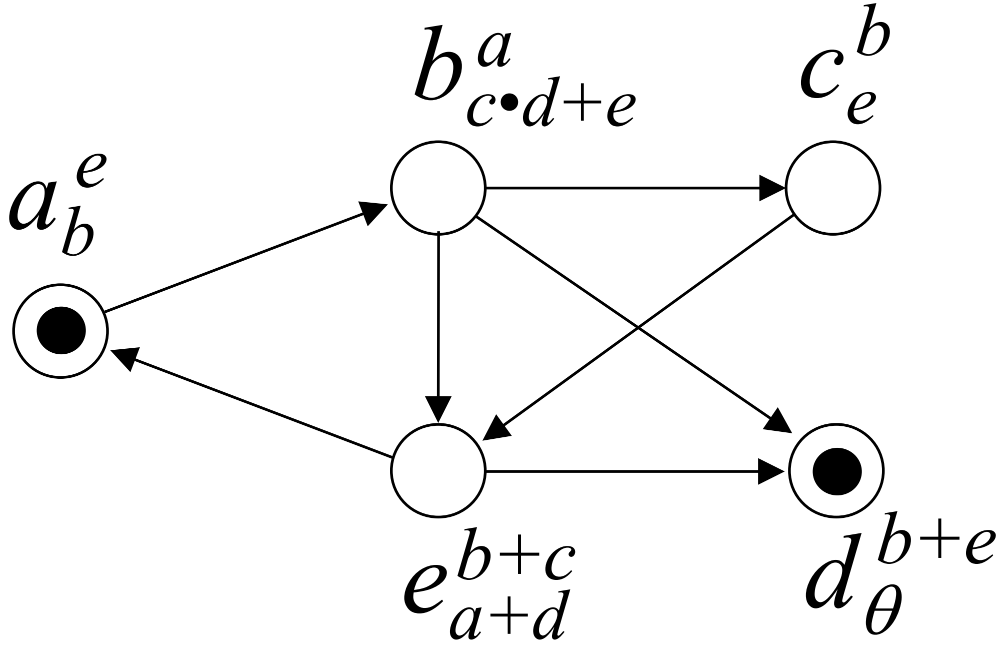




a_b^e
$b_{c\bullet d+e}^a$
c_e^b
e_{a+d}^{b+c}
d_θ^{b+e}


a_b^e
$b_{c\bullet d+e}^a$
c_e^b
e_{a+d}^{b+c}
d_θ^{b+e}


a_b^e
$b_{c\bullet d+e}^a$
c_e^b
e_{a+d}^{b+c}
d_θ^{b+e}



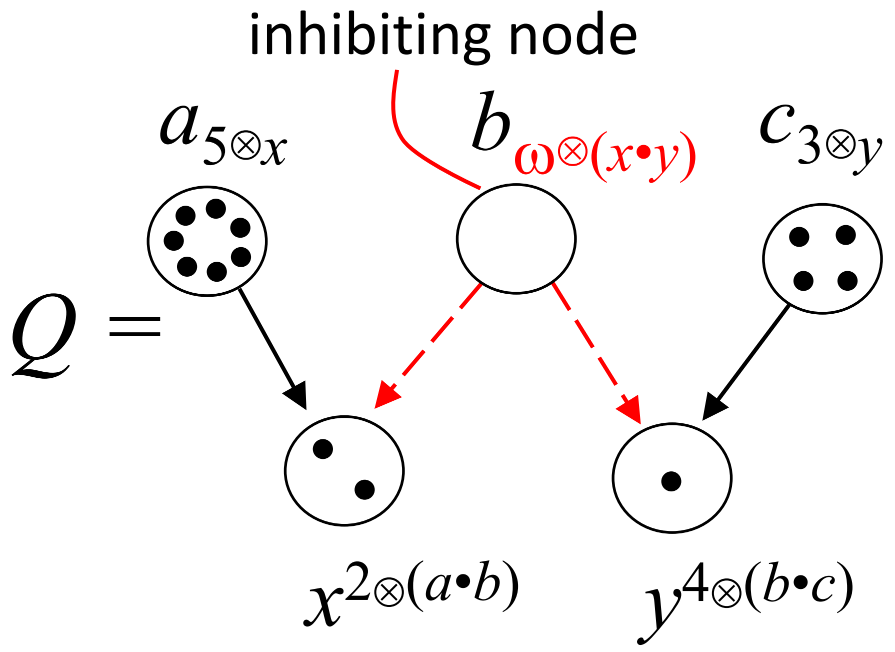
a_b^e
$b^a_{c\bullet d+e}$
c_e^b
e^{b+c}_{a+d}
d^{b+e}_θ

Fring component Q with **weighted** (multiplied) effect and cause monomials:

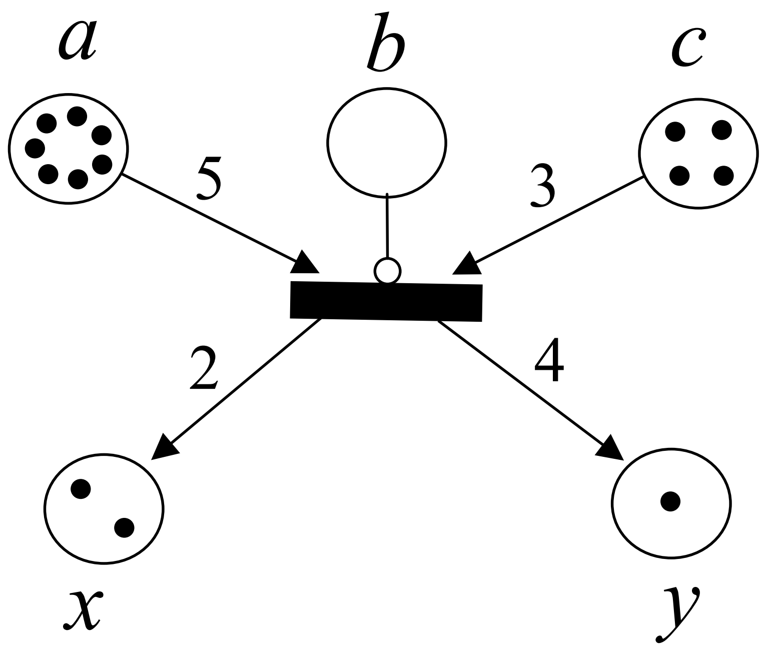
$E_Q(a) = x$ $E_Q(b) = x \bullet y$ $E_Q(c) = y$ $C_Q(x) = a \bullet b$ $C_Q(y) = b \bullet c$

$\overline{E_Q}(a) = 5 \otimes x$ $\overline{E_Q}(b) = \omega \otimes (x \bullet y)$ $\overline{E_Q}(c) = 3 \otimes y$ $\overline{C_Q}(x) = 2 \otimes a \bullet b$ $\overline{C_Q}(y) = 4 \otimes b \bullet c$

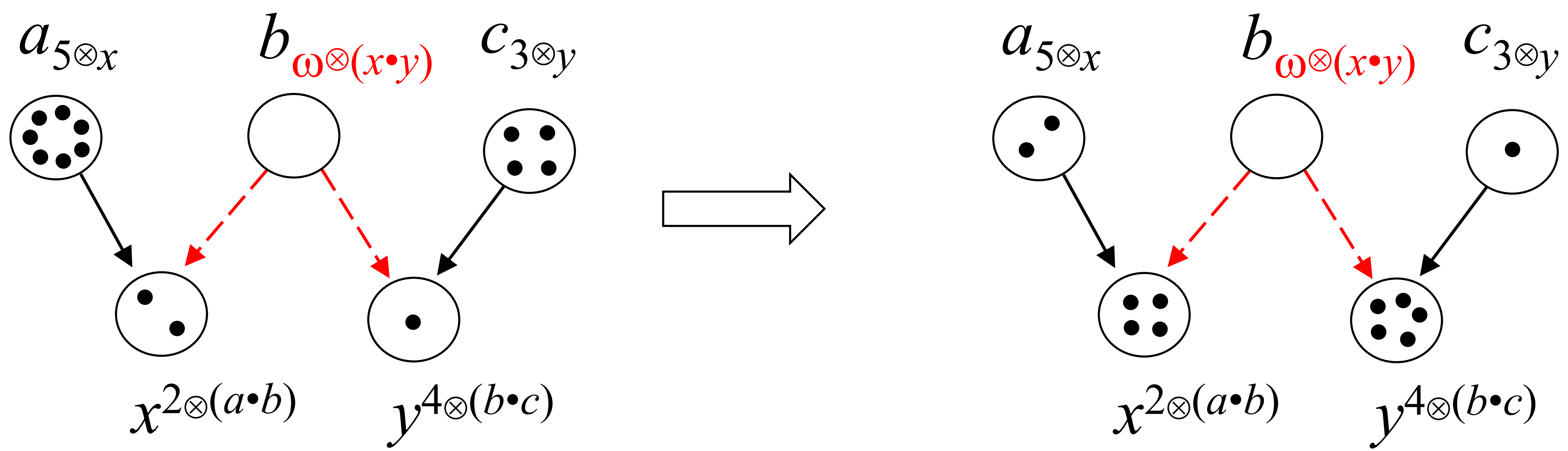
weight of $E_Q(a)$ weight of $E_Q(b)$



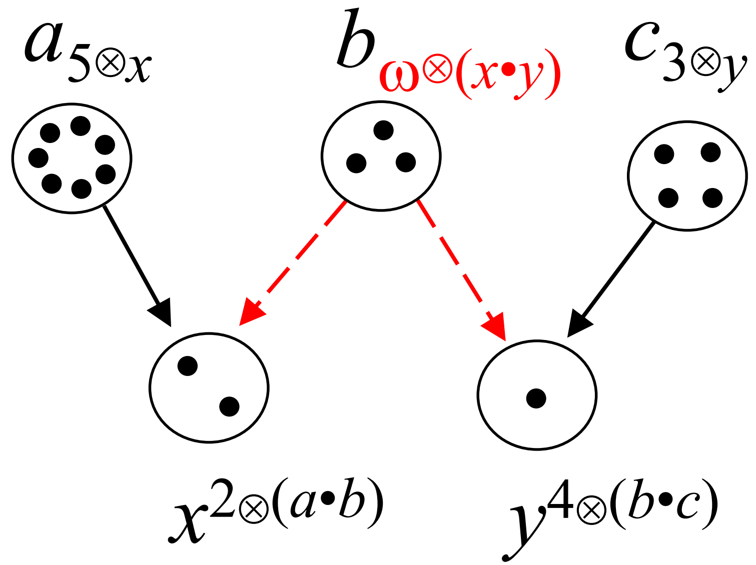
extended c-e structure with inhibiting node b



