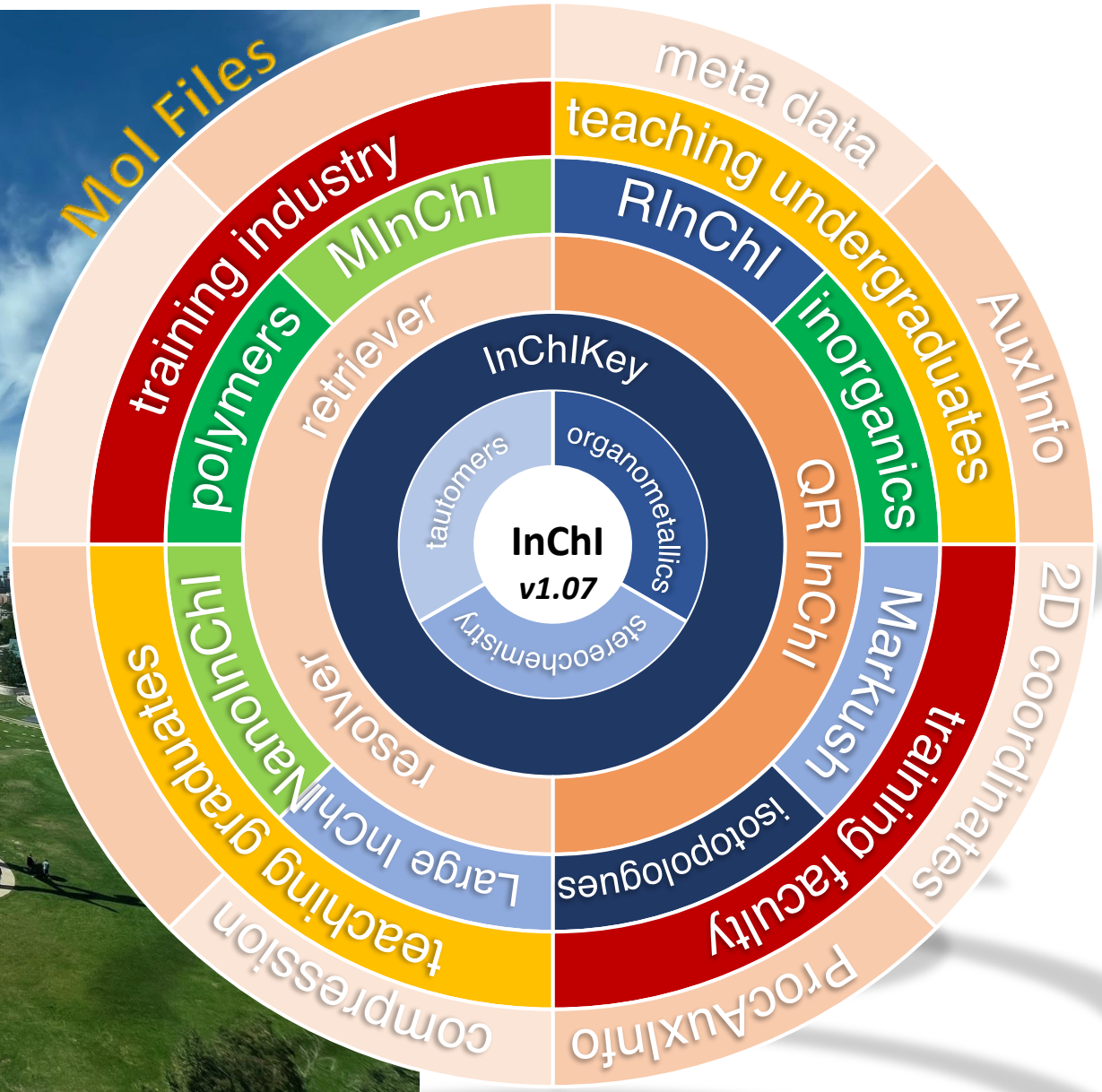
Dynamic InChI: canonical, unique and on-the-fly



Dynamic InChI: canonical, unique and on-the-fly

Symposium: Open Source Chemoinformatics Resources

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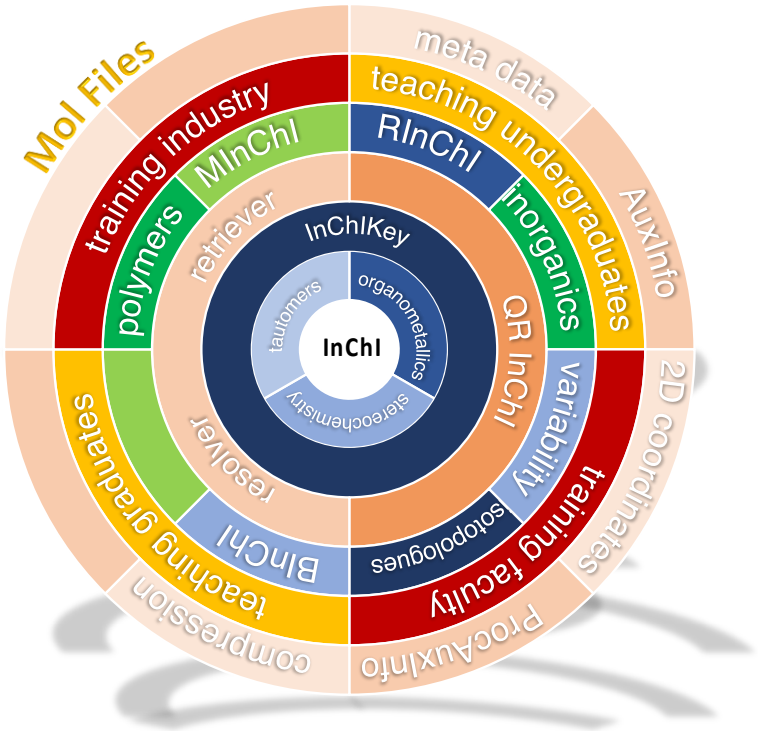
2. Institute of Inorganic Chemistry, RWTH Aachen University, 52074 Aachen, Germany;
3. Yusuf Hamied Department of Chemistry, University of Cambridge, CB2 1EW, UK

InChI: all you need to know



- **Canonical molecular identifier**
  - Unique
    - One InChI for every molecule
    - One molecule for every InChI
  - Interchangeable, ordered molecule collections
  - Used in
    - PubChem, Reaxys, CAS, ZINC, journals, industry databases, compound trader, ….
  - Make your own InChI
    - ChemDraw, Marvin, Biovia/Draw, Elemental, ChemSketch, RDKit, Knime, openBabel, …

How to read an InChI?

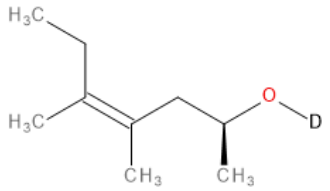
InChI=1S/C9H18O/c1-5-7(2)8(3)6-9(4)10/h9-10H,5-6H2,1-4H3/b8-7-/t9-/m0/s1/i10D

Layered structure:

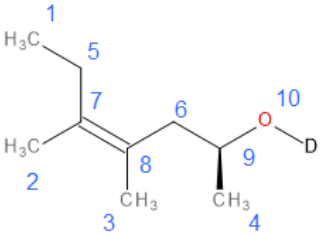
InChI=1S/C9H18O/c1-5-7(2)8(3)6-9(4)10/h9-10H,5-6H2,1-4H3/b8-7-/t9-/m0/s1/i10D
Version /formula/connectivity /hydrogens /Stereochemistry/isotope

InChIKey – hashed InChI

RGTMBYZGSPYLCM-ZBUQKXQUSA-N



canonical numbering



Layered structure:

RGTMBYZGSPYLCM-ZBUQKXQUSA-N
Formula -Stereochemistry -Version -Total charge
Connectivity Isotopes (N = neutral)
Hydrogens Other additional layers

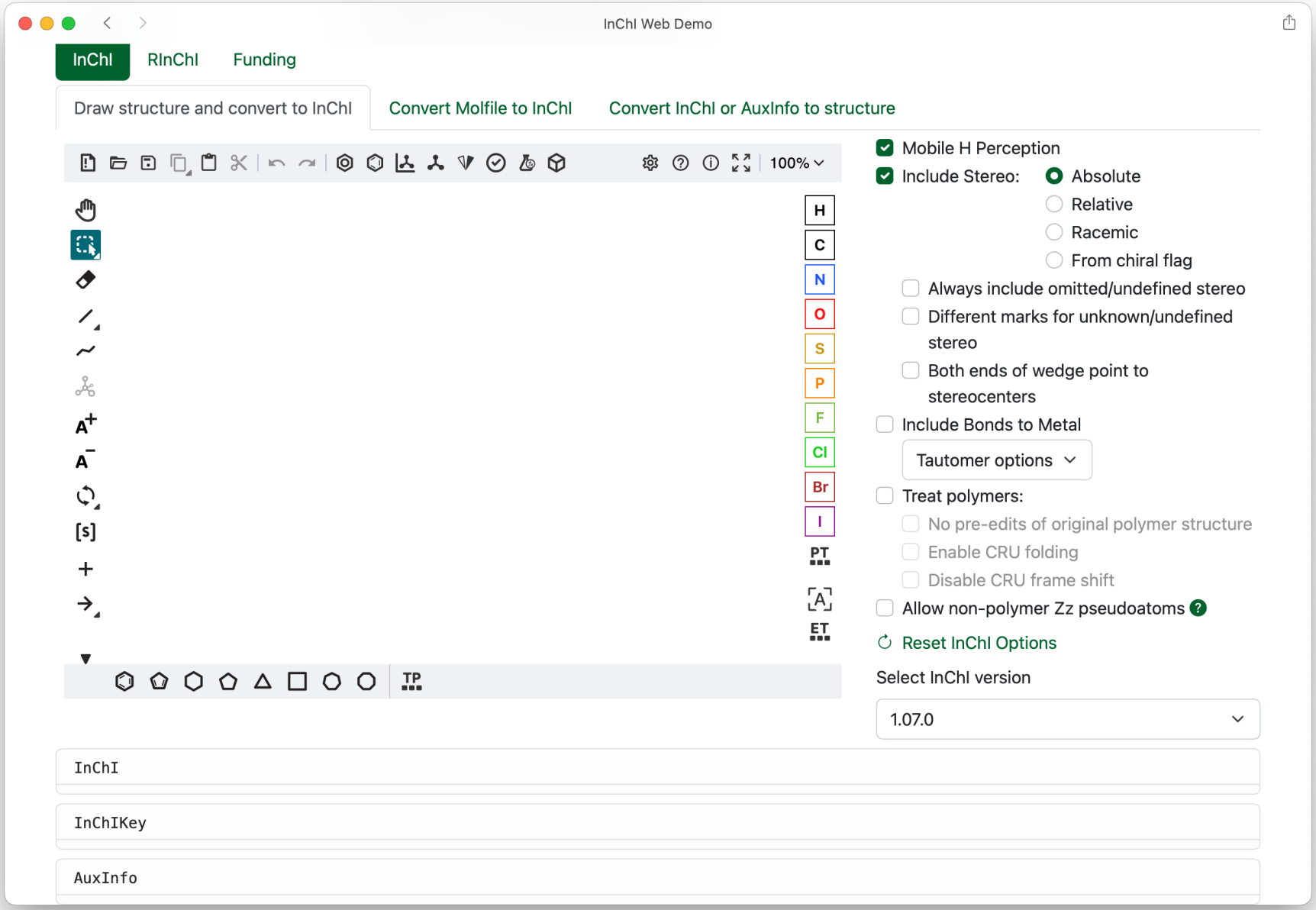
Collisions every few billion structures: none in PubChem

