Electronic Supplementary Material (ESI) for CrystEngComm.

Supplementary Information

Cocrystal design by network-based link prediction

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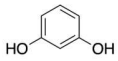
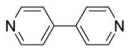
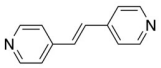
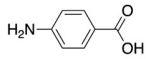
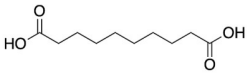
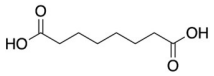
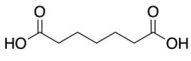
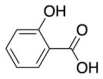
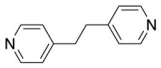
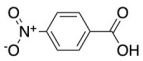
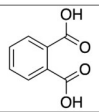
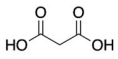
S1 - Materials and syntheses

We first present the materials in Table S1, after which we discuss the protocol used to obtain crystals suitable for single-crystal X-ray diffraction. Besides the two-component structures shown in Table 2, an additional cocrystal dihydrate (**c**) and salt dihydrate (**g**) were found.

Table S1 Materials used in the cocrystallization experiments.

Compound	Structure	Molecular weight	CAS no.	Supplier	Purity
Resorcinol		110.11	108-46-3	Acros Organics	98%
4,4'-bipyridine		156.18	553-26-4	Acros Organics	98%
1,2-di(4-pyridyl)ethylene		182.22	13362-78-2	Fluorchem Ltd.	95%
4-aminobenzoic acid		137.14	150-13-01	Sigma	≥99%
Sebacic acid		202.25	111-20-6	Acros Organics	98%
Suberic acid		174.20	505-48-6	Aldrich	98%
Oxalic acid		90.04	144-62-7	Acros Organics	98%
Pimelic acid		160.17	111-16-0	Sigma-Aldrich Chemie B.V.	97%
Salicylic acid		138.12	67-72-7	Alfa Aesar GmbH & Co KG	≥98%
1,2-bis(4-pyridyl)ethane		184.24	4916-57-8	Sigma-Aldrich Chemie B.V.	≥98%
4-nitrobenzoic acid		167.12	62-23-7	Fluorchem Ltd.	99%
Phthalic acid		166.14	88-99-3	Merck	≥99%
Malonic acid		104.06	141-82-2	Merck	≥99%

Experimental details

a) Cocrystal 4,4'-bipyridine + resorcinol

Colorless needle-like crystals suitable for X-ray diffraction were grown by sublimation of a mixture of 300 mg 4,4'-bipyridine and 230 mg resorcinol. Crystals of the same polymorph can also be grown from solution, but were found to be of lower quality.

b) Cocrystal 1,2-di(4-pyridyl)ethylene + 4-aminobenzoic acid

1,2-di(4-pyridyl)ethylene (40 mg) and 4-aminobenzoic acid (29 mg) were dissolved in ethanol (10 mL). Molecular sieves (Sigma-Aldrich, 3 Å) were used to dry the solution. The solution was subsequently filtered, and left to evaporate in a desiccator flushed with nitrogen gas, yielding colorless needle-like crystals.

c) Cocrystal 1,2-di(4-pyridyl)ethylene + 4-aminobenzoic acid *dihydrate*

1,2-di(4-pyridyl)ethylene (46 mg) was dissolved in 2 mL acetone and was subsequently filtered, resulting in a slightly yellow solution. This solution was added to a second solution, containing 34 mg 4-aminobenzoic acid in acetone. After slow evaporation of the solvent, colorless plate-like crystals were obtained.

d) Cocrystal 1,2-di(4-pyridyl)ethylene + sebacic acid

1,2-di(4-pyridyl)ethylene (55 mg) and sebacic acid (55 mg) were dissolved in methanol (+- 5 mL). The solution was left to slowly evaporate at ambient conditions. Colorless plate-like crystals suitable for X-ray diffraction were obtained after 9 days.

e) Cocrystal 4,4'-bipyridine + suberic acid

7 mL of methanol was added to a mixture of 29 mg of 4,4'-bipyridine and 29 mg of suberic acid. Subsequently, the mixture was dissolved by heating. Slow evaporation yielded colorless crystals that were suitable for single-crystal X-ray diffraction.

