



Socio-legal issues in the application of semantic web technology to chemical safety

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safe

SafePlaceSM

Risk Assessment

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- ▶ Risk assessment is the determination of the risk associated with a given hazard.
- ▶ In the context of chemistry research, risk assessment determines the risk associated with chemical hazards, e.g.,
 - ▶ Explosive,
 - ▶ Flammable,
 - ▶ Carcinogenic,
 - ▶ etc.

COSHH

- ▶ The Control of Substances Hazardous to Health (COSHH) Regulations 2002 are a UK statutory instrument.
- ▶ COSHH requires employers to protect their employees from the effects of exposure to hazardous chemical substances.
 - ▶ (The main mechanism for this is risk assessment.)

COSHH ASSESSMENT FORM				Record No.
SUBSTANCE NAME	PHYSICAL FORM	QUANTITY	NATURE OF HAZARD	
Water	liquid	1000ml	None	
Dextrose	Solid	<20g	possible irritation to eyes and skin	
Caffeine	Solid (tea)	<1g	Harmful if swallowed, induce vomiting.	
Milk	liquid	<100ml	No particular hazards	
NATURE OF PROCESS				
liquid extraction of caffeine, followed by combination with dextrose to produce a sweet drink				
Is there a less hazardous substance? <i>No</i>				
If so, why not use it?				
CONTROL MEASURES REQUIRED <i>No specific measure required</i>				
(Local exhaust ventilation, personal protection, etc.)				

c/o SmartTea project

COSHH Risk Assessment Methodology

0. Plan scientific experiment.
1. Enumerate collection of chemical substances.
2. Discover relevant health and safety information.
3. Interpolate assessment form template.

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c/o SmartTea project			

GHS

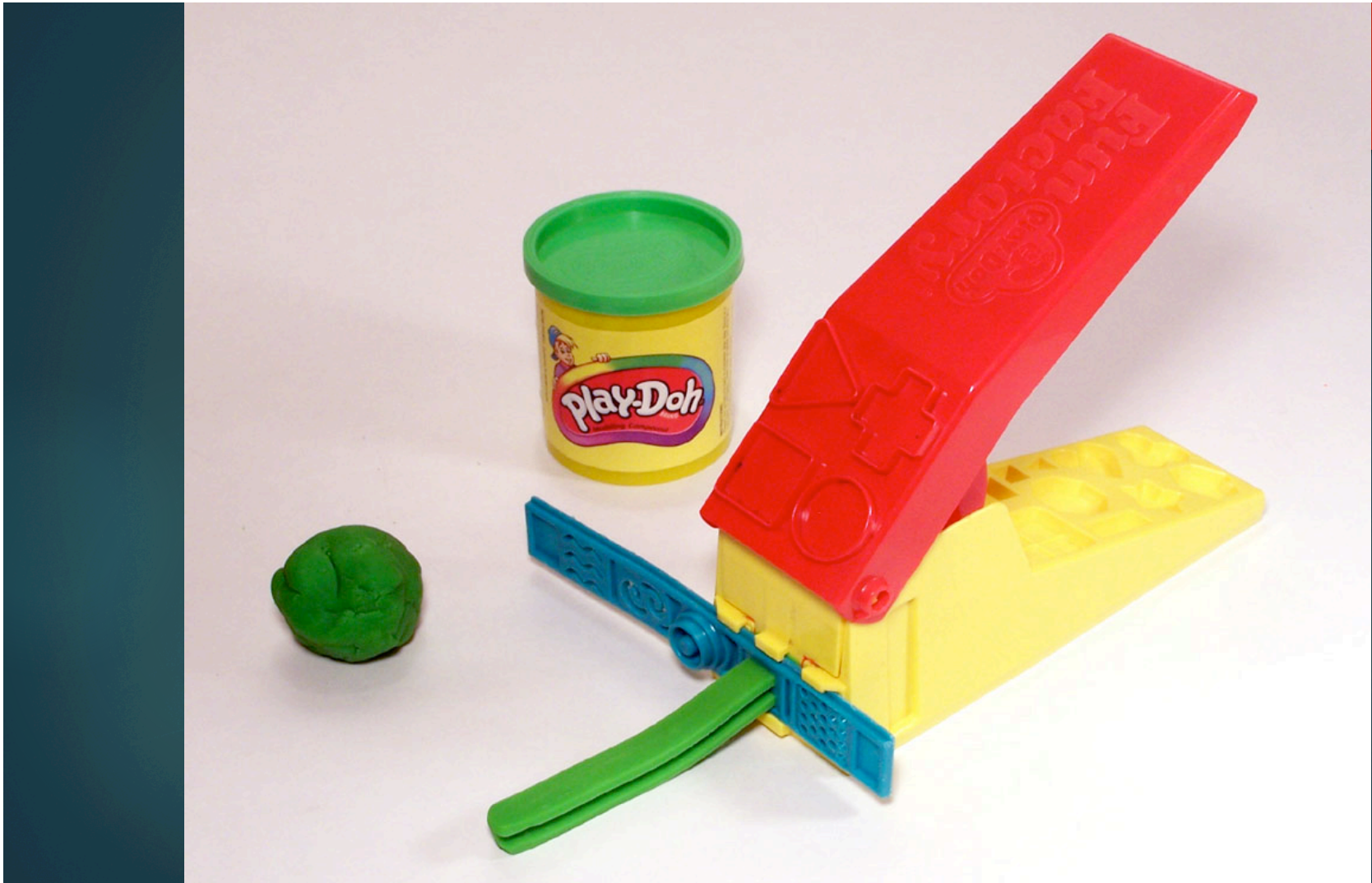
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- ▶ The Globally Harmonized System for Classification and Labelling of Chemicals (GHS) is a UN system.
 - ▶ Designed to supersede the various C&L systems that are currently in use around the world.