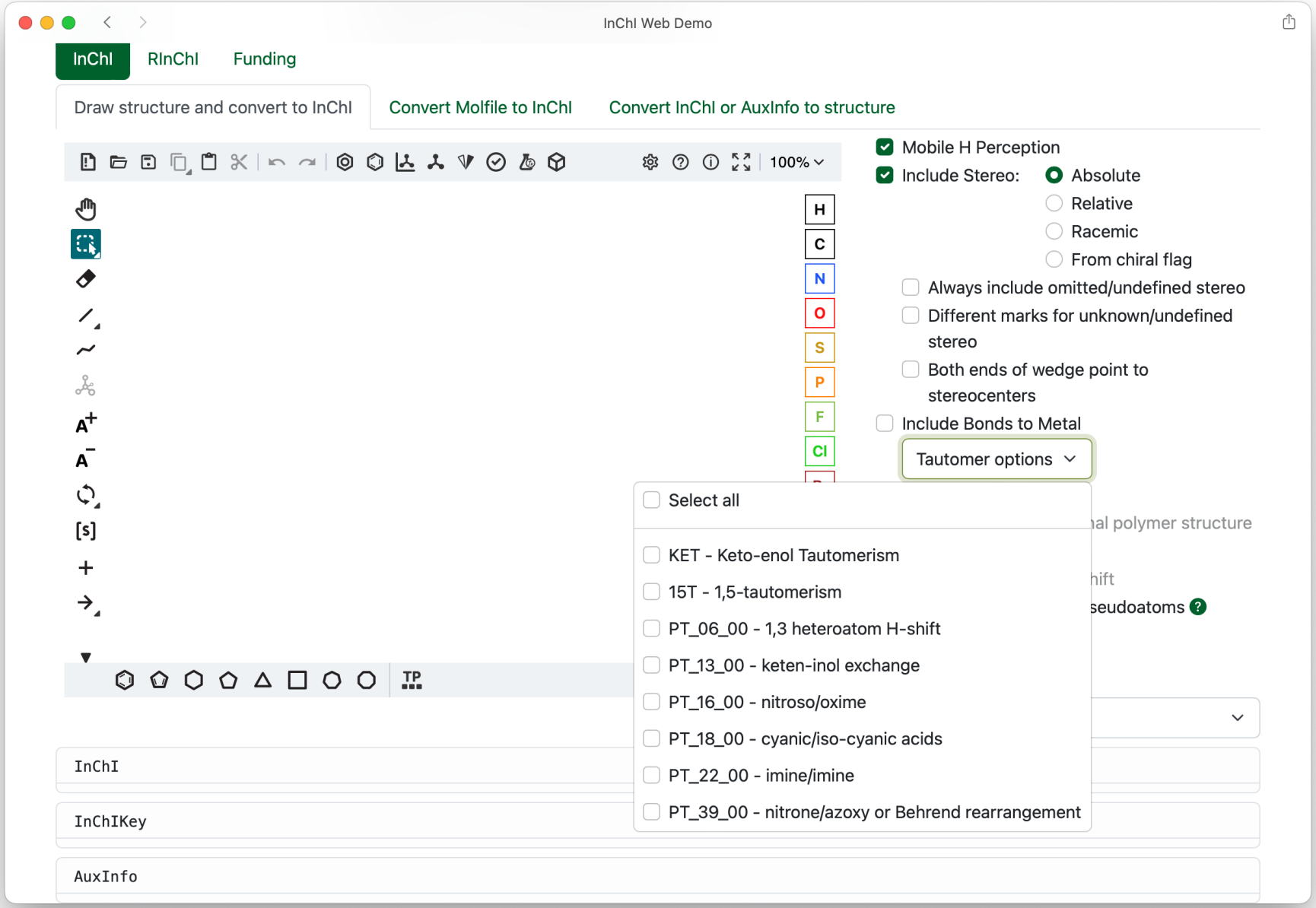
- There a very few known ones in longer peptide chains in terms of stereochemistry

How to read an InChI?

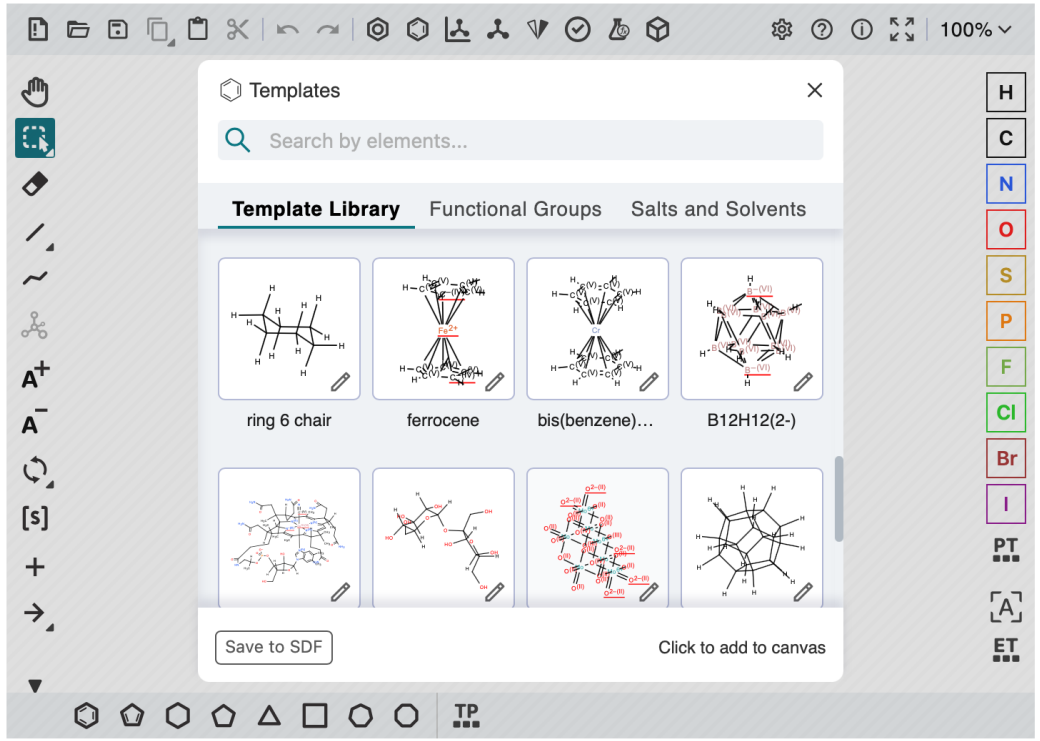
But, don’t do it!

- InChI is meant to be read
  by machines


InChI Web Demo
InChI
RInChI
Funding
Draw structure and convert to InChI
Convert Molfile to InChI
Convert InChI or AuxInfo to structure
100%
H
C
N
O
S
P
F
Cl
Br
I
PT
ET
TP
Mobile H Perception
Include Stereo:
Absolute
Relative
Racemic
From chiral flag
Always include omitted/undefined stereo
Different marks for unknown/undefined stereo
Both ends of wedge point to stereocenters
Include Bonds to Metal
Tautomer options
Treat polymers:
No pre-edits of original polymer structure
Enable CRU folding
Disable CRU frame shift
Allow non-polymer Zz pseudoatoms
Reset InChI Options
Select InChI version
1.07.0
InChI
InChIKey
AuxInfo


InChI Web Demo
InChI
RInChI
Funding
Draw structure and convert to InChI
Convert Molfile to InChI
Convert InChI or AuxInfo to structure
100%
H
C
N
O
S
P
F
Cl
Mobile H Perception
Include Stereo:
Absolute
Relative
Racemic
From chiral flag
Always include omitted/undefined stereo
Different marks for unknown/undefined stereo
Both ends of wedge point to stereocenters
Include Bonds to Metal
Tautomer options
Select all
KET - Keto-enol Tautomerism
15T - 1,5-tautomerism
PT_06_00 - 1,3 heteroatom H-shift
PT_13_00 - keten-inol exchange
PT_16_00 - nitroso/oxime
PT_18_00 - cyanic/iso-cyanic acids
PT_22_00 - imine/imine
PT_39_00 - nitrone/azoxy or Behrend rearrangement
InChI
InChIKey
AuxInfo

InChI Web Demo



- [x] Mobile H Perception
- [x] Include Stereo:
  - (•) Absolute
  - ( ) Relative
  - ( ) Racemic
  - ( ) From chiral flag
- [ ] Always include omitted/undefined stereo
- [ ] Different marks for unknown/undefined stereo
- [ ] Both ends of wedge point to stereocenters
- [ ] Include Bonds to Metal

Tautomer options

- [ ] Treat polymers:
  - [ ] No pre-edits of original polymer structure
  - [ ] Enable CRU folding
  - [ ] Disable CRU frame shift
- [ ] Allow non-polymer Zz pseudoatoms