f) Salt 1,2-di(4-pyridyl)ethylene + oxalic acid

1,2-di(4-pyridyl)ethylene (200 mg) and oxalic acid (100 mg) were sublimated. The obtained crystals were, however, too small for single-crystal X-ray diffraction and therefore 20 mg of the sublimated product was dissolved in 50 mL ethanol. This mixture was heated to 70° C and subsequently filtered. Slow evaporation of the solvent to air at room temperature yielded colorless block-shaped crystals.

g) Salt 1,2-di(4-pyridyl)ethylene + oxalic acid *dihydrate*

1,2-di(4-pyridyl)ethylene (64 mg) and oxalic acid (32 mg) were dissolved in a solution of methanol (2 mL) and water (450 mL). Slow evaporation of the solvent to air yielded yellow needle-shaped crystals after 1 week.

h) Cocrystal 1,2-di(4-pyridyl)ethylene + pimelic acid

A mixture of 1,2-di(4-pyridyl)ethylene (98 mg) and pimelic acid (81 mg) was ground together. Subsequently, 36 mg of the mixture was dissolved in isopropanol (7 mL). Slow evaporation of the solvent at ambient conditions yielded plate-like crystals, containing both coformers (based on ^{1}H-NMR spectroscopy, *vide infra*). The crystals were suitable for single-crystal X-ray diffraction, but exhibit a modulated structure, which is currently being investigated and will form the topic of a future publication.

The cocrystalline nature of the obtained material is proved by comparing the powder diffraction pattern of the cocrystal to those of the reference compounds (Figure S1). The presence of both coformers and absence of isopropanol in the crystal is confirmed by comparing the ^{1}H-NMR spectrum of the dissolved cocrystal to the spectra of the reference compounds (Figure S2).

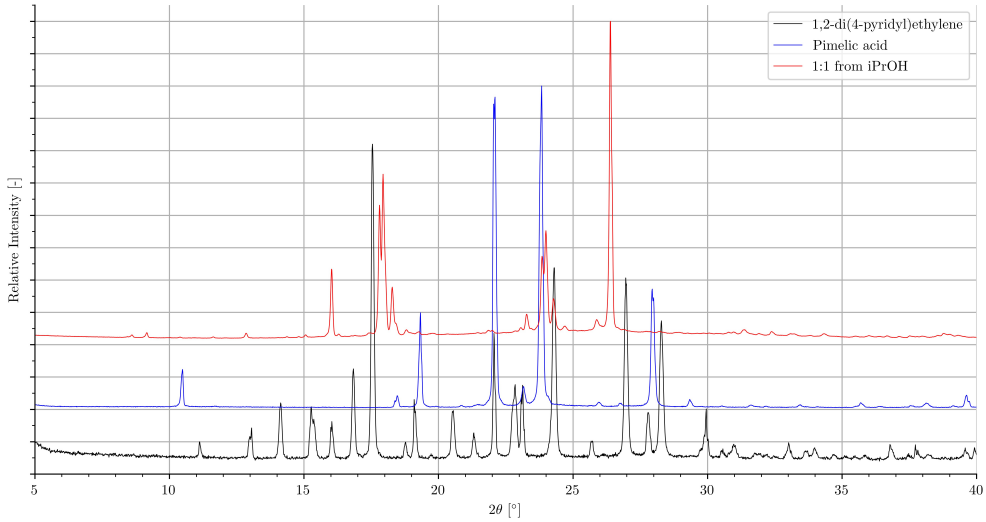
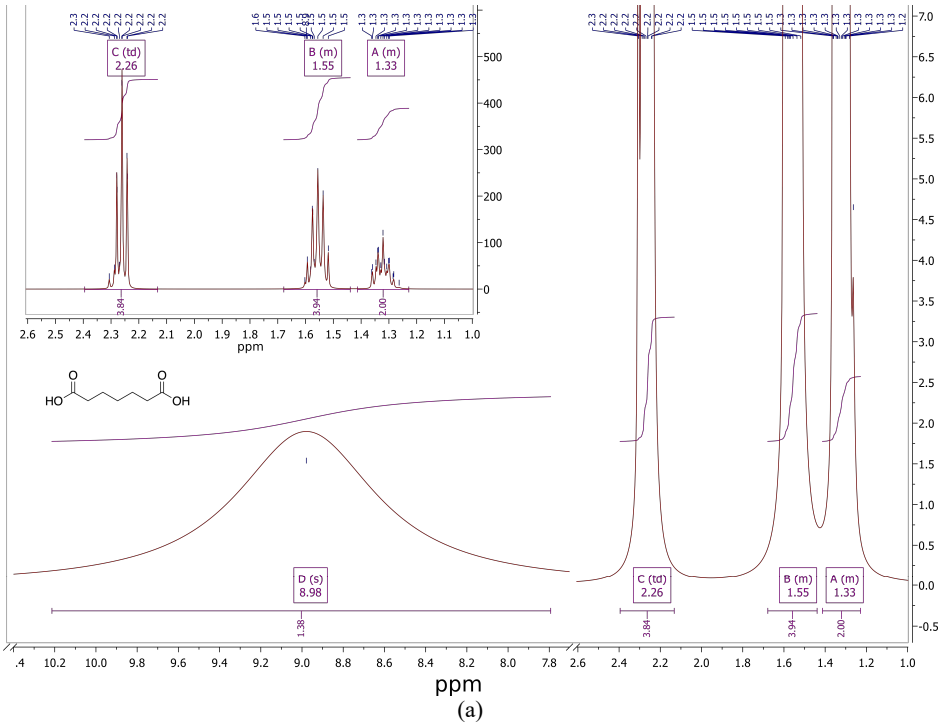