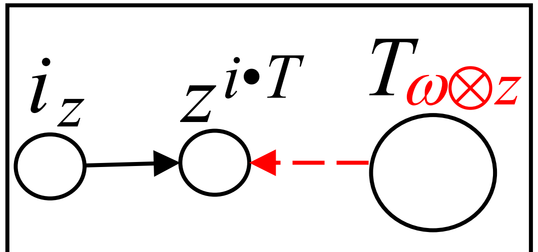
equivalent Petri net with inhibitor arrow enabled



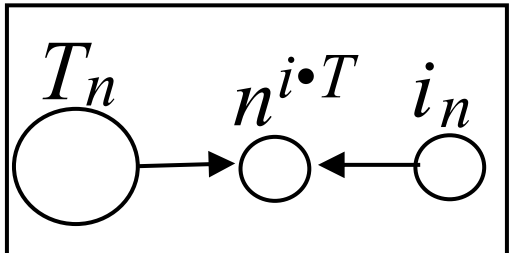
not enabled



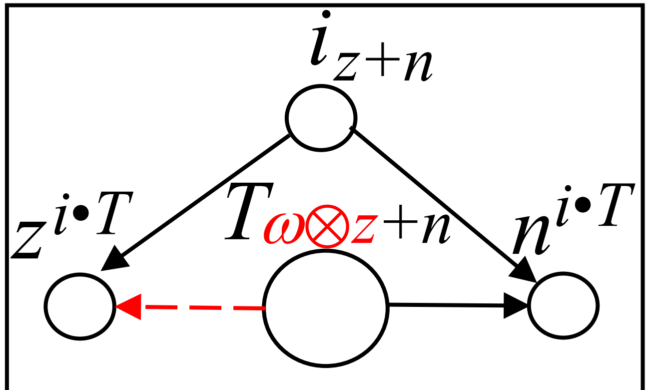
Construction of c-e structure Q_0+Q_1 implementing "test zero".
A token at the node i starts testing contents of T; on termination, the token appears at z (zero) if T is empty and at n (not zero) otherwise. The tested node T plays two roles: inhibiting in Q_0 and ordinary in Q_1. Capacity of T is infinite, whereas of remaining nodes is 1. The empty subscript/superscript θ is skipped. In the Petri net counterpart, the inhibiting arrow enters the left transition.



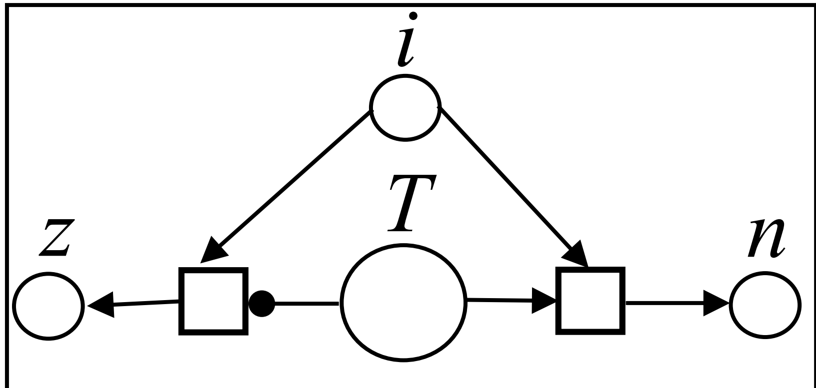
firing component Q_0



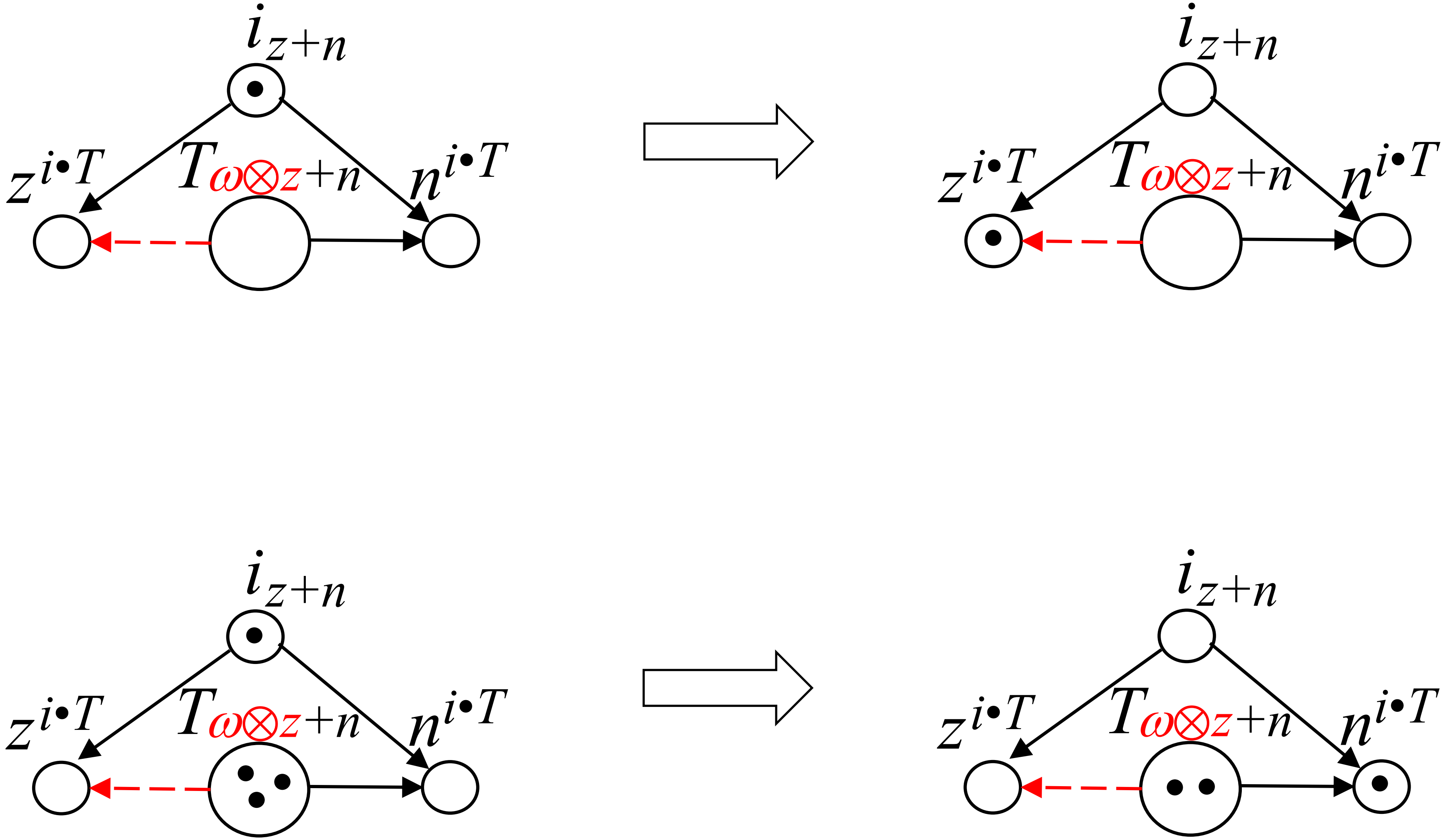
firing component Q_1



c-e structure $Q_0 + Q_1$



Petri net equivalent to $Q_0 + Q_1$



i_{z+n}
$z^{i\bullet T}$
$T_{\omega\otimes z+n}$
$n^{i\bullet T}$
i_{z+n}
$z^{i\bullet T}$
$T_{\omega\otimes z+n}$
$n^{i\bullet T}$
i_{z+n}
$z^{i\bullet T}$
$T_{\omega\otimes z+n}$
$n^{i\bullet T}$
i_{z+n}
$z^{i\bullet T}$
$T_{\omega\otimes z+n}$
$n^{i\bullet T}$

Sketch of formalism

Basic notions of c-e structures

$\mathbb{X}$ - a non-empty enumerable set (of nodes), $\theta \notin \mathbb{X}$ - a neutral symbol.
Any node $x \in \mathbb{X}$ and θ is a formal polynomial; if K and L are formal polynomials, then $(K+L)$ and $(K{\bullet}L)$ are too. Their set is $\mathbf{F}[\mathbb{X}]$.
Addition and multiplication of formal polynomials:
$K \oplus L = (K+L)$, $K \odot L = (K{\bullet}L)$ (use „+" and „•" instead of $\oplus$ and $\odot$).
Let the algebra $\langle \mathbf{F}[\mathbb{X}], +, \bullet, \theta \rangle$ obey the axioms:

(+)	$\theta+K = K+\theta = K$	(•)	$\theta{\bullet}K = K{\bullet}\theta = K$	quasi-semiring
(++)	$K+K = K$	(••)	$x{\bullet}x = x$	
(+++)	$K+L = L+K$	(•••)	$K{\bullet}L = L{\bullet}K$	
(++++)	$K+(L+M) = (K+L)+M$	(••••)	$K{\bullet}(L{\bullet}M) = (K{\bullet}L){\bullet}M$	
(+•)	If $L \neq \theta \Leftrightarrow M \neq \theta$	then	$K{\bullet}(L+M) = K{\bullet}L + K{\bullet}M$	

Definition (cause-effect structure, carrier, set $\mathbf{CE}[\mathbb{X}]$)

A c-e structure over $\mathbb{X}$ is a pair $U = \langle C,E \rangle$ of total functions:

C: $\mathbb{X} \rightarrow \mathbf{F}[\mathbb{X}]$ cause function; nodes in $C(x)$ are causes of x
E: $\mathbb{X} \rightarrow \mathbf{F}[\mathbb{X}]$ effect function; nodes in $E(x)$ are effects of x

such that x occurs in the formal polynomial $C(y)$ iff y occurs in $E(x)$

Carrier of U is the set $car(U) = \{x \in \mathbb{X}\colon C(x) \neq \theta \vee E(x) \neq \theta\}$
The set of all c-e structures over $\mathbb{X}$ is denoted by $\mathbf{CE}[\mathbb{X}]$.
Since $\mathbb{X}$ is fixed, we write just $\mathbf{CE}$

A representation of $U = \langle C,E \rangle$ as a set of annotated nodes is
$\{x^{C(x)}_{E(x)} :\ x \in car(U)\}$

Definition (addition, multiplication, monomial c-e structure)

For c-e structures $U = \langle C_U, E_U \rangle$, $V = \langle C_V, E_V \rangle$, define:

$U+V = \langle C_{U+V}, E_{U+V} \rangle = \langle C_U + C_V, E_U + E_V \rangle$ where

$(C_U + C_V)(x) = C_U(x) + C_V(x)$ and similarly for E

$U \bullet V = \langle C_{U\bullet V}, E_{U\bullet V} \rangle = \langle C_U \bullet C_V, E_U \bullet E_V \rangle$ where

$(C_U \bullet C_V)(x) = C_U(x) \bullet C_V(x)$ and similarly for E

Proposition

System $\langle \mathbf{CE}[\mathbb{X}],+,\bullet,\theta\rangle$ obeys equations for all $U,V,W \in \mathbf{CE}[\mathbb{X}]$, $x,y \in \mathbb{X}$:

(+) $\theta+U = U+\theta = U$

(++) $U+U = U$

(+++) $U+V = V+U$

(++++) $U+(V+W) = (U+V)+W$

(•) $\theta\bullet U = U\bullet\theta = U$

(••) $(x\to y)\bullet(x\to y) = (x\to y)$

(•••) $U\bullet V = V\bullet U$

(••••) $U\bullet(V\bullet W) = (U\bullet V)\bullet W$

(+•) If $C_V(x) \neq \theta \Leftrightarrow C_W(x) \neq \theta$ and $E_V(x) \neq \theta \Leftrightarrow E_W(x) \neq \theta$ then

$$U\bullet(V+W) = U\bullet V + U\bullet W$$

This is the quasi-semiring of c-e structures

Definition (partial order ≤; substructure, set SUB[V], firing component, set $\mathbf{FC}$, pre-set and post-set)

For $U,V \in \mathbf{CE}$ let $U \leq V \Leftrightarrow V = U+V$; $\leq$ is a partial order in $\mathbf{CE}$.