Reset InChI Options

Select InChI version

1.07.0

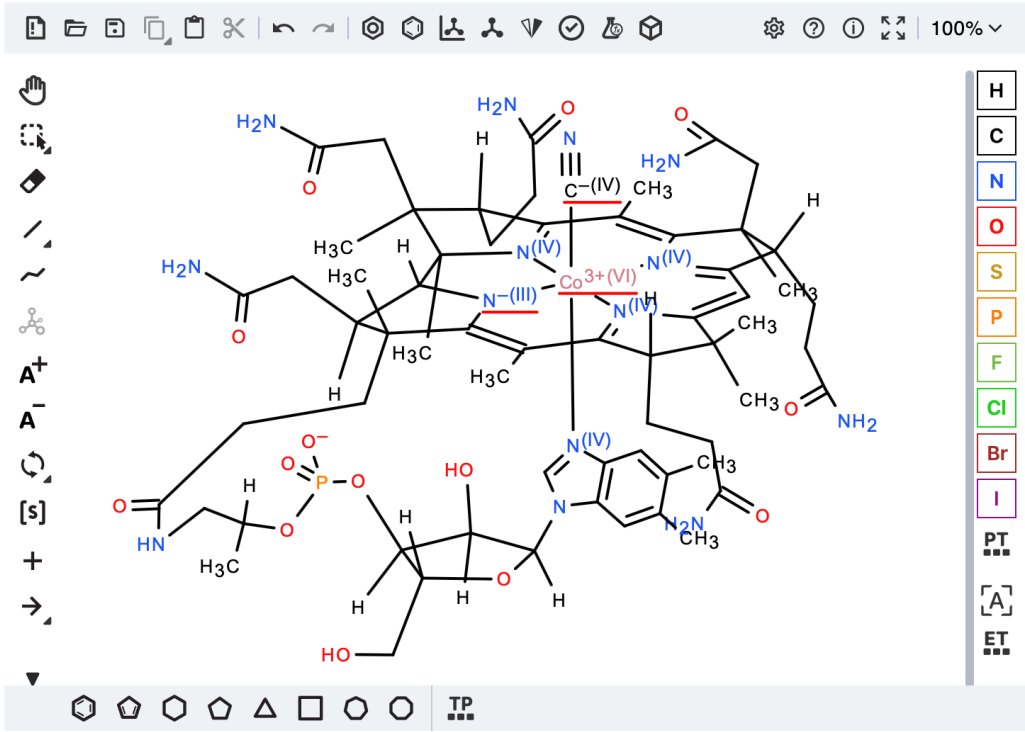
InChI

InChIKey

AuxInfo

Log

InChI Web Demo



100%

- [x] Mobile H Perception
- [x] Include Stereo:
  - (•) Absolute
  - ( ) Relative
  - ( ) Racemic
  - ( ) From chiral flag
- [ ] Always include omitted/undefined stereo
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  - [ ] Disable CRU frame shift
- [ ] Allow non-polymer Zz pseudoatoms
- Reset InChI Options

Select InChI version

1.07.0

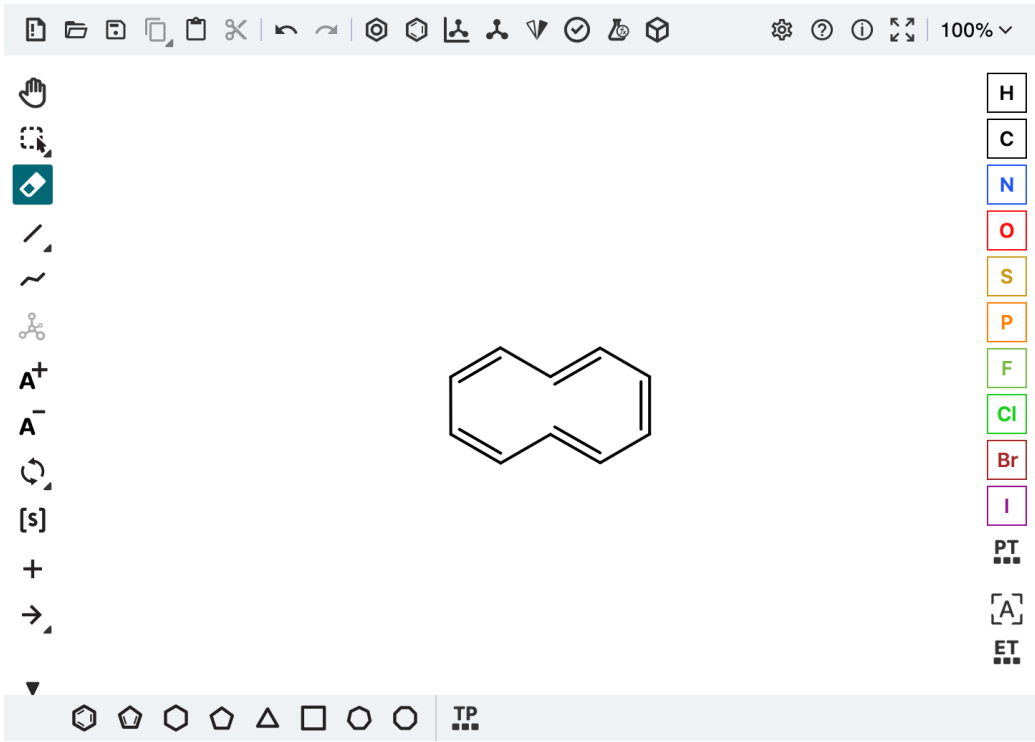
InChI

```
InChI=1S/C62H90N13O14P.CN.Co/c1-29-20-39-40(21-30(29)2)75(28-70-39)57-52(84)53(41(27-76)87-57)89-90(85,86)88-31(3)26-69-49(83)18-19-59(8)37(22-46(66)80)56-62(11)61(10,25-48(68)82)36(14-17-45(65)79)51(74-62)33(5)55-60(9,24-47(67)81)34(12-15-43(63)77)38(71-55)23-42-58(6,7)35(13-16-44(64)78)50(72-42)32(4)54(59)73-56;1-2;/h20-21,23,28,31,34-37,41,52-53,56-57,76,84H,12-19,22,24-27H2,1-11H3,(H15,63,64,65,66,67,68,69,71,72,73,74,77,78,79,80,81,82,83,85,86);;/q;-1;+3/p-2/t31-,34-,35-,36-,37+,41-,52-,53-,56-,57+,59-,60+,61+,62+;;/m1../s1
```

InChIKey

```
FDJOLVPMNUYSCM-WZHZPDAFSA-L
```

InChI Web Demo



Mobile H Perception
Include Stereo: Absolute / Relative / Racemic / From chiral flag
Always include omitted/undefined stereo
Different marks for unknown/undefined stereo
Both ends of wedge point to stereocenters
Include Bonds to Metal
Tautomer options
Treat polymers:
No pre-edits of original polymer structure
Enable CRU folding
Disable CRU frame shift
Allow non-polymer Zz pseudoatoms
Reset InChI Options
Select InChI version
1.07.0

InChI
InChI=1S/C10H10/c1-2-4-6-8-10-9-7-5-3-1/h1-10H/b2-1-,3-1-,4-2-,5-3+,6-4+,7-5+,8-6+,9-7-,10-8-,10-9-

InChIKey
ZYRKBGIIBMTQHN-HGJACCJQSA-N

AuxInfo
AuxInfo=1/0/N:8,10,7,9,5,1,6,3,4,2/E:(1,2,3,4,5,6,7,8,9,10)/rA:10nCCCCCCCCCC/rB:;d1s2;d2;;s4d5;s5;d7;s1;s8d9;/rC:8.5598,-5.0751,-11.625;10.2902,-5.0746,-11.625;9.4266,-4.575,-11.625;10.2902,-6.0755,-11.625;8.5598,-6.08,-11.625;9.4288,-6.575,-11.625;7.6919,

InChI is alive!

- **InChI 1.07.0 released end of Q2 2024**
  - About 3,000 issues (errors, warnings and hints were fixed)
    - Google fuzz issues resolved
  - 6 tautomer transformation added for testing
  - Base for the further development
- **InChI moved to GitHub**
  - InChI v1.07 and its source code available under MIT license
    - https://github.com/IUPAC-InChI/InChI/releases
  - Vital for enabling future collaborative development
  - Comprehensive test environment
    - InChI Web Demo
      - Early test access to developments
    - Docker test suit ready for download

InChI development status

- **InChI**
  - Released 1.07.0
    - Code clean-up (1.07)
    - 6 Tautomer transformations for testing
  - Under development
    - Requirements (nearly) ready
      - Molecular inorganics
      - Stereochemistry
      - Tautomers
      - Sgroups and Sgroup data
      - Isotopologues
    - Longer evaluations
      - Variable molecules / Markush InChIs
        - Prototypes being tested
        - https://github.com/topics/inchi
      - Large molecules

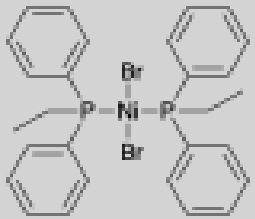
- **InChI Application Framework**
  - Released
    - RInChI 1.0
    - InChI Web Demo
      - https://iupac-inchi.github.io/InChI-Web-Demo/
  - Published
    - QR code
  - Test phase
    - Resolver
      - https://github.com/inchiresolver/inchiresolver#readme
    - RInChI (1.1)
      - https://github.com/IUPAC-InChI/RInChI
  - Awaiting coding
    - MInChI
      - Prototype released
        - https://github.com/cdd/mixtures
    - RInChI (1.2)
  - Active evaluations
    - NanoInChI (NInChI)