Figure S1 PXRD measurements of the new cocrystal phase and its reference materials.



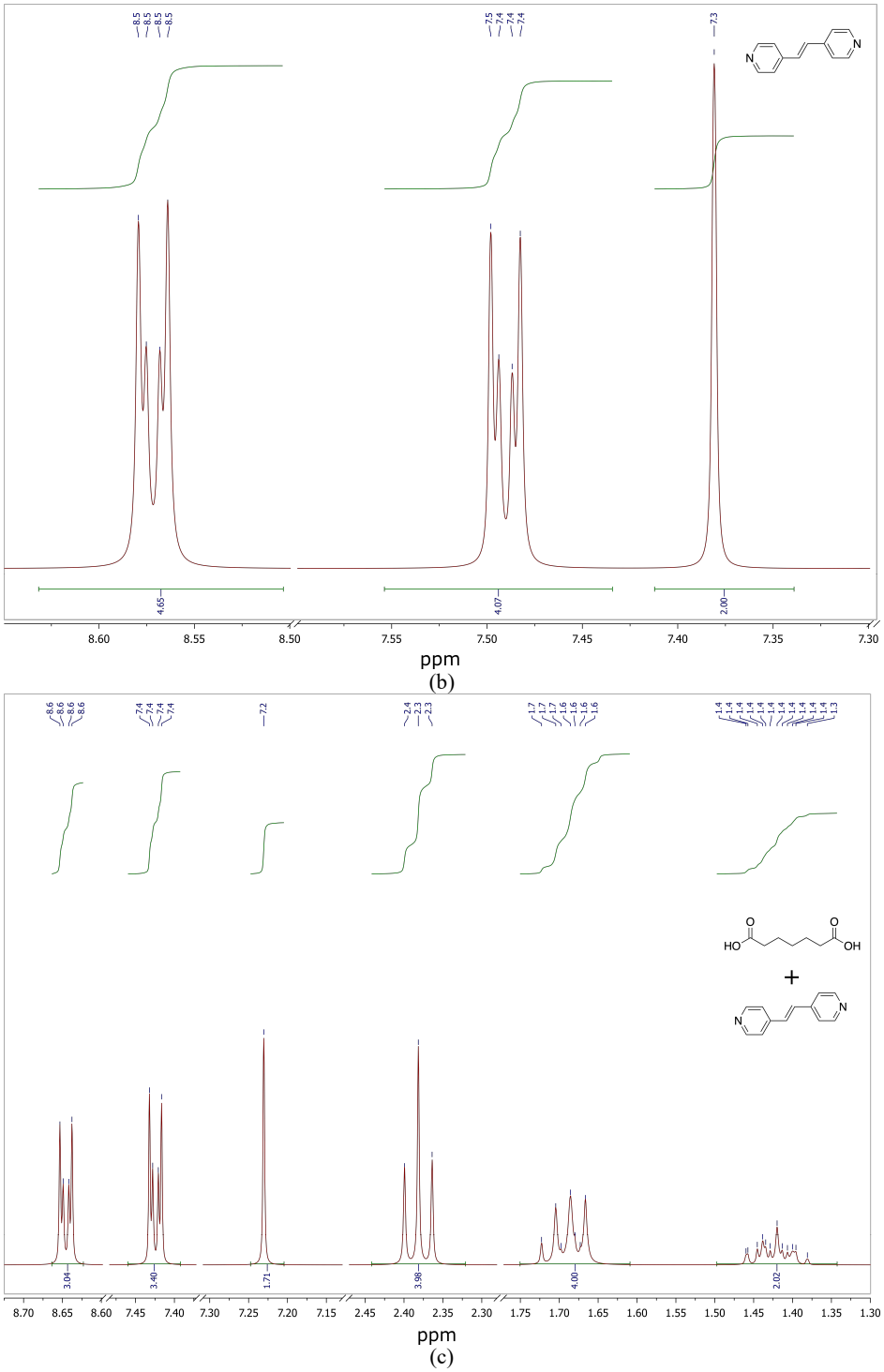


Figure S2 [1]H-NMR spectra of (a) pimelic acid, (b) 1,2-di(4-pyridyl)ethylene and (c) the cocrystal. The peaks of both reference materials emerge in (c), and no signals of solvent or water are seen. The signal of the hydroxyl moiety proton of pimelic acid in (a) is rather weak and was not observed in (c). Based on integration of the peaks, an equimolar cocrystal stoichiometry is most likely.

i) Cocrystal 1,2-bis(4-pyridyl)ethane + salicylic acid
27 mg of 1,2-bis(4-pyridyl)ethane and 20 mg of salicylic acid were dissolved in ethanol (+- 5 mL) and the solution was left to slowly evaporate at ambient conditions. Colorless needle-like crystals suitable for single crystal X-ray diffraction were obtained after several days.

j) Cocrystal 1,2-di(4-pyridyl)ethylene + 4-nitrobenzoic acid
Equimolar amounts of 1,2-di(4-pyridyl)ethylene (18 mg) and 4-nitrobenzoic acid (16 mg) were added to 5 mL of methanol. The solution was filtered and the filtrate was left to slowly evaporate at ambient conditions, resulting in plate-like crystals.

k) Cocrystal 1,2-di(4-pyridyl)ethylene + phthalic acid
1,2-di(4-pyridyl)ethylene (27 mg) and phthalic acid (26 mg) were dissolved in methanol (+- 5 mL). After slow evaporation of the solvent, orange needle-like crystals were retrieved.

l) Cocrystal 1,2-di(4-pyridyl)ethylene + malonic acid
30 mg of 1,2-di(4-pyridyl)ethylene and 16 mg of malonic acid were added together in methanol (+- 5 mL). Slow evaporation of the solvent resulted in orange block-like crystals suitable for single-crystal X-ray diffraction.

S2 - Single-crystal X-ray structure determinations, ORTEP plots and H-bonding

The crystallographic data of all new structures is presented in Table S2. In some cases, the extent to which proton transfer takes place is not 100% (e.g. **i** or **k**). For structure (**f**), the proton is situated on the aromatic nitrogen of the pyridine moiety, hence indicating a salt. Labeled ORTEP plots (at 50% probability) and hydrogen bonding details are systematically presented at the end of this section. For clarity, minor conformations of the coformers are omitted in the former.

Table S2 Crystallographic data and refinement details of the cocrystals discussed above.