If $U \leq V$ then U is a substructure of V;

$\mathbf{SUB}[V] = \{U: U \leq V\}$ is the set of all substructures of V.

For $A \subseteq \mathbf{CE}$: $V \in A$ is minimal (wrt ≤) in A iff $\forall W \in A$: $(W \leq V \Rightarrow W = V)$.

A minimal in $\mathbf{CE} \setminus \{\theta\}$ c-e structure $Q = \langle C_Q, E_Q \rangle$ is a firing component iff Q is a monomial c-e structure and $C_Q(x) = \theta \Leftrightarrow E_Q(x) \neq \theta$ for any $x \in car(Q)$. The set of all firing components is $\mathbf{FC}$, thus the set of all firing components of $U \in \mathbf{CE}$ is $FC[U] = \mathbf{SUB}[U] \cap \mathbf{FC}$.

Let for $Q \in \mathbf{FC}$ and $G \subseteq \mathbf{FC}$:

${}^{\bullet}Q = \{x \in car(Q)\colon C_Q(x) = \theta\}$ (pre-set or causes of Q)

$Q^{\bullet} = \{x \in car(Q)\colon E_Q(x) = \theta\}$ (post-set or effects of Q)

${}^{\bullet}Q^{\bullet} = {}^{\bullet}Q \cup Q^{\bullet}$

${}^{\bullet}G = \bigcup_{Q \in G} {}^{\bullet}Q$ (pre-set or causes of G)

$G^{\bullet} = \bigcup_{Q \in G} Q^{\bullet}$ (post-set or effects of G)

${}^{\bullet}G^{\bullet} = \bigcup_{Q \in G} {}^{\bullet}Q^{\bullet}$

Definition (state of c-e structures)

A <u>state</u> of a c-e structure U is a total function $s: car(U) \to \mathbb{N}$, thus a multiset over $car(U)$. The set of all states of U is $\mathbb{S}$

Definition (weights of monomials and capacity of nodes)

For a c-e structure $U = \langle C,E \rangle$ and firing component $Q \in \mathbf{FC}[U]$, let with the pre-set ${}^{\bullet}Q$ and post-set $Q^{\bullet}$, multisets $\overline{{}^{\bullet}Q} : {}^{\bullet}Q \to \mathbb{N} \cup \{\omega\}$ and $\overline{Q^{\bullet}} : Q^{\bullet} \to \mathbb{N} \cup \{\omega\}$ be given as additional information. The value $\overline{{}^{\bullet}Q}(x)$ is a <u>weight</u> of monomial $E_Q(x)$ and the value $\overline{Q^{\bullet}}(x)$ - a <u>weight</u> of monomial $C_Q(x)$

An <u>effect</u> monomial $E_Q(x)$ of a node $x \in {}^{\bullet}Q$ with weight $\overline{{}^{\bullet}Q}(x)$ is denoted by $\overline{{}^{\bullet}Q}(x) \otimes E_Q(x)$

Similarly for a <u>cause</u> monomial.

The coefficient representing weight will be abandoned if it is 1.

Definition (inhibitors)

For a firing component $Q \in \mathbf{FC}[U]$

$inh[Q] = \{x \in {}^{\bullet}Q : {}^{\bullet}\overline{Q}(x)\} = \omega\}$

thus a set of nodes in the pre-set of Q, whose effect monomials $E_Q(x)$ are of weight ω.

The nodes in $inh[Q]$ will play role of inhibiting nodes of firing component Q.

Definition (enabled firing components)

For a firing component $Q \in \mathbf{FC}[U]$ and state s define the formula:

$$enabled[Q](s) \overset{def}{\Leftrightarrow}$$

$$\forall x \in inh[Q]:\ s(x) = 0 \wedge$$
$$\forall x \in {}^{\bullet}Q \setminus inh[Q]:\ s(x) > 0 \wedge \overline{{}^{\bullet}Q}(x) \leq s(x) \leq cap(U)(x) \wedge$$
$$\forall x \in Q^{\bullet}:\ \overline{Q^{\bullet}}(x) + s(x) \leq cap(U)(x)$$

So, Q is enabled in the state s iff none of inhibiting nodes $x \in {}^\bullet Q$ contains a token and each remaining node in ${}^\bullet Q$ contains, with no fewer tokens than is the weight of its effect monomial $E_Q(x)$ and no more than capacity of each $x \in {}^\bullet Q$

Moreover, none of $x \in Q^\bullet$ holds more tokens than their number when increased by the weight of the cause monomial $C_Q(x)$ exceeds capacity of x

Definition (Sequential and parallel semantics of c-e structures)

Sequential. For $Q \in \mathbf{FC}[U]$ let $[[Q]] \subseteq \mathbb{S} \times \mathbb{S}$ be a binary relation defined as: $(s,t) \in [[Q]]$ iff

$enabled[Q](s) \wedge t = (s - {}^{\bullet}\overline{Q} + \overline{Q}^{\bullet} \leq cap(U)$ (Q transforms state s into t).

Semantics $[[U]]$ of $U \in \mathbf{CE}$ is $[[U]] = \bigcup_{Q \in \mathbf{FC}[U]} [[Q]]$

Parallel. Firing components Q and P detached iff ${}^{\bullet}Q^{\bullet} \cap {}^{\bullet}P^{\bullet} = \emptyset$.

For any non-empty set $G \subseteq \mathbf{FC}$ of pairwise detached firing components, the relations $[[G]]$ and $[[U]]_{par}$ are defined in the same way as $[[Q]]$ and $[[U]]$ in the sequential case, but with Q replaced with G and $\mathbf{FC}[U]$ replaced with the set of all pairwise detached non-empty firing components of U.

Reaction systems
Sketch of formalism and examples

Definition (reaction system)

Reaction system **(RE)** A is a pair of sets:

$A = (\mathbb{B}, \mathbb{R})$ where:

$\mathbb{B}$ - background (comprises the so-called entities)

$\mathbb{R}$ - set of reactions

$r \in \mathbb{R}$ - reaction created of three sets:

$r = (R_r, I_r, P_r)$ where:

$R_r \subseteq \mathbb{B}$ - set of reactants

$I_r \subseteq \mathbb{B}$ - set of inhibitors where:

$R_r \cap I_r = \varnothing$

$P_r \subseteq \mathbb{B}$ is a set of products

The initial state of the system A is a set $\mathbb{S}_0 \subseteq \mathbb{B}$

Definition (state of **RE** and enabled reactions)

State $\mathbb{S}$ of reaction system A is a subset of its background:

$\mathbb{S} \subseteq \mathbb{B}$

The intention is that $\mathbb{S}$ be the set of those background's members, which comprise entities.

A reaction $r = (R_r, I_r, P_r)$ is <u>enabled</u> in a state $\mathbb{S}$ iff

$R_r \subseteq \mathbb{S}$ and $I_r \cap \mathbb{S} = \varnothing$

Definition (semantics of reaction systems - change of state)

The <u>result</u> of a reaction $r = (R_r, I_r, P_r)$ in a state $\mathbb{S}$ is the set P_r if r is enabled in $\mathbb{S}$ and the empty set $\varnothing$ otherwise.

This result is denoted by

$$res_r(\mathbb{S}) = \begin{cases} P_r & \text{if } r \text{ is enabled in the state } \mathbb{S} \\ \varnothing & \text{otherwise} \end{cases}$$

The result of the reaction system A in a state $\mathbb{S}$ is the union of all its reactions in this state:

$$res_A(\mathbb{S}) = \bigcup_{r \in \mathbb{R}} res_r(\mathbb{S})$$

Remarks

1. On completion (if it exists) of reaction system work, the entities in the difference of sets $\mathbb{S} \backslash res_A(\mathbb{S})$ disappear.

2. Features differing the reaction systems from cause-effect structures (or Petri nets):

- the lack of conflicts
- possible absorption of reactants by products.

These features will be taken into account in definition of semantics of reaction c-e structures.

Example (test zero)

The "test zero" task may be realized in the reaction system $A = (\mathbb{B}, \mathbb{R})$ with $\mathbb{B} = \{i, z, n, T\}$, $\mathbb{R} = \{r1, r2\}$ where

$r1 = (\{i\}, \{T\}, \{z\})$, $r2 = (\{i, T\}, \varnothing, \{n\})$

Result of this system's work depends on the initial state $\mathbb{S}_0$ (i.e. what the environment supplies):

If $\mathbb{S}_0 = \{i, T\}$ then the result is $\{n\}$ ("not zero" - presence of entity at T).

If $\mathbb{S}_0 = \{i\}$ then result is $\{z\}$ ("zero" – absence of entity at T).

Reactant i initiates work of the system, while T is tested for presence/absence of entity.