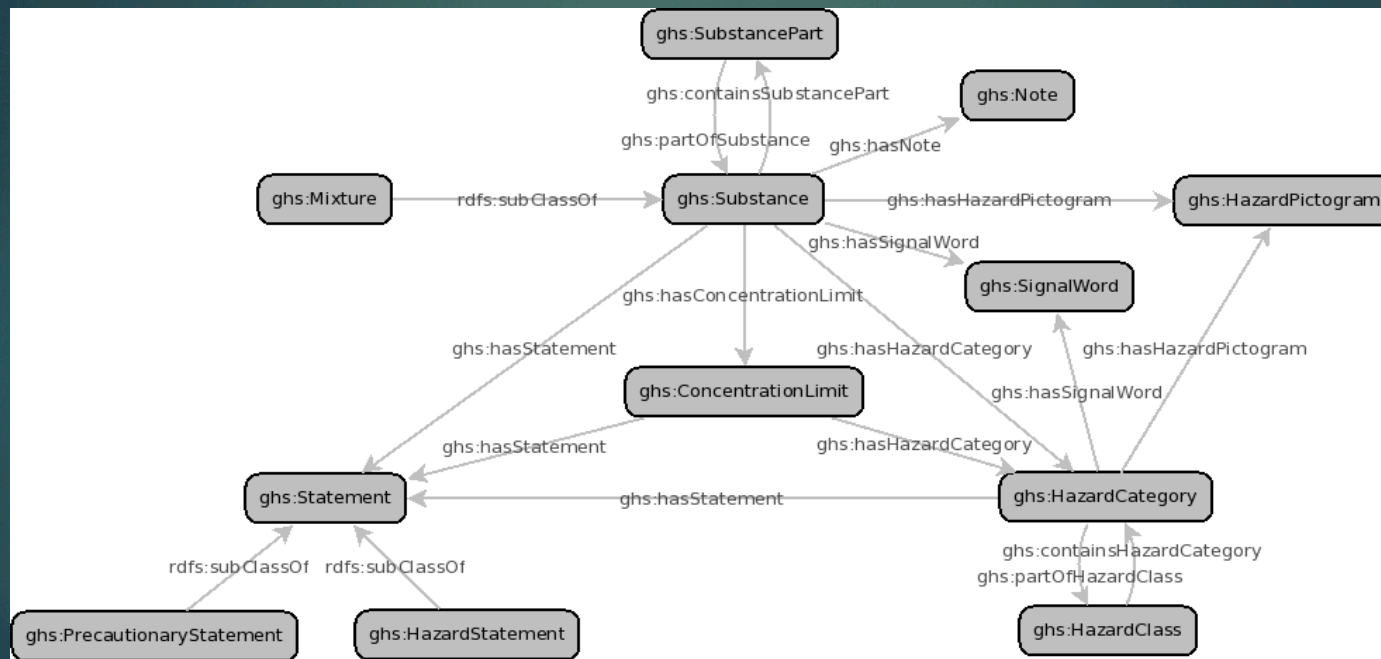
Problem Statement

- ▶ For humans, performing a risk assessment has two main drawbacks:
 - ▶ Less time spent performing experiments; and,
 - ▶ Potential for human error, e.g.,
 - ▶ Incomplete enumeration of chemical substances;
 - ▶ Use of incorrect information;
 - ▶ Transcription errors; and,
 - ▶ Tacit assumption of “common” elements.



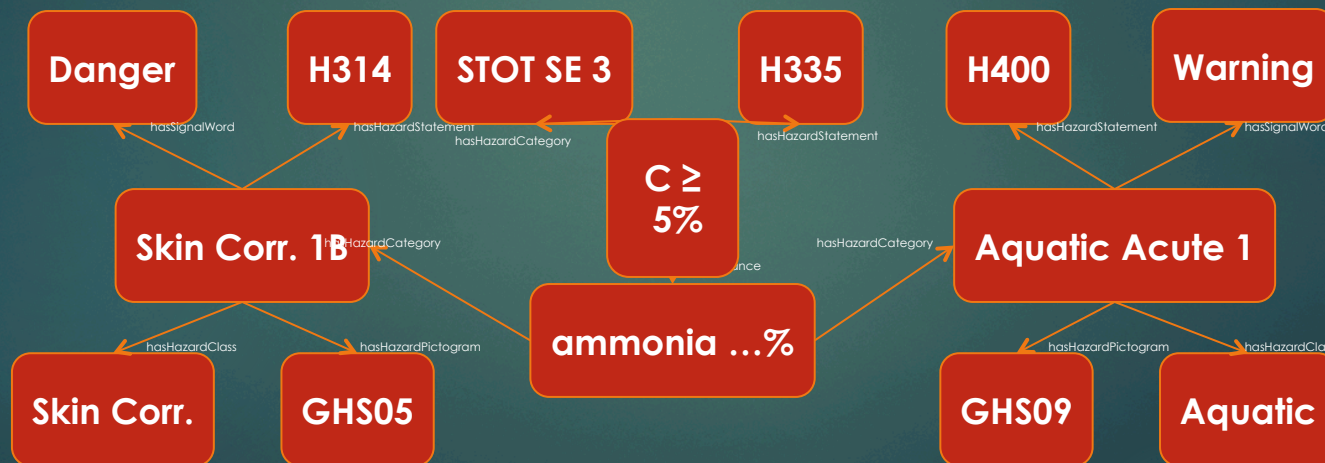
“ghs” Ontology

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“EC (No) 007-001-01-2”

Index No	International Chemical Identification	EC No	CAS No	Classification		Labelling			Specific Conc. Limits, M-factors	Notes
				Hazard Class and Category Code(s)	Hazard statement Code(s)	Pictogram, Signal Word Code(s)	Hazard statement Code(s)	Suppl. Hazard statement Code(s)		
007-001-01-2	ammonia ...%	215-647-6	1336-21-6	Skin Corr. 1B Aquatic-Acute 1	H314 H400	GHS05 GHS09 Dgr	H314 H400		STOT SE 3; H335: C ≥ 5 %	B