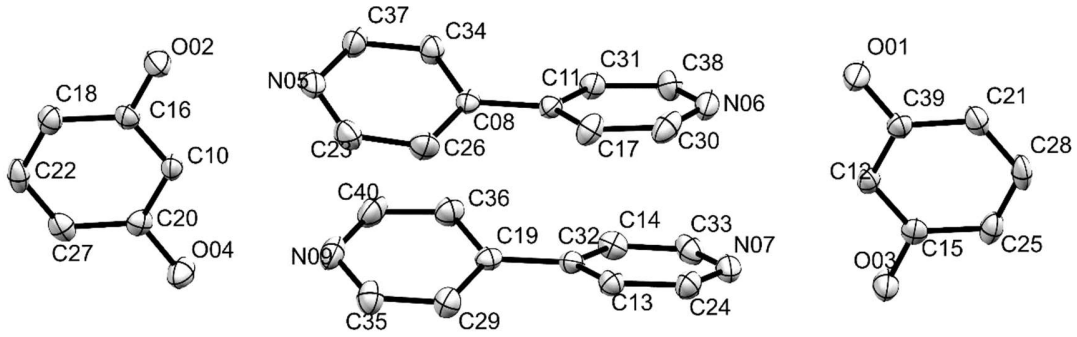
	a	b	c	d
Crystal data				
CCDC deposition no.	1940959	1940950	1940956	1940954
Chemical formula	$C_{10}H_8N_2 \cdot C_6H_6O_2$	$C_{12}H_{10}N_2 \cdot C_7H_7NO_2$	$3(C_{12}H_{10}N_2) \cdot 2(C_7H_7NO_2) \cdot 2(H_2O)$	$C_{10}H_{18}O_4 \cdot C_{12}H_{10}N_2$
M_r	266.29	319.35	852.93	384.46
Crystal system, space group	Monoclinic, $P2_1$	Triclinic, *P-1*	Triclinic, *P-1*	Triclinic, *P-1*
Temperature (K)	150	150	150	150
a, *b*, *c* (Å)	7.5267 (6), 9.8209 (7), 18.1895 (14)	8.4722 (8), 8.6319 (8), 11.8009 (12)	11.4554 (6), 14.1808 (7), 15.2055 (8)	9.5773 (5), 10.7505 (6), 10.9564 (6)
α, β, γ (°)	90, 90.747 (3), 90	108.849 (3), 98.114 (3), 97.134 (3)	104.905 (2), 94.946 (2), 111.852 (2)	96.199 (2), 97.7308 (19), 113.7266 (18)
V (Å^3)	1344.43 (18)	795.17 (13)	2169.4 (2)	1006.87 (10)
Z	4	2	2	2
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.09	0.09	0.09	0.09
Crystal size (mm)	0.56 × 0.12 × 0.07	0.54 × 0.37 × 0.17	0.57 × 0.43 × 0.12	0.44 × 0.26 × 0.07
Data collection				
Diffractometer	Bruker D8 Quest Apex3	Bruker D8 Quest Apex3	Bruker D8 Quest Apex3	Bruker D8 Quest Apex3
Absorption correction	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10	Multi-scan Sheldrick, G. M. (2012). TWINABS. Version 2012/1. Georg-August-Universität Göttingen, Göttingen, Germany	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10
T_{min}, T_{max}	0.680, 0.746	0.664, 0.746	0.51, 0.75	0.711, 0.747
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	50251, 6665, 5315	14502, 3941, 2925	7876, 7876, 5641	35723, 7668, 5433
R_{int}	0.053	0.034	n.a.	0.028
(sin θ/λ)max (Å^{-1})	0.667	0.668	0.610	0.771
Refinement				
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.041, 0.123, 0.88	0.054, 0.146, 1.08	0.061, 0.178, 1.04	0.045, 0.141, 1.01
No. of reflections	6665	3941	7876	7668
No. of parameters	373	304	595	259
No. of restraints	1	38	n.a.	n.a.
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement. Hydrogen positions of water molecule O63 could not be determined.	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.26, −0.22	0.31, −0.24	0.47, −0.32	0.43, −0.30
Special remarks	Two resorcinol and two 4,4'-bipyridene molecules linked by O-H..N H-bonds are found in the asymmetric unit.	The asymmetric unit contains one 4-aminobenzoic acid molecule, disordered about an inversion centre and two half 1,2-di(4-pyridyl)ethylene molecules, one of which is disordered and each lying about inversion centres.	The asymmetric unit consists of two 4-aminobenzoic acid components, two (complete) 1,2-di(4-pyridyl)ethylene molecules, two half 1,2-di(4-pyridyl)ethylene molecules lying about an inversion centre, and two water molecules.	