Evolution of the system $A = (\underbrace{\{i,z,n,T\}}_{\mathbb{B}}, \underbrace{\{r1,r2\}}_{\mathbb{R}})$ with initial state $\{i,T\}$ is the following:

$res_{r1}(\{i,T\}) = \varnothing$ (because $\{i\} \subseteq \{i,T\}$ and $\{T\} \cap \{i,T\} \neq \varnothing$)
$res_{r2}(\{i,T\}) = \{n\}$ (because $\{i,T\} \subseteq \{i,T\}$ and $\varnothing \cap \{i,T\} = \varnothing$)
thus
$res_A(\{i,T\}) = res_{r1}(\{i,T\}) \cup res_{r2}(\{i,T\}) = \{n\}$ ("not zero")

Evolution of the system A with initial state $\{i\}$ is the following:

$res_{r1}(\{i\}) = \{z\}$ (because $\{i\} \subseteq \{i\}$ and $\{T\} \cap \{i\} = \varnothing$)
$res_{r2}(\{i\}) = \varnothing$ (because $\{i,T\} \not\subseteq \{i\}$ and $\varnothing \cap \{\mathrm{i}\} = \varnothing$) thus
$res_A(\{i\}) = res_{r1}(\{i\}) \cup res_{r2}(\{i\}) = \{z\}$ ("zero")

Cause-effect structures working similarly to reaction systems

The objective: to build a system structurally identical with c-e structures but working like reaction systems.

They are reaction c-e structures, denoted by **RECE**

The counterparts of some concepts of **RECE** and **RE**:

nodes	↔ elements of background
firing components	↔ reactions
causes in a firing component	↔ reactants in a reaction
effects in a firing component	↔ products in a reaction
inhibitors in a firing component	↔ inhibitors in a reaction
tokens	↔ entities

Definition (state of **RECE**)

A state of reaction c-e structure U is a total function $s\colon car(U) \to \{0,1,\omega\}$. The set of all states of U is $\mathbb{S}$.

Symbols 0 and 1 will be treated as logical values of ***false*** and ***true*** respectively and operations of propositional calculus on them will be applied. Operations ∨, ∧ on ω, are defined as:

$0 \vee \omega = \omega \vee 0 = \omega, \quad 0 \wedge \omega = \omega \wedge 0 = 0, \; 1 \vee \omega = \omega \vee 1 = \omega, \; 1 \wedge \omega = \omega \wedge 1 = 1,$

$\omega \vee \omega = \omega \wedge \omega = \omega, \quad \neg\omega = 0.$

ω will be used for inhibiting actions. Interpretation of 0 and 1 as ***false*** and ***true*** is justified by absorption property of entities in reaction systems and will be made formal later.

Definition (weights of monomials and inconsistent firing components)

For a c-e structure $U = \langle C,E\rangle$ and firing component $Q\in\mathbf{FC}[U]$, functions

$\overline{{}^{\bullet}Q} : {}^{\bullet}Q \to \{0,1,\omega\}$ and $\overline{Q^{\bullet}} : Q^{\bullet} \to \{0,1,\omega\}$ are given as additional information. The value $\overline{{}^{\bullet}Q}(x)$ is a weight of monomial $E_Q(x)$ and the value $\overline{Q^{\bullet}}(x)$ - a weight of monomial $C_Q(x)$

As formerly, ω is interpreted as a "disable signal" and used for defining inhibiting nodes.

Firing components Q and P are inconsistent if for a certain $x\in {}^{\bullet}Q^{\bullet}\cap{}^{\bullet}P^{\bullet}$ weights $\overline{{}^{\bullet}Q}(x)$ and $\overline{{}^{\bullet}P}(x)$ or $\overline{Q^{\bullet}}(x)$ and $\overline{P^{\bullet}}(x)$ are different.

The lack of conflicts requires introducing for reaction c-e structures concept called here "volley"

Definition (volley - simultaneous firing, extension of weight functions)

Any set $G \subseteq \mathbf{FC}$ without inconsistent firing components is called a volley. The family of volleys is $\mathbf{FCV}$.

If $G \subseteq \mathbf{FC}[U]$ then $\mathbf{FCV}[U]$ is a set of volleys in U.

The pre-set ${}^{\bullet}G$ and post-set $G^{\bullet}$ of a volley G are defined as before.

Extension of the weight functions ${}^{\bullet}\overline{Q}$ and $\overline{Q}^{\bullet}$ onto the volley G are:

$$
{}^{\bullet}\overline{G}(x) = \begin{cases} {}^{\bullet}\overline{Q}(x) & for\ arbitrary\ Q\ if\ it\ belongs\ to\ G \\ 0 & else \end{cases}
$$

$$
\overline{G^{\bullet}}(x) = \begin{cases} \overline{Q^{\bullet}}(x) & for\ arbitrary\ Q\ if\ it\ belongs\ to\ G \\ 0 & else \end{cases}
$$

This is a correct definition since for any firing components Q and P in G:

$^{\bullet}\overline{Q}(x) = {^{\bullet}\overline{P}}(x)$ if $x \in {^{\bullet}G}$ and $\overline{Q^{\bullet}}(x) = \overline{P^{\bullet}}(x)$ if $x \in G^{\bullet}$

Functions $^{\bullet}\overline{G}$ and $\overline{G^{\bullet}}$ will be used in definition of reaction c-e structures semantics.

Inhibitors for **RECE** are the same as for **CE**:

For a firing component $Q \in \mathbf{FC}[U]$

$inh[Q] = \{x \in {}^{\bullet}Q : {}^{\bullet}\overline{Q}(x)\} = \omega\}$

thus a set of nodes in the pre-set of Q, whose effect monomials $E_Q(x)$ are of weight ω.

Definition (enabled firing components and enabled volleys)

For a firing component $Q \in \mathbf{FC}[U]$ and state *s* let the formula $enabled[Q](s)$ be defined as:

$$\forall x \in inh[Q]:\ s(x) = 0 \wedge \forall x \in {}^{\bullet}Q \setminus inh[Q]:\ s(x) = 1$$

For a volley $G \in \mathbf{FCV}[U]$, the formula $enabled[G](s)$ is defined as above by replacing Q with G and $\mathbf{FC}[U]$ with $\mathbf{FCV}[U]$

Definition (semantics [[…]] of reaction c-e structures)

For a volley $G \in \mathbf{FCV}[U]$, $G \neq \emptyset$ let $[[G]] \subseteq \mathbb{S} \times \mathbb{S}$ be a binary relation defined as: $(s,t) \in [[G]]$ iff

$$enabled[G](s) \wedge \forall x \in car(U): \quad t(x) = (s(x) \wedge \neg^{\bullet}\overline{G}(x)) \vee \overline{G^{\bullet}}(x)$$

Semantics $[[U]]$ of $U \in \mathbf{RECE}$ is $\bigcup_{G \in \mathbf{FCV}[U]} [[G]]$

for any maximal volley G, i.e. if $G \subseteq G' \in \mathbf{FCV}[U]$ and $(s,t) \in [[G']]$ then $G = G'$

Description of semantics by means of this propositional formula is justified by the properties of reaction systems:

1. Presence of token ("entity") at a node absorbs another token arriving in this node.
2. Lack of conflicts between different reactions, takes place in reaction c-e structures due to the lack of inconsistent firing components in $G \in \mathbf{FCV}[U]$

Example (reaction c-e structure assembling a chemical molecule)

Description of creating chemical molecules by the reaction system

$A = (\{C, H, O, U, V, W, X, Y, Z\}, \{r1, r2, r3, r4, r5, r6\})$

with reactions defined as:

$r1 = (\{C, H\}, \varnothing, \{U\})$ U contains molecule CH (methylidyne)

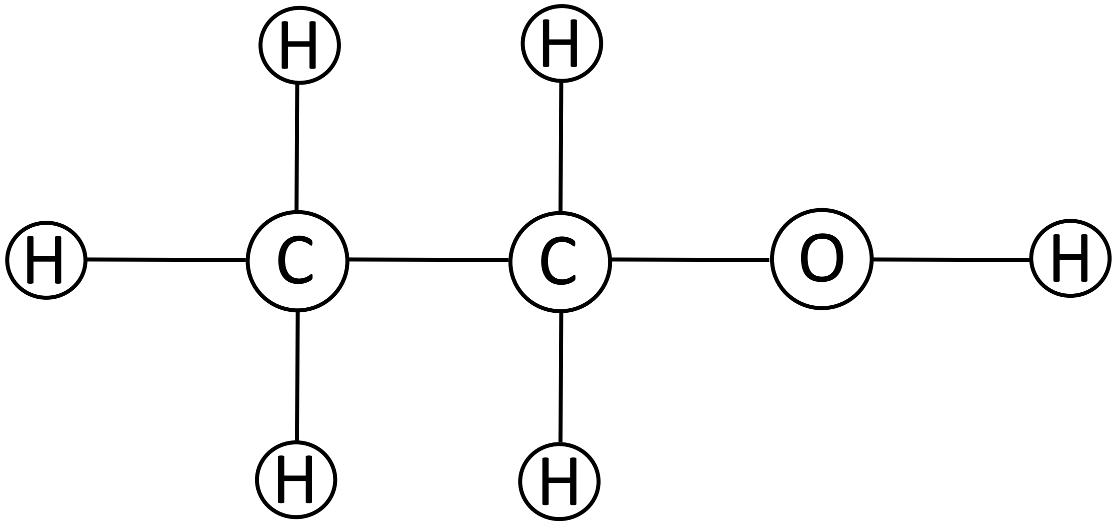
$r2 = (\{U, C, H\}, \varnothing, \{V\})$ V contains molecule C_2H_2 (acetylene)

$r3 = (\{V, H\}, \varnothing, \{W\})$ W contains molecule C_2H_3 (ethylenyl)

$r4 = (\{W, H\}, \varnothing, \{X\})$ X contains molecule C_2H_4 (ethylene)

$r5 = (\{X, H, O\}, \varnothing, \{Y\})$ Y contains molecule C_2H_5O (ethoxide)

$r6 = (\{Y, H\}, \varnothing, \{Z\})$ Z contains molecule C_2H_5OH (ethanol) is given by successive steps of this reaction system evolution shown at the following slides. This evolution assembles the molecule:



Starting with initial state $\{C,H,O\}$, the results of reactions are:

$res_{r1}(\{C,H,O\}) = \{U\}$ (since $\{C,H\} \subseteq \{C,H,O\}$ and $\emptyset \cap \{C,H,O\} = \emptyset$)

$res_{r2}(\{C,H,O\}) = res_{r3}(\{C,H,O\}) = res_{r4}(\{C,H,O\}) = res_{r5}(\{C,H,O\}) =$

$res_{r6}(\{C,H,O\}) = \emptyset$

thus

$res_{A}(\{C,H,O\}) = \{U\}$

Continuing with the state $\{C,H,O,U\}$, the results of reactions are:

$res_{r1}(\{C,H,O,U\})=\{U\}$ (since $\{C,H\}\subseteq\{C,H,O,U\}$ and $\emptyset\cap\{C,H,O,U\}=\emptyset$)