United Kingdom Home > 12540 - Benzene

12540 FLUKA

Benzene

analytical standard

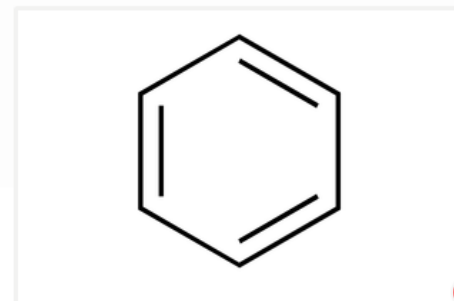
[DOWNLOAD MSDS \(PDF\)](#)

CAS Number [71-43-2](#) | Empirical Formula (Hill Notation) [C₆H₆](#) | Molecular Weight [78.11](#)

Bellstein Registry Number [969212](#) | EC Number [200-753-7](#) | MDL number [MFCD00003009](#)

PubChem Substance ID [24847664](#)

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Safety Information

Symbol	GHS08 GHS02, GHS07, GHS08
Signal word	Danger
Hazard statements	H225-H304-H315-H319-H340-H350-H372
Precautionary statements	P201-P210-P301 + P310-P305 + P351 + P338-P308 + P313-P331
Personal Protective Equipment	Eyeshields, Faceshields, full-face respirator (US), Gloves, multi-purpose combination respirator cartridge (US), type ABEK (EN14387) respirator filter
Hazard Codes (Europe)	F,T
Risk Statements (Europe)	45-46-11-36/38-48/23/24/25-65

QR-InChI

Standard QR code readers will interpret the QR code to give the string which will be recognised as a url

Resolve the url

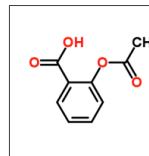


Landing Page
Basic
Information
on the InChI
Key

Note: This InChI key must have been registered with the site since the link from InChI key to InChI is not computable.

Resolve the link

Aspirin



Std. InChIKey: BSYNRYMUTXBXSQ-UHFFFAOYSA-N
Std. InChI: InChI=1S/C9H8O4/c1-6(10)13-8-5-3-2-4-7(9)/9(11)12/h2-5H,1H3,(H,11,12)
SMILES: CC(=O)OC1=CC=CC=C1C(=O)O

<http://inchi.scisharp.org/BSYNRYMUTXBXSQ-UHFFFAOYSA-N>

Just to take a
ChemSpider
example

InChI QR Service

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- ▶ The web site/service & API provided for suppliers to enter the molecule and the Molecular formation they wish to link to the InChI Key

InChI QR Codes
03/02/2014



Standard QR code readers will interpret the QR code to give the string which will be recognised as a url

Resolve the url



Landing Page
Basic Information
on the InChI Key

Note: This InChI key must have been registered by the supplier who provides the basic information according to an InChI Trust standard

Supplier: Sigma Aldrich
Product ID: A5376
Batch ID: 2929278373
Amount: 100g
Purity: 99%

The URL is broken down as follows

sid:	Supplier ID
pid:	Product ID
bid:	Batch ID
am:	Amount as number with unit.
pure:	Purity (default to express as percentage)

[http://inchi.scisharp.org/BSYNRYMUTXBXSQ-UHFFFAOYSA-N?
sid=sigmaaldrich&pid=A5376&bid=2929278373&am=100g&pure=99.0](http://inchi.scisharp.org/BSYNRYMUTXBXSQ-UHFFFAOYSA-N?sid=sigmaaldrich&pid=A5376&bid=2929278373&am=100g&pure=99.0)

Alert user to supplied link

Resolve the url

Landing Page Basic Information on the InChI Key



<http://inchi.scisharp.org/BSYNRYMUTXBXSQ-UHFFFAOYSA-N?lpid=ecrystals&link=doi%3A10.5258%2Fecrystals%2F145&desc=Crystal+Structure>

Note: This InChI key must have been registered by the supplier who provides a link on to a suitable source web site