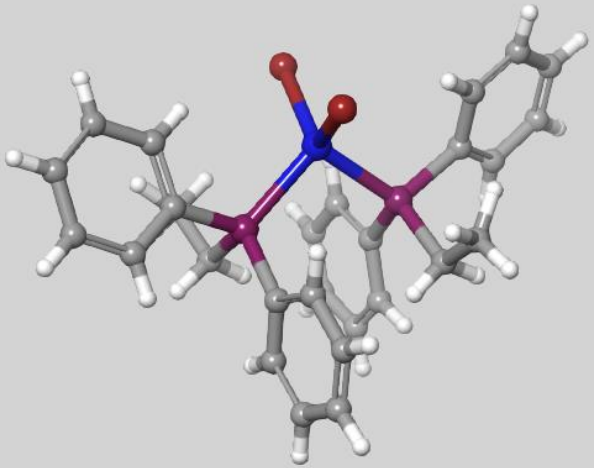
Molecular Inorganics

InChI v1.07

InChI=1S/2C14H15P.2BrH.Ni
/c2*1-2-15(13-9-5-3-6-10-13)14-11-7-4-8-12-14;;;
/h2*3-12H,2H2,1H3;2*1H;/q;;;;+2/p-2
InChIKey=LRGOJBHMPWNRJJ-UHFFFAOYSA-L

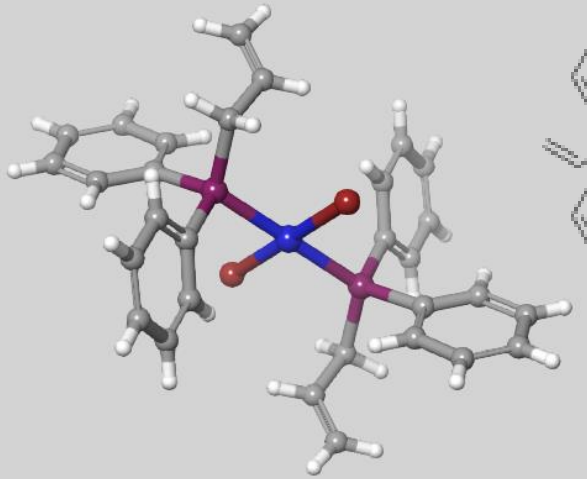
No stereoisomers

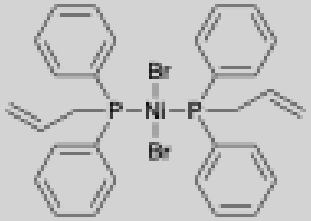




CSD refcode: KOMHEZ
J.-O.Malm, V.Alfredsson, G.Svensson, J.Albertsson (1992) *Acta Crystallogr.,Sect.C:Cryst.Struct.Commun.*,**48**,406

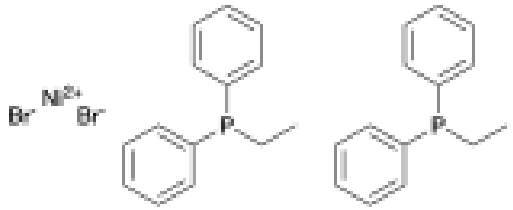
InChI=1S/2C15H15P.2BrH.Ni
/c2*1-2-13-16(14-9-5-3-6-10-14)15-11-7-4-8-12-15;;;
/h2*2-12H,1,13H2;2*1H;/q;;;;+2/p-2
InChIKey=PUFLLCFASVLTJA-UHFFFAOYSA-L



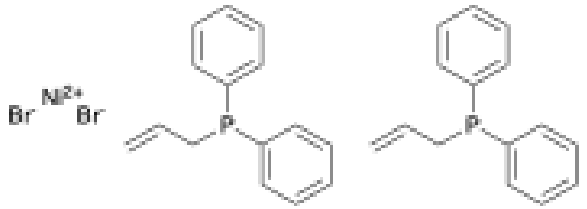


Possibility of *cis / trans* stereoisomers

CSD refcode: XIKWEX
M.L.Clapson, D.J.Nelson, M.W.Drover (2023) *ACS Org. Inorg. Au*,**3**,217

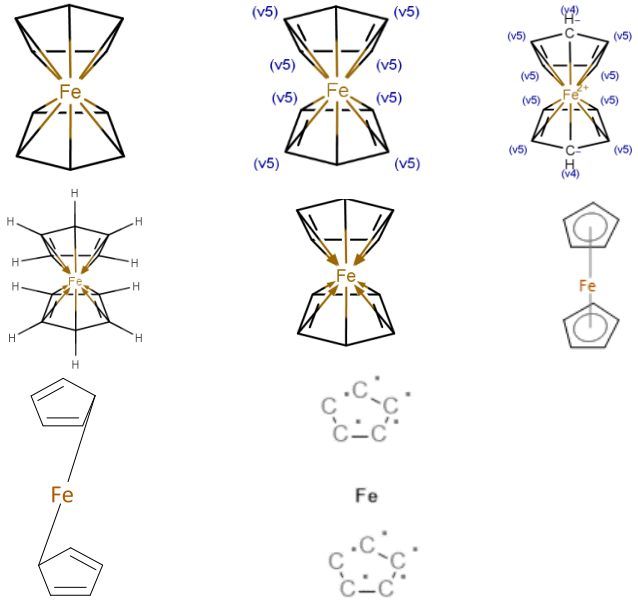


The change in nickel geometry probably reflects a change in the electronic state of the nickel, which is very sensitive to the ligands



Molecular Inorganics

- **Current standard InChI deletes all bonds to metal atoms**
  - Information of metal coordination is lost
    - Stereochemistry of molecular inorganics cannot be
- **Guidelines for identifying equivalent representations finalised 2022**
  - Example Ferrocene
    - Depictions interpreted as identical representations



(V3 molfile)

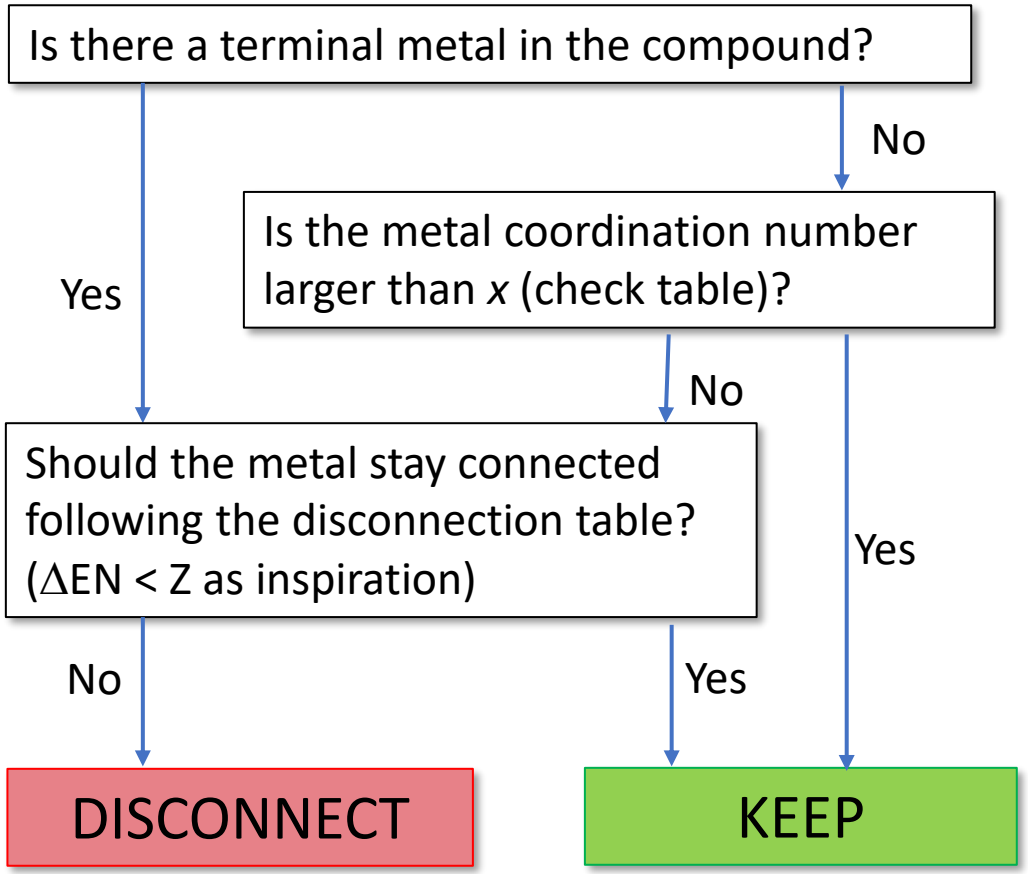
    - Depictions seen as other substances

Molecular Inorganics

- **Keep connectivity for inorganics and organometallics**
  - Keep explicitly drawn Hydrogens
    - Hydrogen atoms must be drawn explicitly
    - Exception: H atoms bound to atoms of organic elements like C, N, O where the H count is determined by the atom valence and the actual bond order of the atom
  - Exception of connectivity: see simple flow chart