$res_{r2}(\{C,H,O,U\})=\{V\}$ (since $\{C,H,U\}\subseteq\{C,H,O,U\}$ and $\emptyset\cap\{C,H,O,U\}=\emptyset$)

$res_{r3}(\{C,H,O,U\})= res_{r4}(\{C,H,U\})=res_{r5}(\{C,H,O,U\})=res_{r6}(\{C,H,O,U\})=\emptyset$

thus

$res_{A}(\{C,H,O,U\})=\{U,V\}$

Continuing with the state $\{C,H,O,U,V\}$, the results of reactions are:

$res_{r1}(\{C,H,O,U,V\})=\{U\}$ (since $\{C,H\}\subseteq\{C,H,O,U,V\}$ and $\emptyset\cap\{C,H,O,U,V\}=\emptyset$)

$res_{r2}(\{C,H,O,U,V\})=\{V\}$ (since $\{C,H,U\}\subseteq\{C,H,O,U,V\}$ and $\emptyset\cap\{C,H,O,U,V\}=\emptyset$)

$res_{r3}(\{C,H,O,U,V\})=\{W\}$ (since $\{H,V\}\subseteq\{C,H,O,U,V\}$ and $\emptyset\cap\{C,H,O,U,V\}=\emptyset$)

$res_{r4}(\{C,H,O,U,V\})=res_{r5}(\{C,H,O,U,V\})=res_{r6}(\{C,H,O,U,V\})=\emptyset$

thus

$res_{A}(\{C,H,O,U.V\})=\{U,V,W\}$

Continuing with the state $\{C,H,O,U,V,W\}$, the results of reactions are:

$res_{r1}(\{C,H,O,U,V,W\})=\{U\}$ (since $\{C,H\}\subseteq\{C,H,O,U,V,W\}$ and $\emptyset\cap\{C,H,O,U,V,W\}=\emptyset$)

$res_{r2}(\{C,H,O,U,V,W\})=\{V\}$ (since $\{C,H,U\}\subseteq\{C,H,O,U,V,W\}$ and $\emptyset\cap\{C,H,O,U,V,W\}=\emptyset$)

$res_{r3}(\{C,H,O,U,V,W\})=\{W\}$ (since $\{H,V\}\subseteq\{C,H,O,U,V,W\}$ and $\emptyset\cap\{C,H,O,U,V,W\}=\emptyset$)

$res_{r4}(\{C,H,O,U,V,W\})=\{X\}$ (since $\{H,W\}\subseteq\{C,H,O,U,V,W\}$ and $\emptyset\cap\{C,H,O,U,V,W\}=\emptyset$)

$res_{r5}(\{C,H,O,U,V,W\})= res_{r6}(\{C,H,O,U,V,W\})=\emptyset$

thus

$res_{A}(\{C,H,O,U,V,W\})=\{U,V,W,X\}$

Continuing with the state $\{C,H,O,U,V,W,X\}$, the results of reactions are:

$res_{r1}(\{C,H,O,U,V,W,X\})=\{U\}$ (since $\{C,H\}\subseteq\{C,H,O,U,V,W,X\}$ and $\emptyset\cap\{C,H,O,U,V,W,X\}=\emptyset$)

$res_{r2}(\{C,H,O,U,V,W,X\})=\{V\}$ (since $\{C,H,U\}\subseteq\{C,H,O,U,V,W,X\}$ and $\emptyset\cap\{C,H,O,U,V,W,X\}=\emptyset$)

$res_{r3}(\{C,H,O,U,V,W,X\})=\{W\}$ (since $\{H,V\}\subseteq\{C,H,O,U,V,W,X\}$ and $\emptyset\cap\{C,H,O,U,V,W,X\}=\emptyset$)

$res_{r4}(\{C,H,O,U,V,W,X\})=\{X\}$ (since $\{H,W\}\subseteq\{C,H,O,U,V,W,X\}$ and $\emptyset\cap\{C,H,O,U,V,W,X\}=\emptyset$)

$res_{r5}(\{C,H,O,U,V,W,X\})=\{Y\}$ (since $\{H,O,X\}\subseteq\{C,H,O,U,V,W,X\}$ and $\emptyset\cap\{C,H,O,U,V,W,X\}=\emptyset$)

$res_{r6}(\{C,H,O,U,V,W,X\})=\emptyset$

thus

$res_{A}(\{C,H,O,U,V,W,W,X\})=\{U,V,W,X,Y\}$

Continuing with the state $\{C,H,O,U,V,W,X,Y\}$, the results of reactions are:

$res_{r1}(\{C,H,O,U,V,W,X,Y\})=\{U\}$ (since $\{C,H\}\subseteq\{C,H,O,U,V,W,X,Y\}$ and $\emptyset\cap\{C,H,O,U,V,W,X,Y\}=\emptyset$)

$res_{r2}(\{C,H,O,U,V,W,X,Y\})=\{V\}$ (since $\{C,H,U\}\subseteq\{C,H,O,U,V,W,X,Y\}$ and $\emptyset\cap\{C,H,O,U,V,W,X,Y\}=\emptyset$)

$res_{r3}(\{C,H,O,U,V,W,X,Y\})=\{W\}$ (since $\{H,V\}\subseteq\{C,H,O,U,V,W,X,Y\}$ and $\emptyset\cap\{C,H,O,U,V,W,X,Y\}=\emptyset$)

$res_{r4}(\{C,H,O,U,V,W,X,Y\})=\{X\}$ (since $\{H,W\}\subseteq\{C,H,O,U,V,W,X,Y\}$ and $\emptyset\cap\{C,H,O,U,V,W,X,Y\}=\emptyset$)

$res_{r5}(\{C,H,O,U,V,W,X,Y\})=\{Y\}$ (since $\{H,O,X\}\subseteq\{C,H,O,U,V,W,X,Y\}$ and $\emptyset\cap\{C,H,O,U,V,W,X,Y\}=\emptyset$)

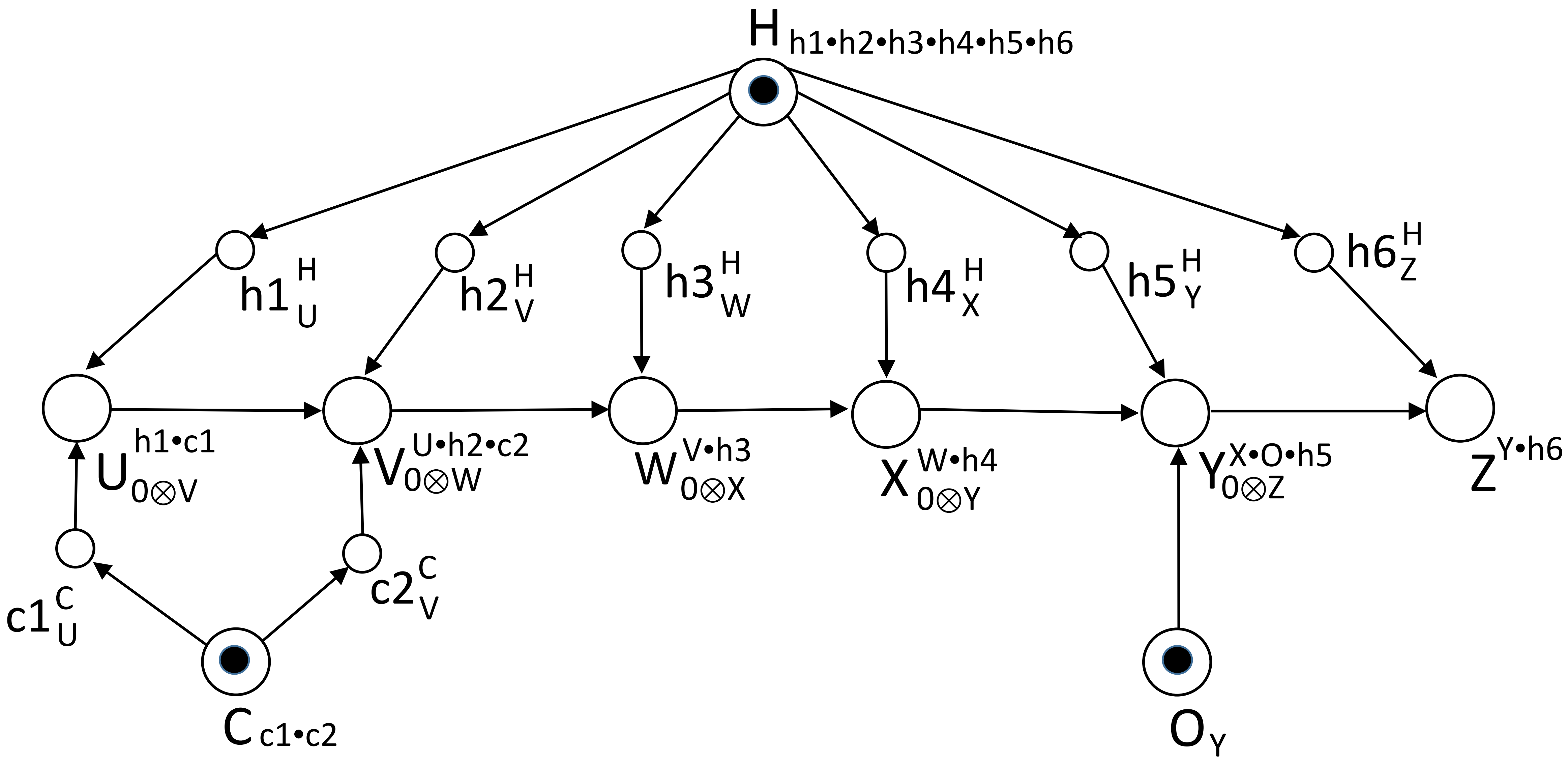
$res_{r6}(\{C,H,O,U,V,W,X,Y\})\ \{Z\}$ (since $\{H,Y\}\subseteq\{C,H,O,U,V,W,X,Y\}$ and $\emptyset\cap\{C,H,O,U,V,W,X,Y\}=\emptyset$)