InChI QR

benzo-15-crown-5

InChI Link
Crystal Structure
doi:10.5258/ecrystals/145

Std. InChIKey: FNEPSTUXZLEUCK-UHFFFAOYSA-N
Std. InChI: InChI=1S/C14H20O5/c1-2-4-14-13(3-1)18-11-9-16-7-5-15-6-8-17-10

Link to the eCrystals Web site

eCrystals University of Southampton

6,7,9,10,12,13,15,16-Octahydro-benzo-1,4,7,10,13-pentaoxacyclodecine

Sample Originator: Esther Rivory^a and Jeremy G. Frey^a
Data Collection: Simon J. Cole^a
Structure Determination: Simon J. Cole^a and Michael B. Hursthouse^a
University of Southampton^a
C₁₄H₂₀O₅
InChI=1C14H20O5/c1-2-4-14-13(3-1)18-11-9-16-7-5-15-6-8-17-10-12-13-14(13)-2(2)

Identification: 10.5258/ecrystals/145

Controlled: crown ethers, crown
Keywords:
Date: 07 October 2004
Created:
Deposited On: 21 Jan 2008 15:29
Deposited By: Dr Simon J. Cole

Available Files

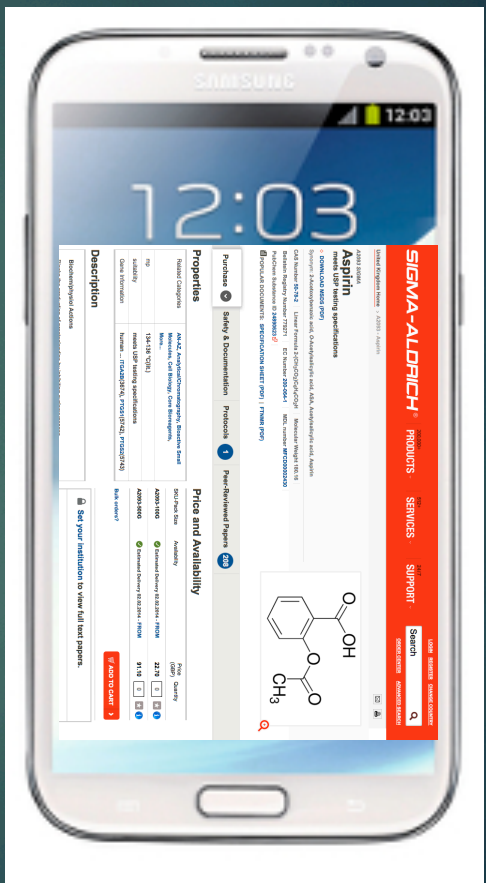
File Name	Size
Final Result	
646c831.cif	13k
646c831.cml	6k
646c831.hf.txt	105k
646c831_checkcif.htm	7k

Validation

Parameter	Value
Chemical formula	C14H20O5
Crystal morphology	Plate
Crystal system	Orthorhombic
Space group symbol	Pbcn
Cell length a	16.496(16)
Cell length b	8.325(3)

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InChI QR Codes
03/02/2014



App provides detailed information



App recognizes the url



Licence?
 Note: The supplier would not in this case need to have registered the InChI QR Key with the trust