Molecular Inorganics

- **Disconnection flow chart**

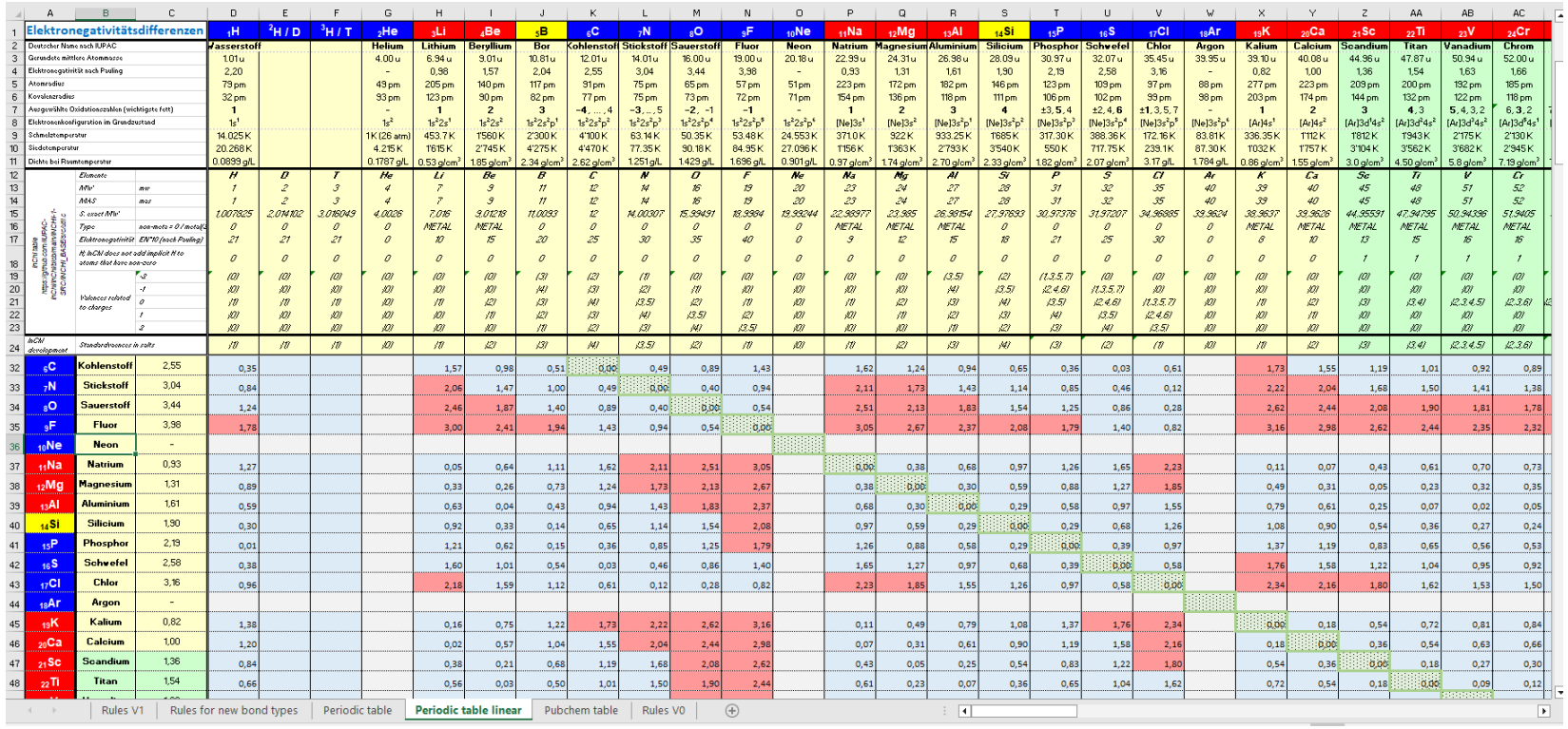


To be noted:

- This flow chart has to be run for every metal.
- The „Disconnection Table“ step has to be run for every bond to a metal.
- If atoms are not connected in the input, they stay disconnected. No new bonds are formed that are not already in the input.

Molecular Inorganics

- **Disconnection table**



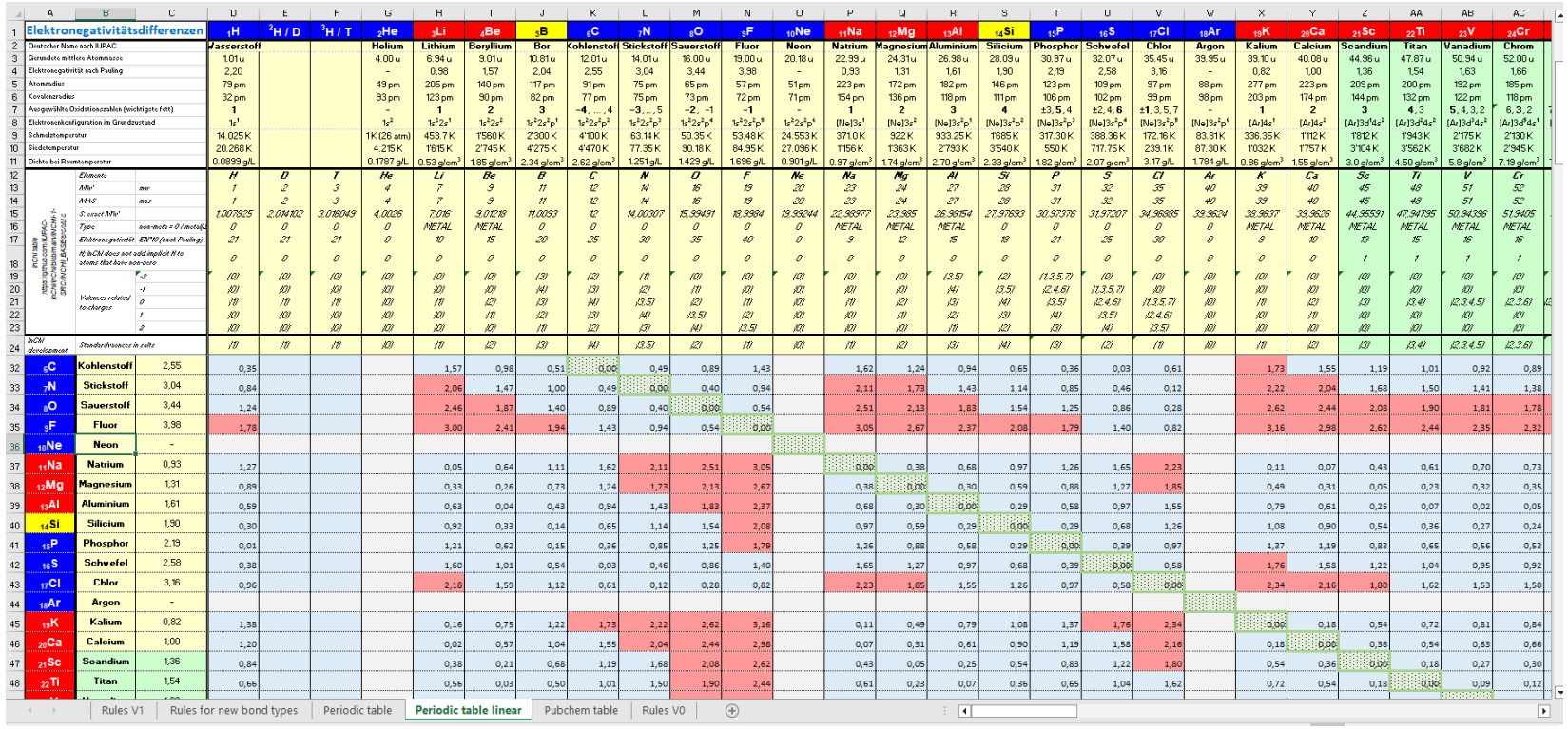
Elektronegativitätsdifferenzen	1H	2H / D	3H / T	2He	3Li	4Be	5B	6C	7N	8O	9F	10Ne	11Na	12Mg	13Al	14Si	15P	16S	17Cl	18Ar	19K	20Ca	21Sc	22Ti	23V	24Cr
Deutscher Name nach IUPAC	Wasserstoff			Helium	Lithium	Beryllium	Bor	Kohlenstoff	Stickstoff	Sauerstoff	Fluor	Neon	Natrium	Magnesium	Aluminium	Silicium	Phosphor	Schwefel	Chlor	Argon	Kalium	Calcium	Scandium	Titan	Vanadium	Chrom
Gerundete mittlere Atommasse	1,01 u			4,00 u	6,94 u	9,01 u	10,81 u	12,01 u	14,01 u	16,00 u	19,00 u	20,18 u	22,99 u	24,31 u	26,98 u	28,09 u	30,97 u	32,07 u	35,45 u	39,95 u	39,10 u	40,08 u	44,96 u	47,87 u	50,94 u	52,00 u
Elektronegativität nach Pauling	2,20			-	0,98	1,57	2,04	2,55	3,04	3,44	3,98	-	0,93	1,31	1,61	1,90	2,19	2,58	3,16	-	0,82	1,00	1,36	1,54	1,63	1,66
Atomradius	79 pm			49 pm	205 pm	140 pm	117 pm	91 pm	75 pm	65 pm	57 pm	51 pm	223 pm	172 pm	182 pm	146 pm	123 pm	109 pm	97 pm	88 pm	277 pm	223 pm	209 pm	200 pm	192 pm	185 pm
Kovalenzradius	32 pm			93 pm	123 pm	90 pm	82 pm	77 pm	75 pm	73 pm	72 pm	71 pm	154 pm	136 pm	118 pm	111 pm	106 pm	102 pm	99 pm	98 pm	203 pm	174 pm	144 pm	132 pm	122 pm	118 pm
Ausgewählte Oxidationszahlen (wichtigste fett)	**1**			-	**1**	**2**	**3**	**−4**, ... , 4	**−3**, ... , 5	**−2**, −1	**−1**	-	**1**	**2**	**3**	**4**	±3, **5**, 4	±2, 4, **6**	**±1**, 3, 5, 7	-	**1**	**2**	**3**	**4**, 3	**5**, 4, 3, 2	6, **3**, 2
Elektronenkonfiguration im Grundzustand	$1s^1$			$1s^2$	$[He]2s^1$	$[He]2s^2$	$[He]2s^2p^1$	$[He]2s^2p^2$	$[He]2s^2p^3$	$[He]2s^2p^4$	$[He]2s^2p^5$	$[He]2s^2p^6$	$[Ne]3s^1$	$[Ne]3s^2$	$[Ne]3s^2p^1$	$[Ne]3s^2p^2$	$[Ne]3s^2p^3$	$[Ne]3s^2p^4$	$[Ne]3s^2p^5$	$[Ne]3s^2p^6$	$[Ar]4s^1$	$[Ar]4s^2$	$[Ar]3d^14s^2$	$[Ar]3d^24s^2$	$[Ar]3d^34s^2$	$[Ar]3d^54s^1$
Schmelztemperatur	14,025 K			1K (26 atm)	453,7 K	1'560 K	2'300 K	4'100 K	63,14 K	50,35 K	53,48 K	24,553 K	371,0 K	922 K	933,25 K	1685 K	317,30 K	388,36 K	172,16 K	83,81 K	336,35 K	1'112 K	1'812 K	1'943 K	2'175 K	2'130 K
Siedetemperatur	20,268 K			4,215 K	1'615 K	2'745 K	4'275 K	4'470 K	77,35 K	90,18 K	84,95 K	27,096 K	1'156 K	1'363 K	2'793 K	3'540 K	550 K	717,75 K	239,1 K	87,30 K	1'032 K	1'757 K	3'104 K	3'562 K	3'682 K	2'945 K
Dichte bei Raumtemperatur	0,0899 g/L			0,1787 g/L	0,53 g/cm³	1,85 g/cm³	2,34 g/cm³	2,62 g/cm³	1,251 g/L	1,429 g/L	1,696 g/L	0,901 g/L	0,97 g/cm³	1,74 g/cm³	2,70 g/cm³	2,33 g/cm³	1,82 g/cm³	2,07 g/cm³	3,17 g/L	1,784 g/L	0,86 g/cm³	1,55 g/cm³	3,0 g/cm³	4,50 g/cm³	5,8 g/cm³	7,19 g/cm³
InChI layer: Elements					*Li*	*Be*	*B*	*C*	*N*	*O*	*F*	*Ne*	*Na*	*Mg*	*Al*	*Si*	*P*	*S*	*Cl*	*Ar*	*K*	*Ca*	*Sc*	*Ti*	*V*	*Cr*
InChI layer: Nfix					7	9	11	12	14	16	19	20	23	24	27	28	31	32	35	40	39	40	45	48	51	52
InChI layer: Nhyd					7	9	11	12	14	16	19	20	23	24	27	28	31	32	35	40	39	40	45	48	51	52