thus

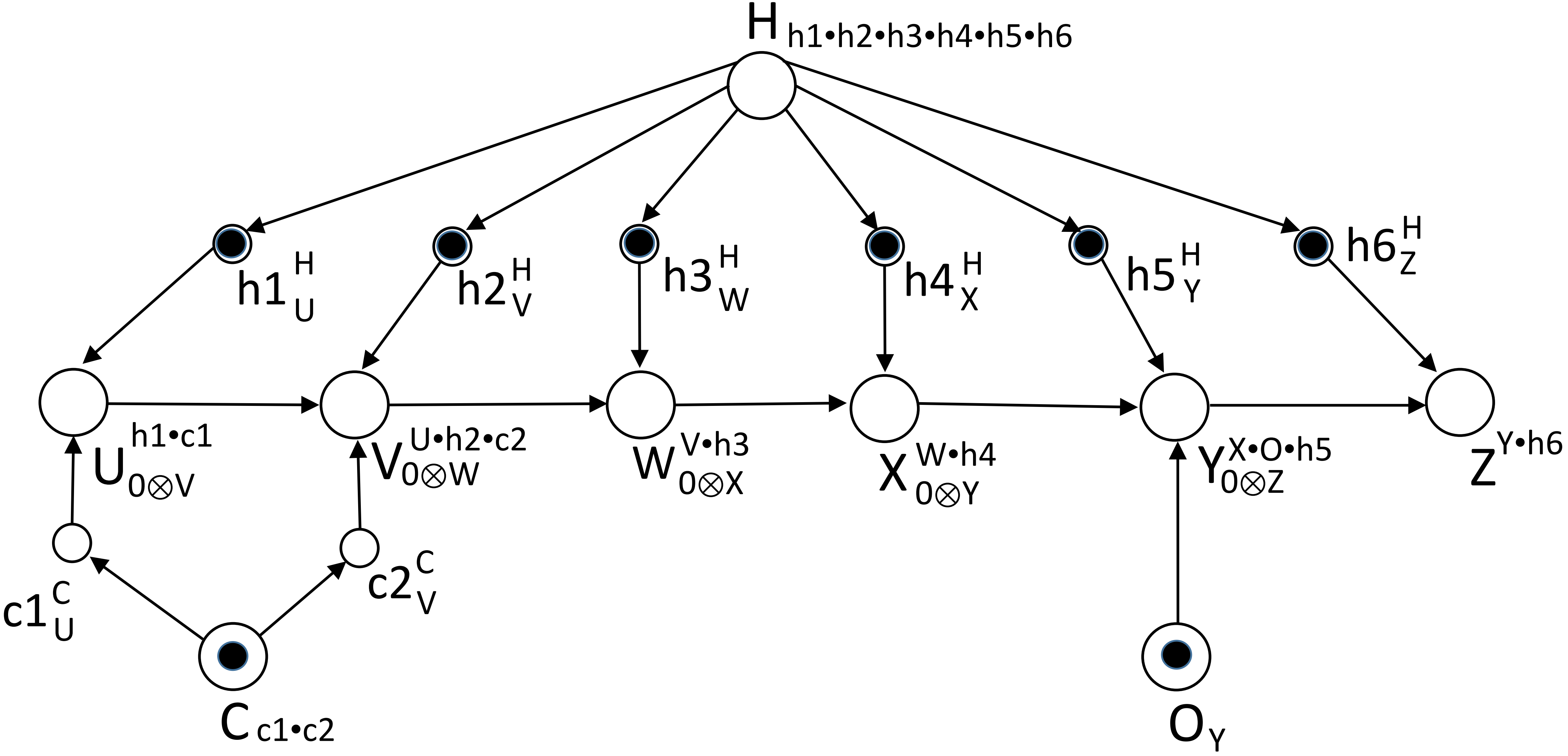
$res_{A}(\{C,H,O,U,V,W,W,X,Y\})=\{U,V,W,X,Y,Z\}$

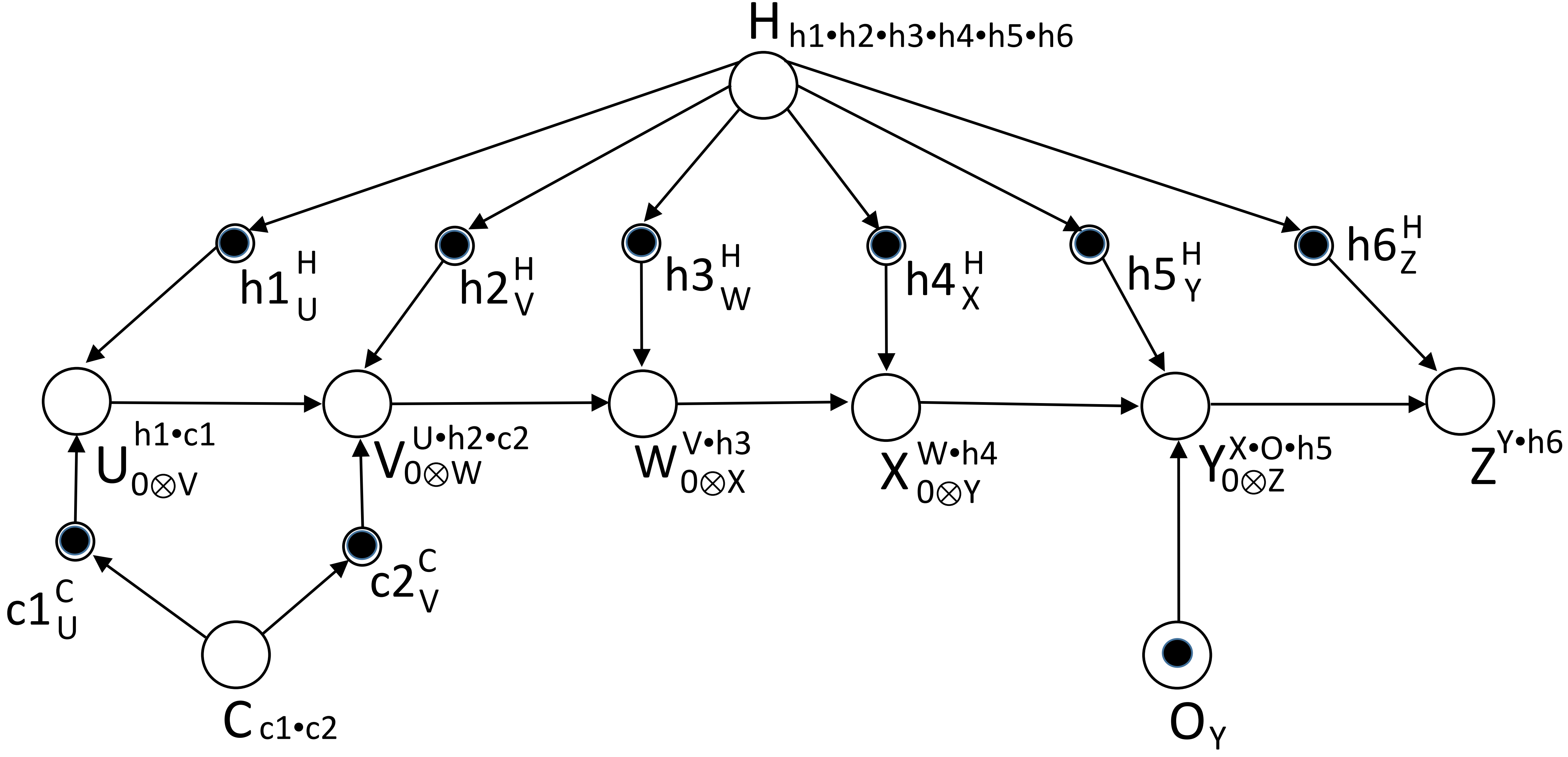
The next slides present the animated evolution of the c-e structure with initial state $s(C) = s(H) = s(O) = 1$ (and empty remaining nodes) imitating behaviour of reaction system *A* passing successive states. Regarding it as a translation of *A*, note that small nodes *c*1, *c*2, *h*1, *h*2, *h*3, *h*4, *h*5, *h*6 are some "artifacts" of this translation and have no counterparts in *A*. Intuitively, they might be seen as holding single atoms taken from *C* and *H*. The big nodes *C,H,O* may be seen as stores for atoms of carbon, hydrogen and oxygen.

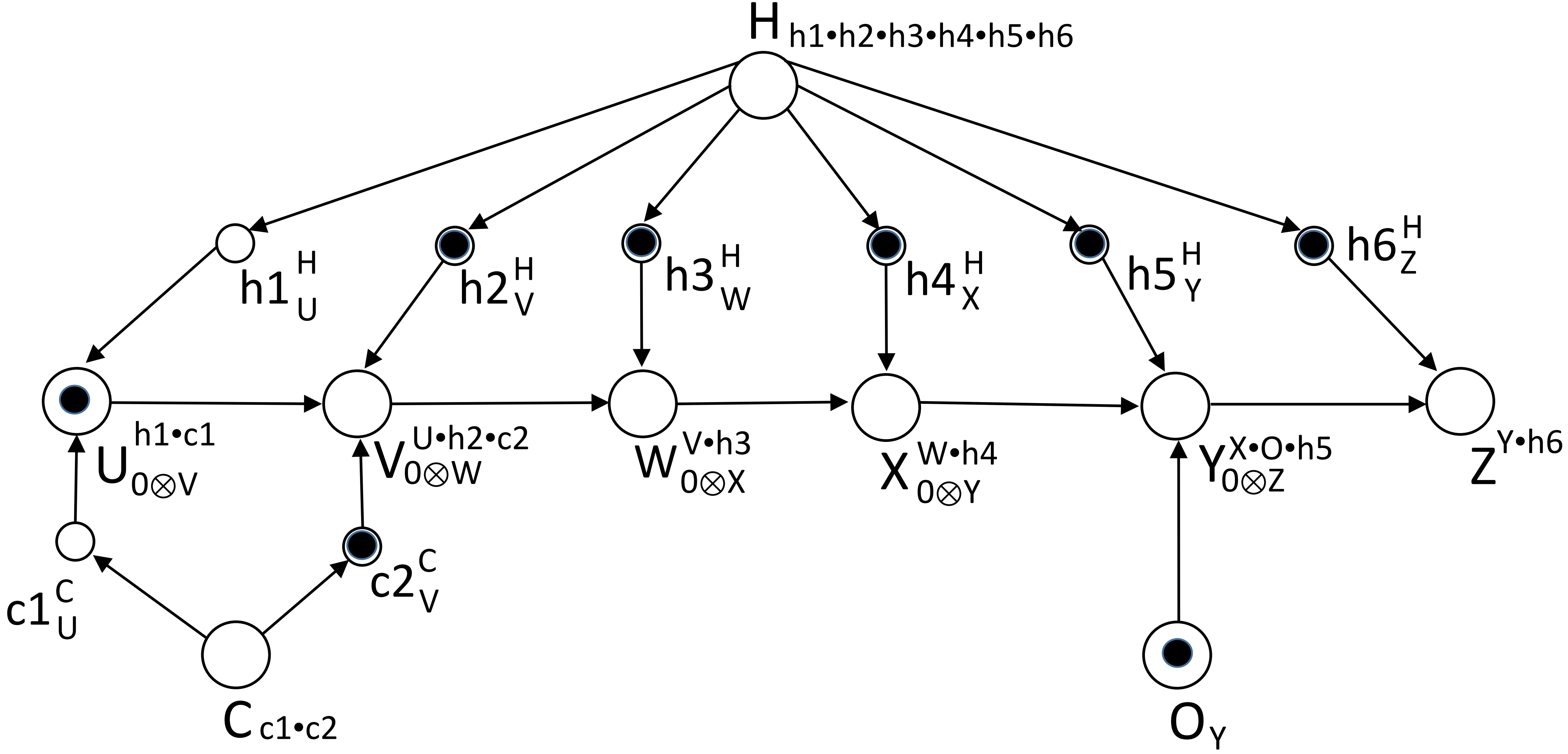
Remember that coefficient 0 in lower polynomials of nodes *U,V,W,X,Y*, permanently sustains tokens at them (according to definition of semantics of c-e structures).