<http://inchi.scisharp.org/BSYNRYMUTXBXSQ-UHFFFAOYSA-N>

Issues

Legal

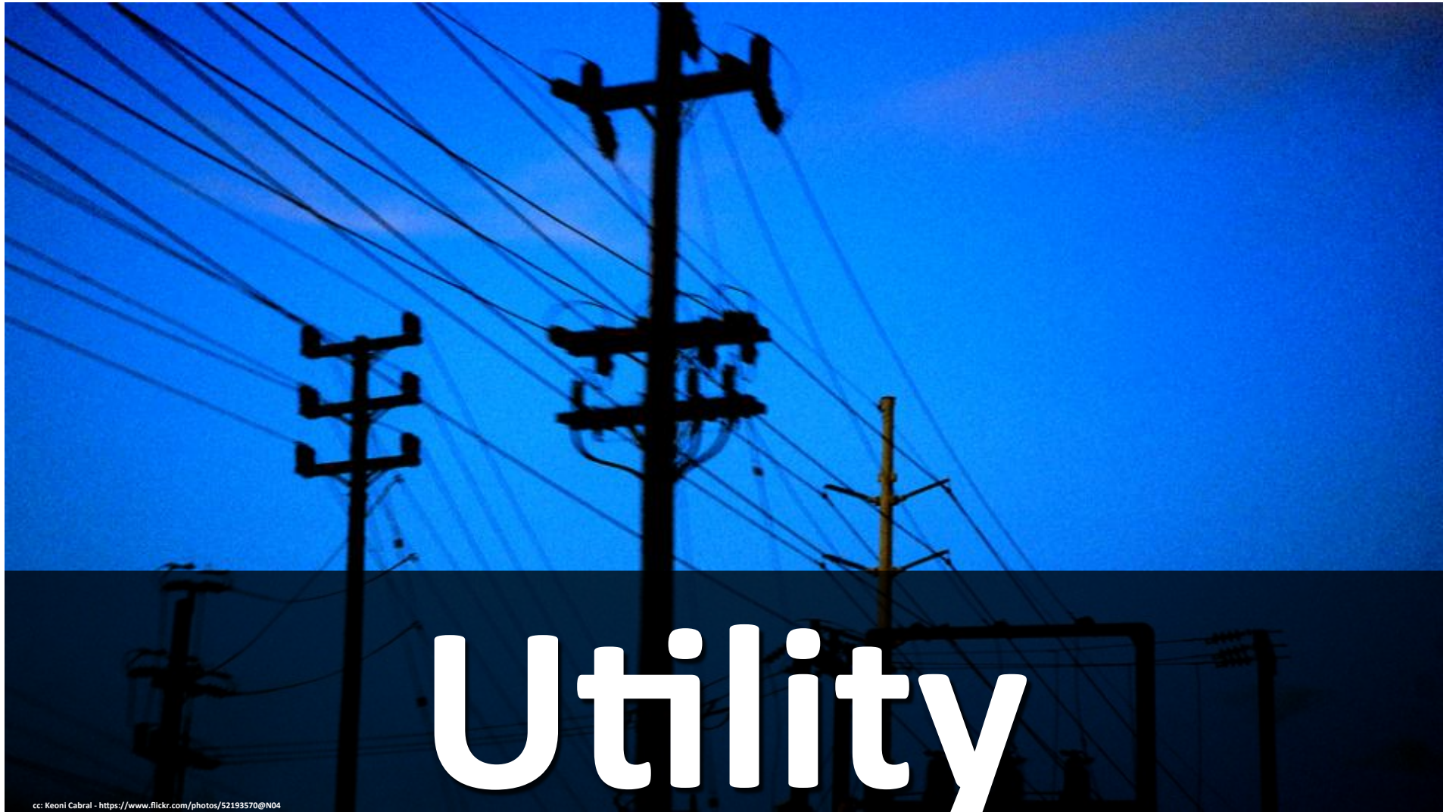
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InChI QR Codes
03/02/2014

- ▶ QR Code is an unenforced patent
- ▶ Would the Trust want/need to review the validity of the data/links provided?
- ▶ What commitment to longevity would be made by the Trust and Suppliers?
- ▶ How “public” should the QR code contents to be?
- ▶ Potentially hold supplier information in aggregate that could be significant (i.e. whole catalogues of many suppliers)

A top-down view of several wooden Scrabble tiles scattered on a dark surface. The tiles are arranged to spell out the word 'DATA' in the center. Other tiles with various letters and numbers are scattered around. The word 'DATA' is formed by tiles with 'D' (4 points), 'A' (1 point), 'T' (1 point), and 'A' (1 point).