InChI layer: S, exact Nfix					7,016	9,0128	11,0093	12	14,00307	15,99491	18,9984	19,99244	22,98977	23,985	26,98154	27,97693	30,97376	31,97207	34,96885	39,9624	38,9637	39,9626	44,95591	47,94795	50,94396	51,9405
InChI layer: Type					METAL	METAL	0	0	0	0	0	0	METAL	METAL	METAL	0	0	0	0	0	METAL	METAL	METAL	METAL	METAL	METAL
InChI layer: Elektronegativität					10	15	20	25	30	35	40	0	9	12	15	18	21	25	30	0	8	10	13	15	16	16
InChI layer: H, InChI does not add implicit H to atoms that have non-zero					0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	1
InChI layer: Valences related to charges	-3				(0)	(0)	(3)	(3)	(1)	(0)	(0)	(0)	(0)	(0)	(0)	(0)	(3,5)	(2)	(1,3,5,7)	(0)	(0)	(0)	(0)	(0)	(0)	(0)
	-1				(0)	(0)	(4)	(3)	(2)	(1)	(0)	(0)	(0)	(0)	(4)	(3,5)	(2,4,6)	(1,3,5,7)	(0)	(0)	(0)	(0)	(0)	(0)	(0)	(0)
	0				(1)	(1)	(3)	(4)	(3,5)	(2)	(1)	(0)	(1)	(2)	(3)	(4)	(3,5)	(2,4,6)	(1,3,5,7)	(0)	(1)	(2)	(3)	(3,4)	(2,3,4,5)	(2,3,6)
	1				(0)	(1)	(2)	(3)	(4)	(3)	(2)	(0)	(1)	(2)	(3)	(4)	(3,5)	(2,4,6)	(0)	(0)	(0)	(0)	(0)	(0)	(0)	(0)
	2				(0)	(0)	(1)	(2)	(3)	(4)	(3,5)	(0)	(0)	(0)	(1)	(2)	(3)	(4)	(3,5)	(0)	(0)	(0)	(0)	(0)	(0)	(0)
InChI development	Standardnonce in salts				(1)	(1)	(1)	(1)	(1)	(2)	(3)	(4)	(3,5)	(2)	(1)	(0)	(1)	(2)	(3)	(4)	(3)	(2)	(1)	(0)	(1)	(2)	(3)	(3,4)	(2,3,4,5)	(2,3,6)
6C	Kohlenstoff	2,55				1,57	0,98	0,51	0,00	0,49	0,89	1,43		1,62	1,24	0,94	0,65	0,35	0,03	0,61		1,73	1,55	1,19	1,01	0,92	0,89
7N	Stickstoff	3,04				2,06	1,47	1,00	0,49	0,00	0,40	0,94		2,11	1,73	1,43	1,14	0,85	0,46	0,12		2,22	2,04	1,68	1,50	1,41	1,38
8O	Sauerstoff	3,44				2,46	1,87	1,40	0,89	0,40	0,00	0,54		2,51	2,13	1,83	1,54	1,25	0,86	0,28		2,62	2,44	2,08	1,90	1,81	1,78
9F	Fluor	3,98				3,00	2,41	1,94	1,43	0,94	0,54	0,00		3,05	2,67	2,37	2,08	1,79	1,40	0,82		3,16	2,98	2,62	2,44	2,35	2,32
10Ne	Neon	-																									
11Na	Natrium	0,93				0,05	0,64	1,11	1,62	2,11	2,51	3,05		0,00	0,38	0,68	0,97	1,26	1,65	2,23		0,11	0,07	0,43	0,61	0,70	0,73
12Mg	Magnesium	1,31				0,33	0,26	0,73	1,24	1,73	2,13	2,67		0,38	0,00	0,30	0,59	0,88	1,27	1,85		0,49	0,31	0,05	0,23	0,32	0,35
13Al	Aluminium	1,61				0,63	0,04	0,43	0,94	1,43	1,83	2,37		0,68	0,30	0,00	0,29	0,58	0,97	1,55		0,79	0,61	0,25	0,07	0,02	0,05
14Si	Silicium	1,90				0,92	0,33	0,14	0,65	1,14	1,54	2,08		0,97	0,59	0,29	0,00	0,29	0,68	1,26		1,08	0,90	0,54	0,36	0,27	0,24
15P	Phosphor	2,19				1,21	0,62	0,15	0,36	0,85	1,25	1,79		1,26	0,88	0,58	0,29	0,00	0,39	0,97		1,37	1,19	0,83	0,65	0,56	0,53
16S	Schwefel	2,58				1,60	1,01	0,54	0,03	0,46	0,86	1,40		1,65	1,27	0,97	0,68	0,39	0,00	0,58		1,76	1,58	1,22	1,04	0,95	0,92
17Cl	Chlor	3,16				2,18	1,59	1,12	0,61	0,12	0,28	0,82		2,23	1,85	1,55	1,26	0,97	0,58	0,00		2,34	2,16	1,80	1,62	1,53	1,50
18Ar	Argon	-																									
19K	Kalium	0,82				0,16	0,75	1,22	1,73	2,22	2,62	3,16		0,11	0,49	0,79	1,08	1,37	1,76	2,34		0,00	0,18	0,54	0,72	0,81	0,84
20Ca	Calcium	1,00				0,02	0,57	1,04	1,55	2,04	2,44	2,98		0,07	0,31	0,61	0,90	1,19	1,58	2,16		0,18	0,00	0,36	0,54	0,63	0,66
21Sc	Scandium	1,36				0,38	0,21	0,68	1,19	1,68	2,08	2,62		0,43	0,05	0,25	0,54	0,83	1,22	1,80		0,54	0,36	0,00	0,18	0,27	0,30
22Ti	Titan	1,54				0,56	0,03	0,50	1,01	1,50	1,90	2,44		0,61	0,23	0,07	0,36	0,65	1,04	1,62		0,72	0,54	0,18	0,00	0,09	0,12