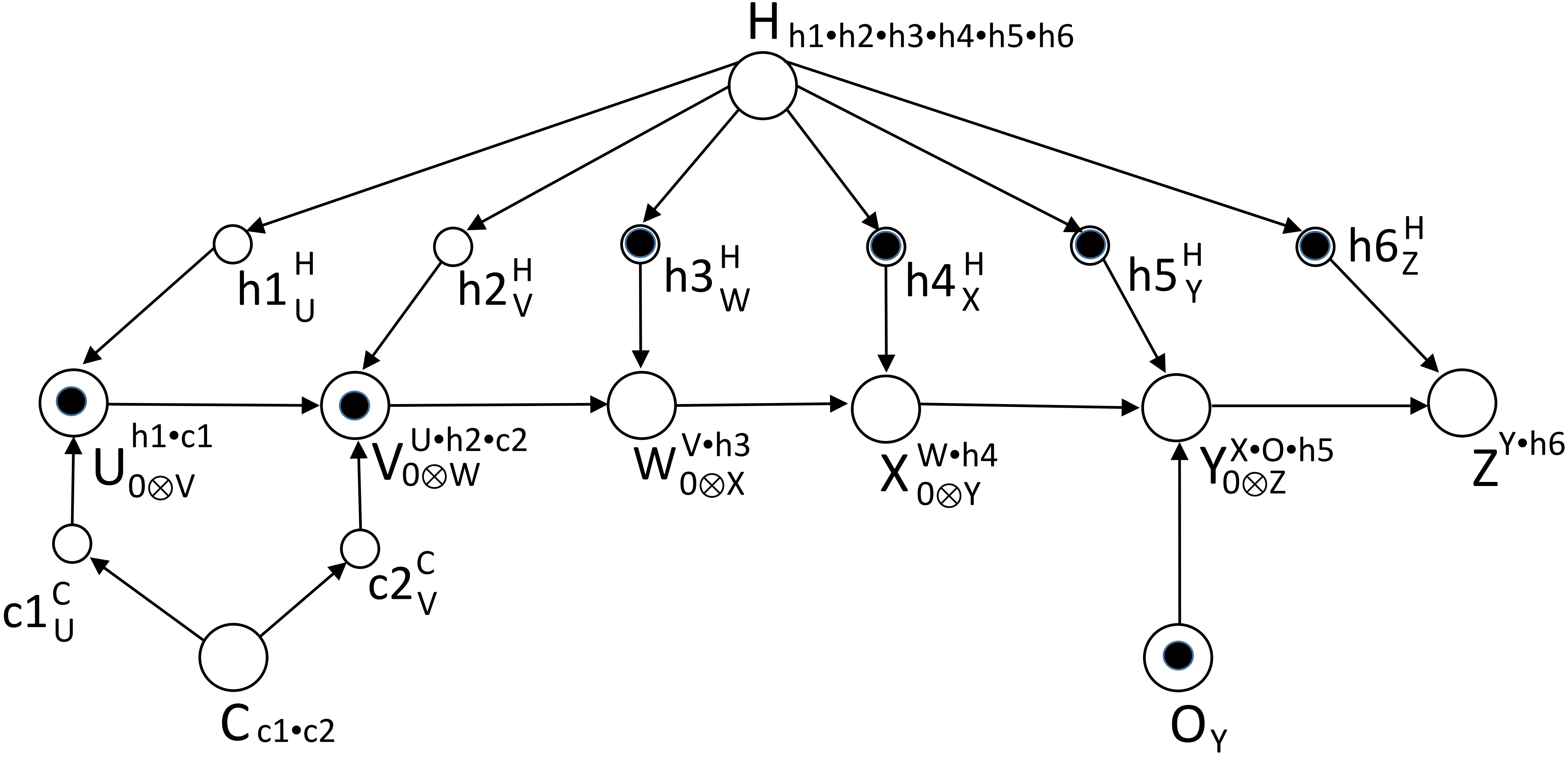
H h1•h2•h3•h4•h5•h6
h1 H U
h2 H V
h3 H W
h4 H X
h5 H Y
h6 H Z
U h1•c1 0⊗V
V U•h2•c2 0⊗W
W V•h3 0⊗X
X W•h4 0⊗Y
Y X•O•h5 0⊗Z
Z Y•h6
c1 C U
c2 C V
C c1•c2
O Y


H h1•h2•h3•h4•h5•h6
h1 H U
h2 H V
h3 H W
h4 H X
h5 H Y
h6 H Z
U h1•c1 0⊗V
V U•h2•c2 0⊗W
W V•h3 0⊗X
X W•h4 0⊗Y
Y X•O•h5 0⊗Z
Z Y•h6
c1 C U
c2 C V
C c1•c2
O Y

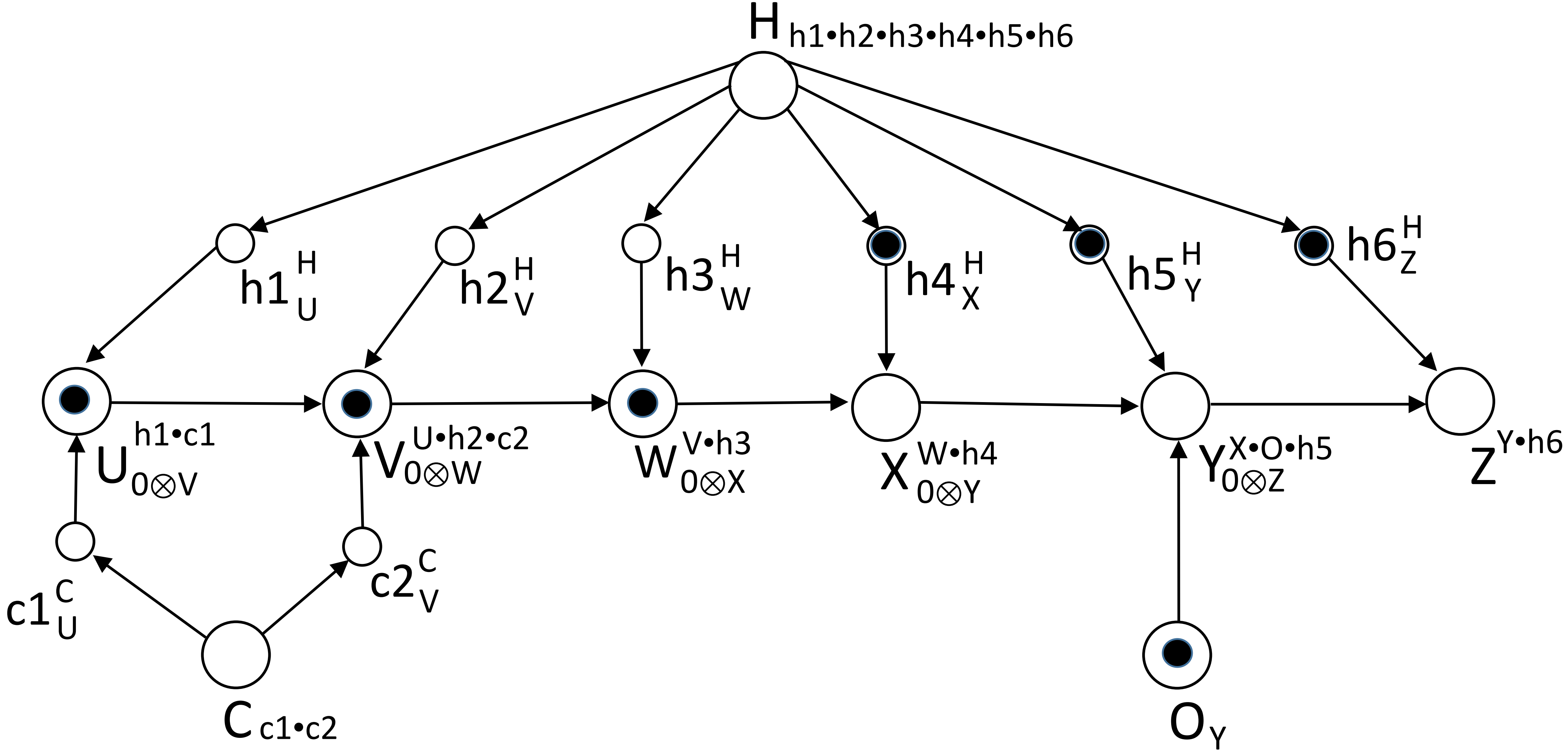

H h1•h2•h3•h4•h5•h6
h1 H U
h2 H V
h3 H W
h4 H X
h5 H Y
h6 H Z
U h1•c1 0⊗V
V U•h2•c2 0⊗W
W V•h3 0⊗X
X W•h4 0⊗Y
Y X•O•h5 0⊗Z
Z Y•h6
c1 C U
c2 C V
C c1•c2
O Y