Data



Utility

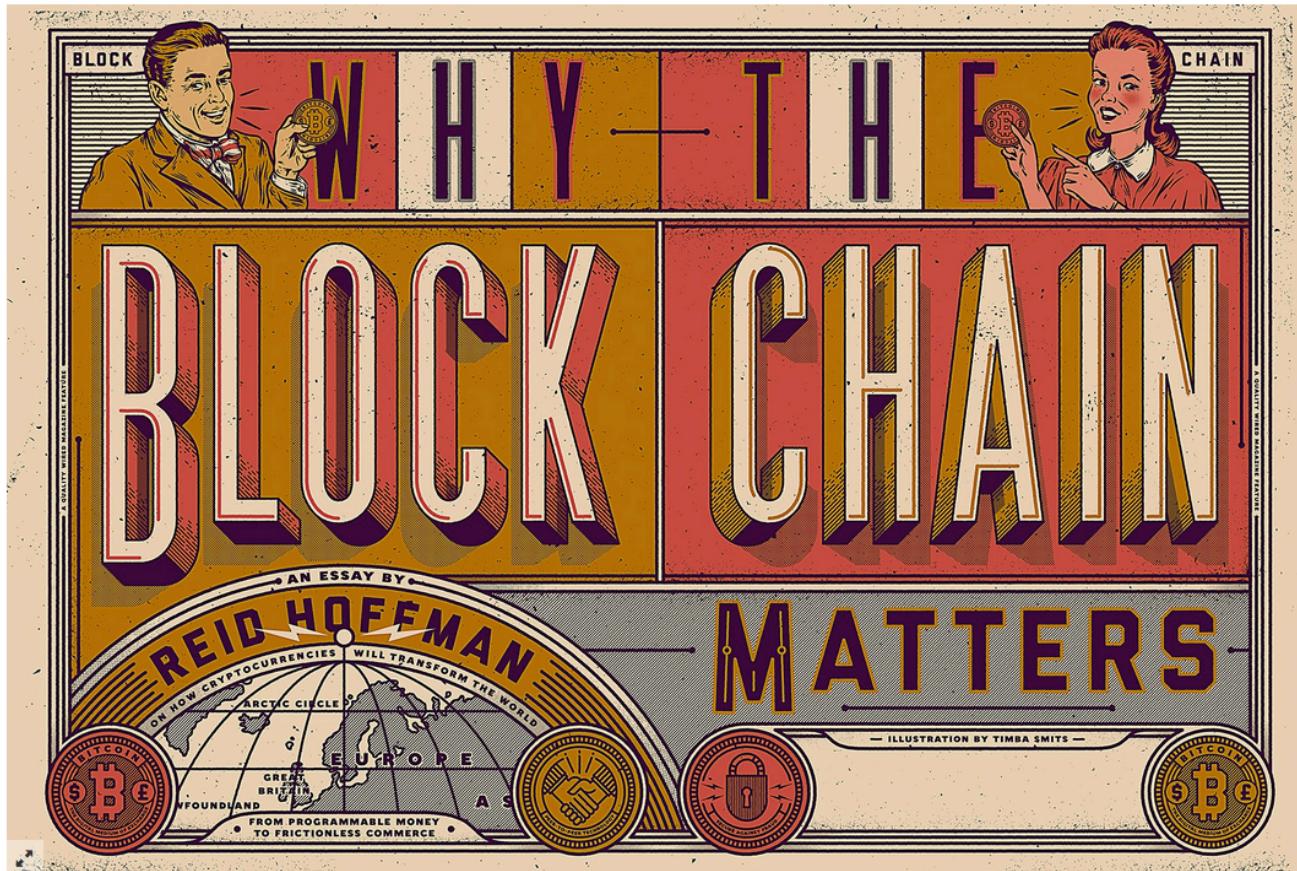
cc: Keoni Cabral - <https://www.flickr.com/photos/52193570@N04>



Reid Hoffman: Why the block chain matters

MAGAZINE / 15 MAY 15 / by REID HOFFMAN

      3546 shares
11 comments



Timba Smits



Thank You