Rules V1 | Rules for new bond types | Periodic table | **Periodic table linear** | Pubchem table | Rules V0

Molecular Inorganics

Cambridge Crystallographic Data Centre

- **Disconnection table**



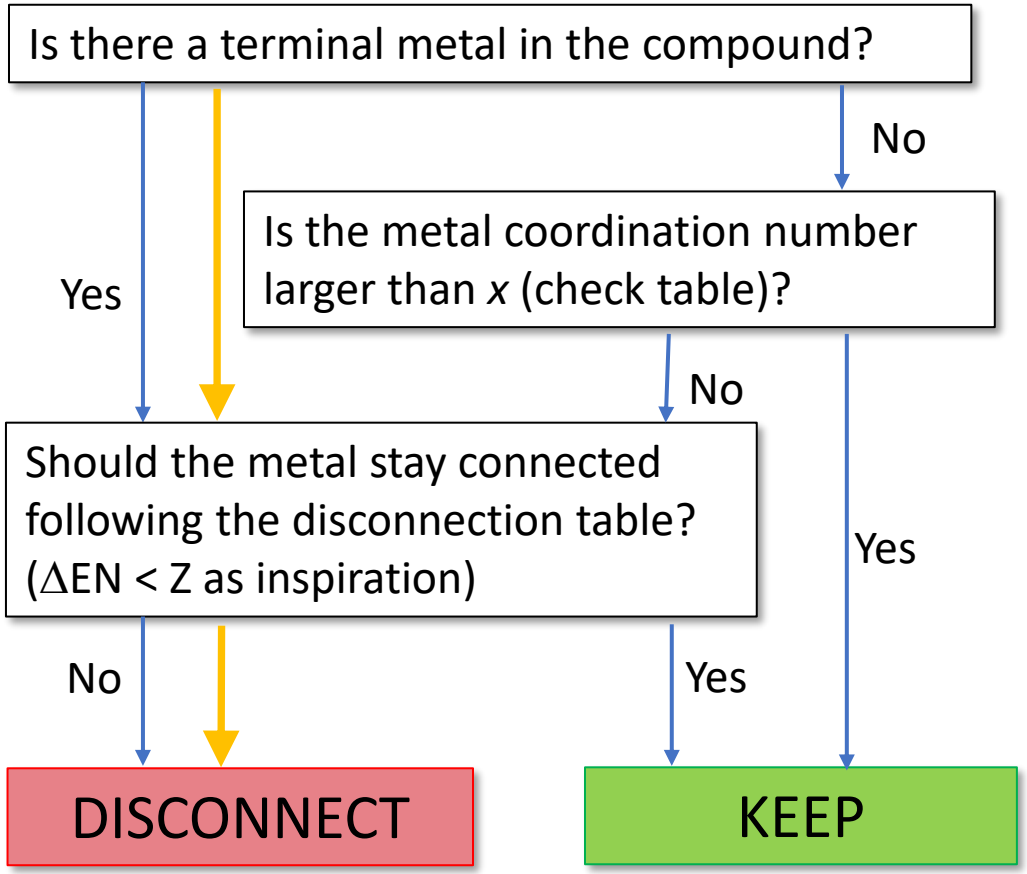
Elektronegativitätsdifferenzen	1H	2H / D	3H / T	2He	3Li	4Be	5B	6C	7N	8O	9F	10Ne	11Na	12Mg	13Al	14Si	15P	16S	17Cl	18Ar	19K	20Ca	21Sc	22Ti	23V	24Cr
Deutscher Name nach IUPAC	Wasserstoff			Helium	Lithium	Beryllium	Bor	Kohlenstoff	Stickstoff	Sauerstoff	Fluor	Neon	Natrium	Magnesium	Aluminium	Silicium	Phosphor	Schwefel	Chlor	Argon	Kalium	Calcium	Scandium	Titan	Vanadium	Chrom
Gerundete mittlere Atommasse	1,01 u			4,00 u	6,94 u	9,01 u	10,81 u	12,01 u	14,01 u	16,00 u	19,00 u	20,18 u	22,99 u	24,31 u	26,98 u	28,09 u	30,97 u	32,07 u	35,45 u	39,95 u	39,10 u	40,08 u	44,96 u	47,87 u	50,94 u	52,00 u
Elektronegativität nach Pauling	2,20			-	0,98	1,57	2,04	2,55	3,04	3,44	3,98	-	0,93	1,31	1,61	1,90	2,19	2,58	3,16	-	0,82	1,00	1,36	1,54	1,63	1,66
Atomradius	79 pm			49 pm	205 pm	140 pm	117 pm	91 pm	75 pm	65 pm	57 pm	51 pm	223 pm	172 pm	182 pm	146 pm	123 pm	109 pm	97 pm	88 pm	277 pm	223 pm	209 pm	200 pm	192 pm	185 pm
Kovalenzradius	32 pm			93 pm	123 pm	90 pm	82 pm	77 pm	75 pm	73 pm	72 pm	71 pm	154 pm	136 pm	118 pm	111 pm	106 pm	102 pm	99 pm	98 pm	203 pm	174 pm	144 pm	132 pm	122 pm	118 pm
Ausgewählte Oxidationszahlen (wichtigste fett)	**1**			-	**1**	**2**	**3**	**−4**, ... , 4	**−3**, ... , 5	**−2**, −1	**−1**	-	**1**	**2**	**3**	**4**	±3, **5**, 4	±2, 4, **6**	**±1**, 3, 5, 7	-	**1**	**2**	**3**	**4**, 3	**5**, 4, 3, 2	6, **3**, 2
Elektronenkonfiguration im Grundzustand	$1s^1$			$1s^2$	$1s^22s^1$	$1s^22s^2$	$1s^22s^22p^1$	$1s^22s^22p^2$	$1s^22s^22p^3$	$1s^22s^22p^4$	$1s^22s^22p^5$	$1s^22s^22p^6$	[Ne]$3s^1$	[Ne]$3s^2$	[Ne]$3s^23p^1$	[Ne]$3s^23p^2$	[Ne]$3s^23p^3$	[Ne]$3s^23p^4$	[Ne]$3s^23p^5$	[Ne]$3s^23p^6$	[Ar]$4s^1$	[Ar]$4s^2$	[Ar]$3d^14s^2$	[Ar]$3d^24s^2$	[Ar]$3d^34s^2$	[Ar]$3d^54s^1$
Schmelztemperatur	14,025 K			1K (26 atm)	453,7 K	1'560 K	2'300 K	4'100 K	63,14 K	50,35 K	53,48 K	24,553 K	371,0 K	922 K	933,25 K	1685 K	317,30 K	388,36 K	172,16 K	83,81K	336,35 K	1'112 K	1'812 K	1'943 K	2'175 K	2'130 K
Siedetemperatur	20,268 K			4,215 K	1'615 K	2'745 K	4'275 K	4'470 K	77,35 K	90,18 K	84,95 K	27,096 K	1'156 K	1'363 K	2'793 K	3'540 K	550 K	717,75 K	239,1 K	87,30 K	1'032 K	1'757 K	3'104 K	3'562 K	3'682 K	2'945 K
Dichte bei Raumtemperatur	0,0899 g/L			0,1787 g/L	0,53 g/cm³	1,85 g/cm³	2,34 g/cm³	2,62 g/cm³	1,251 g/L	1,429 g/L	1,696 g/L	0,901 g/L	0,97 g/cm³	1,74 g/cm³	2,70 g/cm³	2,33 g/cm³	1,82 g/cm³	2,07 g/cm³	3,17 g/L	1,784 g/L	0,86 g/cm³	1,55 g/cm³	3,0 g/cm³	4,50 g/cm³	5,8 g/cm³	7,19 g/cm³
Elemente	*H*	*D*	*T*	*He*	*Li*	*Be*	*B*	*C*	*N*	*O*	*F*	*Ne*	*Na*	*Mg*	*Al*	*Si*	*P*	*S*	*Cl*	*Ar*	*K*	*Ca*	*Sc*	*Ti*	*V*	*Cr*
Mfb'	*mir*	1	2	3	4	7	9	11	12	14	16	19	20	23	24	27	28	31	32	35	40	39	40	45	46	51	52
Mfb's	*mas*	1	2	3	4	7	9	11	12	14	16	19	20	23	24	27	28	31	32	35	40	39	40	45	46	51	52
S. exact Mfb'		*1,007825*	*2,014102*	*3,016049*	*4,0026*	*7,016*	*9,01218*	*11,0093*	*12*	*14,00307*	*15,99491*	*18,9984*	*19,99244*	*22,98977*	*23,985*	*26,98154*	*30,97376*	*31,97207*	*34,96885*	*39,9624*	*38,9637*	*39,9626*	*44,95591*	*47,94795*	*50,94396*	*51,9405*
Typ	*non-meta = 0 / metal=1*	*0*	*0*	*0*	*0*	*METAL*	*METAL*	*0*	*0*	*0*	*0*	*0*	*0*	*METAL*	*METAL*	*0*	*0*	*0*	*0*	*0*	*METAL*	*METAL*	*METAL*	*METAL*	*METAL*	*METAL*
Elektronegativität	*EN*10 (nach Pauling)*	*21*	*21*	*21*	*0*	*10*	*15*	*20*	*25*	*30*	*35*	*40*	*0*	*9*	*12*	*15*	*18*	*21*	*25*	*30*	*0*	*8*	*10*	*13*	*15*	*16*	*16*
H, InChI does not add implicit H to atoms that have non-zero		*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*1*	*1*	*1*	*1*
Valences related to charges	-3	*(0)*	*(0)*	*(0)*	*(0)*	*(0)*	*(0)*	*(3)*	*(3)*	*(1)*	*(0)*	*(0)*	*(0)*	*(0)*	*(0)*	*(0)*	*(3,5)*	*(2)*	*(1,3,5,7)*	*(0)*	*(0)*	*(0)*	*(0)*	*(0)*	*(0)*	*(0)*
	-1	*(0)*	*(0)*	*(0)*	*(0)*	*(0)*	*(0)*	*(4)*	*(3)*	*(2)*	*(1)*	*(0)*	*(0)*	*(0)*	*(0)*	*(4)*	*(3,5)*	*(2,4,6)*	*(1,3,5,7)*	*(0)*	*(0)*	*(0)*	*(0)*	*(2)*	*(0)*	*(0)*	*(0)*
	0	*(1)*	*(1)*	*(1)*	*(0)*	*(1)*	*(2)*	*(3)*	*(4)*	*(3,5)*	*(2)*	*(1)*	*(0)*	*(1)*	*(2)*	*(3)*	*(4)*	*(3,5)*	*(2,4,6)*	*(0)*	*(1)*	*(2)*	*(3)*	*(3,4)*	*(2,3,4,5)*	*(2,3,6)*
	1	*(0)*	*(0)*	*(0)*	*(0)*	*(1)*	*(1)*	*(2)*	*(3)*	*(4)*	*(3,5)*	*(2)*	*(1)*	*(0)*	*(1)*	*(2)*	*(3)*	*(4)*	*(3,5)*	*(2,4,6)*	*(0)*	*(0)*	*(1)*	*(2)*	*(0)*	*(0)*	*(0)*
	2	*(0)*	*(0)*	*(0)*	*(0)*	*(0)*	*(0)*	*(1)*	*(2)*	*(3)*	*(4)*	*(3,5)*	*(0)*	*(0)*	*(0)*	*(1)*	*(2)*	*(3)*	*(4)*	*(3,5)*	*(0)*	*(0)*	*(0)*	*(0)*	*(0)*	*(0)*	*(0)*
InChI development	Standardisierung in salts	*(1)*	*(1)*	*(1)*	*(0)*	*(1)*	*(2)*	*(3)*	*(4)*	*(3,5)*	*(2)*	*(1)*	*(0)*	*(1)*	*(2)*	*(3)*	*(4)*	*(3)*	*(2)*	*(1)*	*(0)*	*(1)*	*(2)*	*(3)*	*(3,4)*	*(2,3,4,5)*	*(2,3,6)*
6C	Kohlenstoff	2,55	0,35			1,57	0,98	0,51	0,00	0,49	0,89	1,43		1,62	1,24	0,94	0,65	0,35	0,03	0,61		1,73	1,55	1,19	1,01	0,92	0,89
7N	Stickstoff	3,04	0,84			2,06	1,47	1,00	0,49	0,00	0,40	0,94		2,11	1,73	1,43	1,14	0,85	0,46	0,12		2,22	2,04	1,68	1,50	1,41	1,38
8O	Sauerstoff	3,44	1,24			2,46	1,87	1,40	0,89	0,40	0,00	0,54		2,51	2,13	1,83	1,54	1,25	0,86	0,28		2,62	2,44	2,08	1,90	1,81	1,78
9F	Fluor	3,98	1,78			3,00	2,41	1,94	1,43	0,94	0,54	0,00		3,05	2,67	2,37	2,08	1,79	1,40	0,82		3,16	2,98	2,62	2,44	2,35	2,32
10Ne	Neon	-																									
11Na	Natrium	0,93	1,27			0,05	0,64	1,11	1,62	2,11	2,51	3,05		0,00	0,38	0,68	0,97	1,26	1,65	2,23		0,11	0,07	0,43	0,61	0,70	0,73
12Mg	Magnesium	1,31	0,89			0,33	0,26	0,73	1,24	1,73	2,13	2,67		0,38	0,00	0,30	0,59	0,88	1,27	1,85		0,49	0,31	0,05	0,23	0,32	0,35
13Al	Aluminium	1,61	0,59			0,63	0,04	0,43	0,94	1,43	1,83	2,37		0,68	0,30	0,00	0,29	0,58	0,97	1,55		0,79	0,61	0,25	0,07	0,02	0,05
14Si	Silicium	1,90	0,30			0,92	0,33	0,14	0,65	1,14	1,54	2,08		0,97	0,59	0,29	0,00	0,29	0,68	1,26		1,08	0,90	0,54	0,36	0,27	0,24
15P	Phosphor	2,19	0,01			1,21	0,62	0,15	0,36	0,85	1,25	1,79		1,26	0,88	0,58	0,29	0,00	0,39	0,97		1,37	1,19	0,83	0,65	0,56	0,53
16S	Schwefel	2,58	0,38			1,60	1,01	0,54	0,03	0,46	0,86	1,40		1,65	1,27	0,97	0,68	0,39	0,00	0,58		1,76	1,58	1,22	1,04	0,95	0,92
17Cl	Chlor	3,16	0,96			2,18	1,59	1,12	0,61	0,12	0,28	0,82		2,23	1,85	1,55	1,26	0,97	0,58	0,00		2,34	2,16	1,80	1,62	1,53	1,50
18Ar	Argon	-																									
19K	Kalium	0,82	1,38			0,16	0,75	1,22	1,73	2,22	2,62	3,16		0,11	0,49	0,79	1,08	1,37	1,76	2,34		0,00	0,18	0,54	0,72	0,81	0,84
20Ca	Calcium	1,00	1,20			0,02	0,57	1,04	1,55	2,04	2,44	2,98		0,07	0,31	0,61	0,90	1,19	1,58	2,16		0,18	0,00	0,36	0,54	0,63	0,66
21Sc	Scandium	1,36	0,84			0,38	0,21	0,68	1,19	1,68	2,08	2,62		0,43	0,05	0,25	0,54	0,83	1,22	1,80		0,54	0,36	0,00	0,18	0,27	0,30
22Ti	Titan	1,54	0,66			0,56	0,03	0,50	1,01	1,50	1,90	2,44		0,61	0,23	0,07	0,36	0,65	1,04	1,62		0,72	0,54	0,18	0,00	0,09	0,12