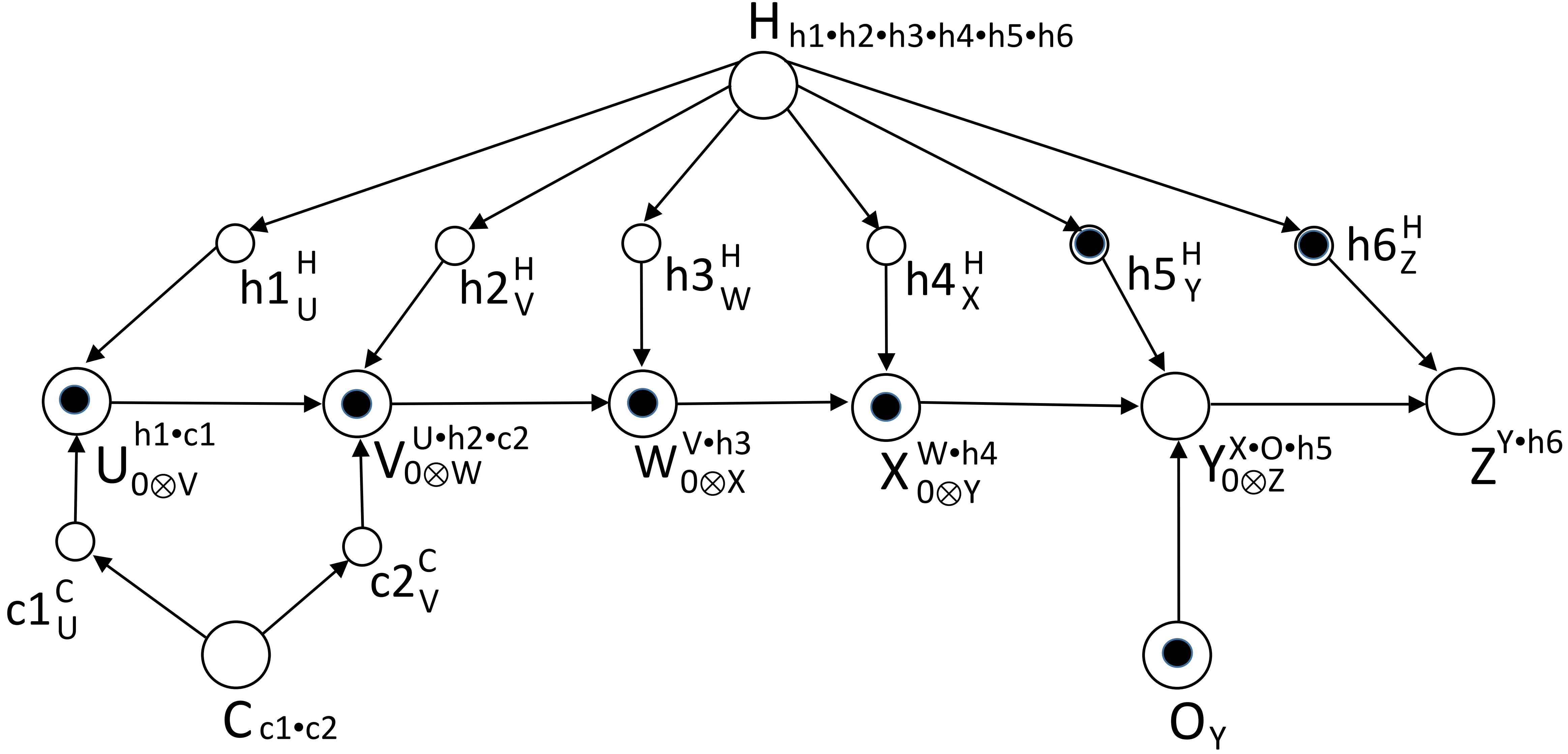
U=CH (methylidyne)



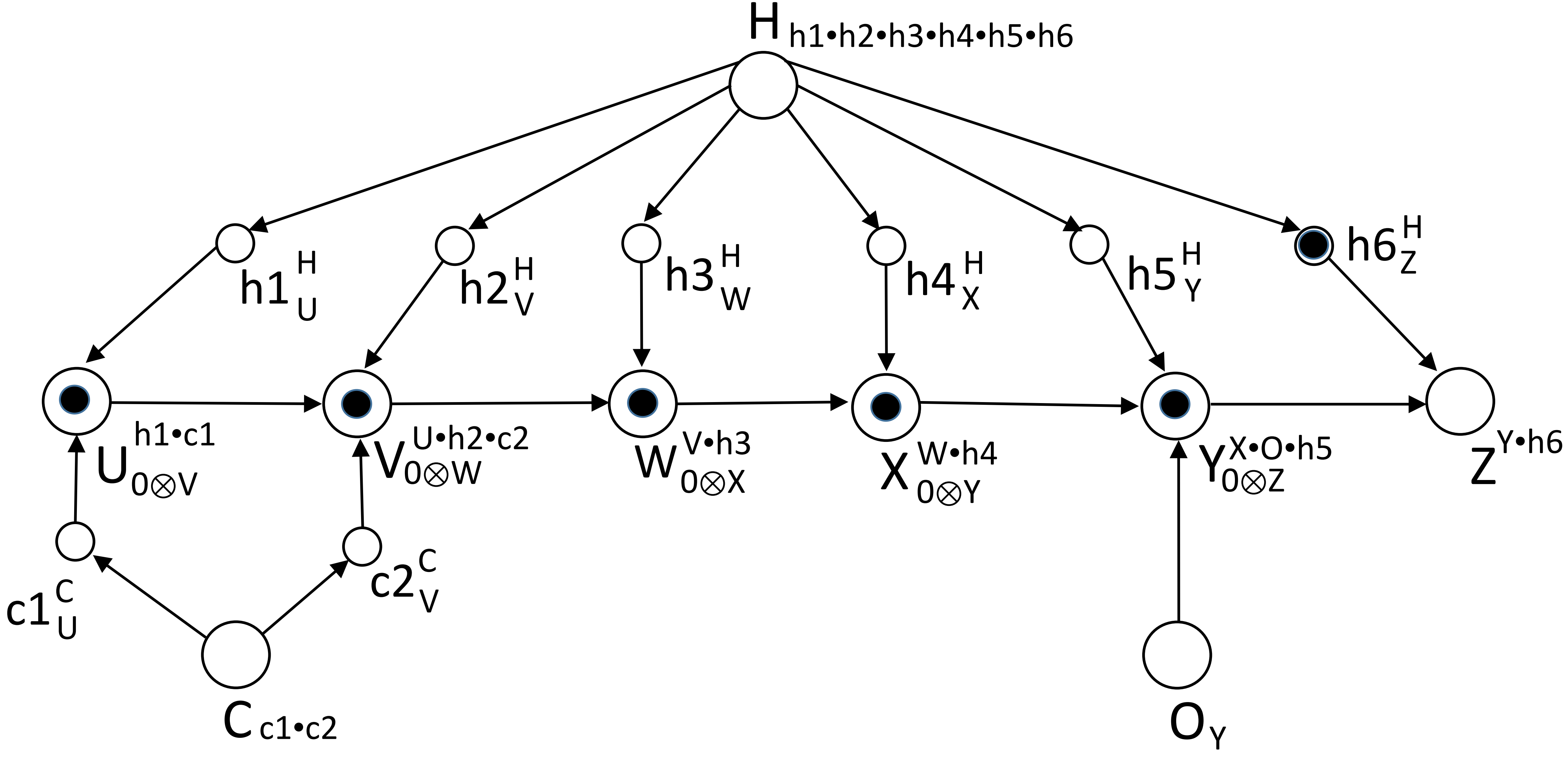
$V = C_2H_2$ (acetylene)



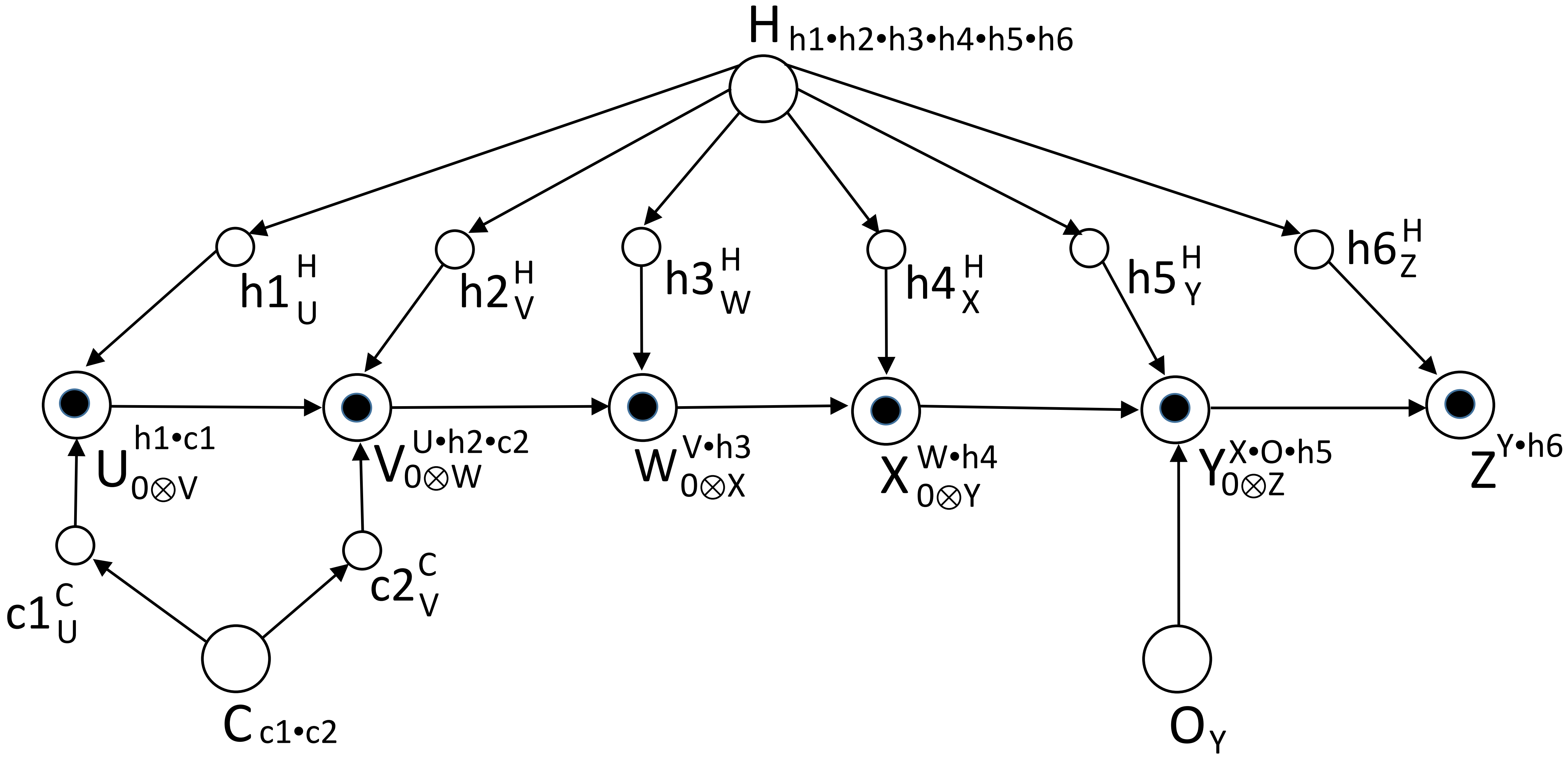
W=C_2H_3 (ethylenyl)



X=C_2H_4 (ethylene)



$Y=C_2H_5O$ (ethoxide)



Z=C_2H_5OH (ethanol)