Rules V1 | Rules for new bond types | Periodic table | **Periodic table linear** | Pubchem table | Rules V0

InChITRUST

Molecular Inorganics

- **Disconnection flow chart**



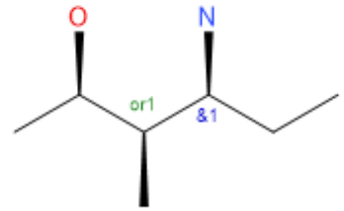
Example: Na-Cl

-> Terminal metal
-> Disconnection table says DISCONNECT

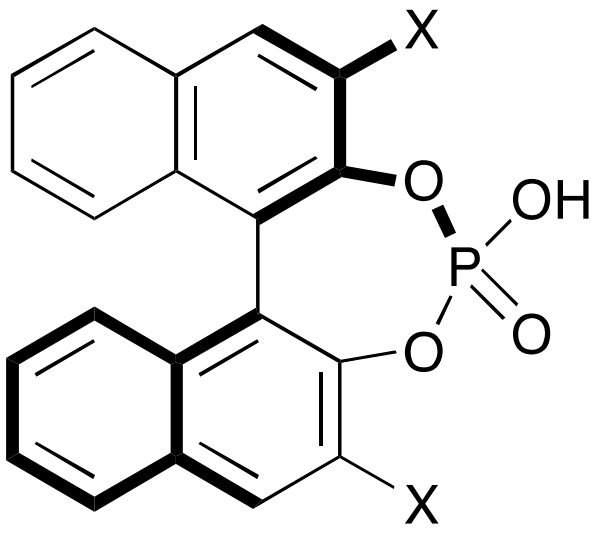
-> Na+ and Cl-

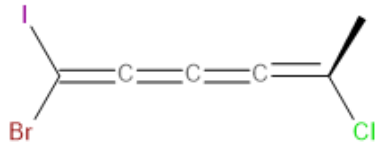
-> InChI=1S/ClH.Na/h1H;/q;+1/p-1-

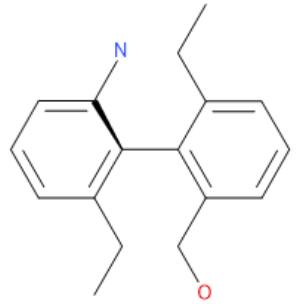
Enhancements in Stereochemistry

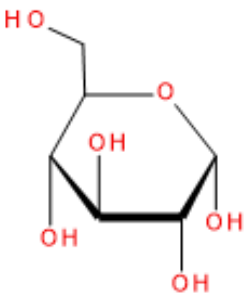


- **Addressing the following entities**
  - (MDL) enhanced stereochemistry
    - ABS, AND, and OR stereocentres
    - Extended V3 molfile handling
  - Cumulenes √
  - Atropisomers
  - Haworth representation for sugars
    - But: Haworth is not handled by the molfile format (molfile are the primary input for InChIs)
  - Additional bug fixes









Status of InChI Application Frameworks

- **Reaction InChI (RInChI)** https://github.com/IUPAC-InChI/RInChI
  - Version 1.0 released
  - Version 1.1 being tested (support of enhanced RXN file format, bug fixes, documentation issues, new tutorial)
  - Version 1.2 awaiting programming (reaction atom mapping, multi-threading, agent-role)
  - Later releases (dependent on further InChI development)
    - Enhanced representation for inorganics and organometallics (important for catalysts)
    - No-structure handling
      - Enzymatic reactions
    - Enhanced stereochemistry
    - Tautomer restrictions
      - The tautomer transformation may go too far for Reaction InChIs

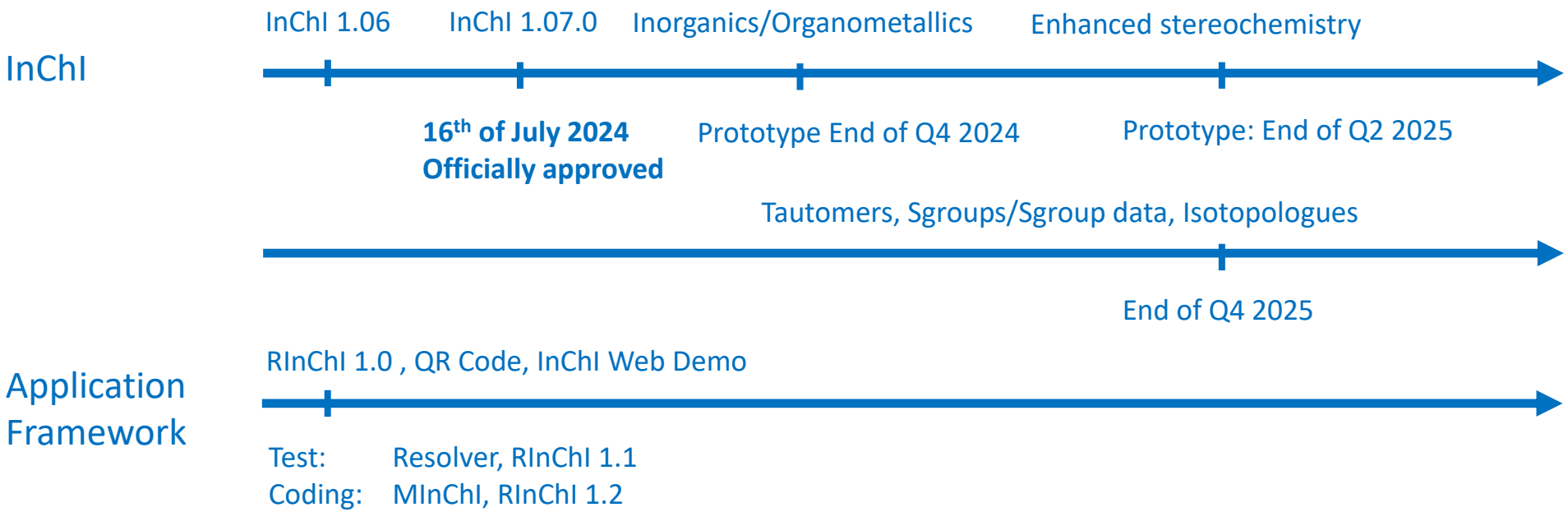
Status of InChI Application Frameworks

- **QR code proposals and Resolver prototype**
  - QR Code proposals published 2022
  - InChI Resolver prototype (available since 2021) – *cf* WorldFAIR Chemical Data Exchange Protocols
- **InChI Web Demo**
  - Interactive Webtool to create InChIs and RInChIs (under development)
  - Access to multiple InChI/RInChI version including development versions for testing
  - https://iupac-inchi.github.io/InChI-Web-Demo/
- **Mixtures InChI (MInChI)**
  - Awaiting coding – prototype at https://github.com/cdd/mixtures (Alex Clark, CDD)

Under investigation/longer evaluations

- **InChI**
  - Variable molecules / Markush InChIs
    - Prototypes have been built for variable molecules and are being tested
      - https://github.com/topics/inchi
  - Large molecules
- **InChI Application Frameworks**
  - Nano InChI (NInChI)
    - Working group funded by IUPAC
    - Working on format proposal

InChI Roadmap



Evaluations:
- Large molecules
- Variable molecules / Markush InChIs
- NanoInChI (NInChI)

All technical developments depend on further funding.

The InChI Project

- **Financial base**
  - Membership fees
  - Contributions in kind
    - Based on open source model
    - Support by Sonja Herres-Pawlis RWTH Aachen university (Germany)
      - Developers Djordje Baljozovic, Nauman Khan (finded by Volkswagen Stiftung)
      - Additional support by Jan Brammer and Frank Lange (NFDI4Chem, DALIA)
    - Support by Beilstein Institute, Frankfurt(Main)
      - Cheminformatician Felix Bänsch (50% FTE)
    - Feedback by other developers on GitHub.

The InChI Project

IUPAC	InChI Trust
Scientific oversight, innovation and governance	Development, adoption and sustainability
IUPAC Divisions and Committees (Div VIII and CPCDS)	Project Director Technical Director Marketing & Outreach Director

InChI Trust Members

CCS 中国化学会 Chinese Chemical Society
CAS A division of the American Chemical Society
NIH National Institutes of Health
IUPAC
RELX Group
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