	e	f	g
Crystal data			
CCDC deposition no.	1940949	1940953	1940955
Chemical formula	$C_8H_{14}O_4 \cdot C_{10}H_8N_2$	$C_{12}H_{12}N_2 \cdot 2(C_2O_4)$	$C_{12}H_{12}N_2 \cdot C_2O_4 \cdot 2(H_2O)$
M_r	330.37	362.29	380.35
Crystal system, space group	Triclinic, *P-1*	Triclinic, *P-1*	Monoclinic, *C*2/*m*
Temperature (K)	150	150	150
a, *b*, *c* (Å)	8.9732 (5), 9.5401 (5), 10.9902 (6)	3.677 (3), 10.505 (7), 10.652 (7)	16.3686 (5), 6.9285 (2), 9.5207 (3)
α, β, γ (°)	82.2592 (19), 72.1344 (17), 65.7070 (16)	66.88 (2), 85.72 (2), 81.68 (2)	90, 123.4486 (12), 90
V (Å^3)	816.12 (8)	374.4	900.91 (5)
Z	2	1	2
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.10	0.13	0.12
Crystal size (mm)	0.59 × 0.45 × 0.20	0.22 × 0.15 × 0.11	0.43 × 0.25 × 0.09
Data collection			
Diffractometer	Bruker D8 Quest Apex3	Bruker D8 Quest Apex3	Bruker D8 Quest Apex3
Absorption correction	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10
T_{min}, T_{max}	0.717, 0.746	0.657, 0.746	0.702, 0.747
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	22341, 4061, 3327	8078, 2605, 1820	11525, 1850, 1629
R_{int}	0.022	0.035	0.022
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.668	0.749	0.770
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.037, 0.116, 1.03	0.60, 0.179, 1.04	0.041, 0.128, 1.09
No. of reflections	4061	2605	1850
No. of parameters	223	124	92
No. of restraints	n.a.	n.a.	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.38, −0.23	1.04, −0.41	0.54, −0.33
Special remarks		The 1,2-di(4-pyridyl)ethylene component lies about an inversion centre.	The 1,2-di(4-pyridyl)ethylene component lies about an inversion centre. The hydrogen atoms of the two water componets are disordered over three sites.

	i	j	k	l
Crystal data				
CCDC deposition no.	1940951	1940958	1940952	1940957
Chemical formula	$C_{12}H_{13.42}N_2 \cdot 2(C_7H_{5.29}O_3)$	3(C12H10N2)·4(C7H5NO4)	$C_{12}H_{11.56}N_2 \cdot 2(C_8H_{5.22}O_4)$	$C_{12}H_{10}N_2 \cdot C_3H_4O_4$
M_r	460.47	1215.14	514.47	286.28
Crystal system, space group	Monoclinic, $P2_1/n$	Triclinic, *P-1*	Monoclinic, $P2_1/n$	Monoclinic, $P2/c$
Temperature (K)	150	150	150	150
a, *b*, *c* (Å)	8.6104 (3), 6.8302 (2), 19.1092 (8)	8.1387 (7), 9.6821 (8), 19.0927 (16)	13.0785 (6), 4.9373 (2), 18.7535 (9)	9.5746 (4), 4.6618 (2), 16.1220 (7)
α, β, γ (°)	90, 101.7599 (14), 90	102.620 (3), 90.125 (3), 107.580 (3)	90, 106.176 (3), 90	90, 107.035 (2), 90
V (Å^3)	1100.24 (7)	1395.8 (2)	1163.02 (9)	688.03 (5)
Z	2	1	2	2
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.10	0.11	0.11	0.10
Crystal size (mm)	0.59 × 0.31 × 0.08	0.38 × 0.21 × 0.04	0.47 × 0.28 × 0.05	0.60 × 0.22 × 0.19
Data collection				
Diffractometer	Bruker D8 Quest Apex3	Bruker D8 Quest Apex3	Bruker D8 Quest Apex3	Bruker D8 Quest Apex3
Absorption correction	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10
T_{min}, T_{max}	0.711, 0.747	0.649, 0.747	0.637, 0.747	0.702, 0.747
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	23889, 4211, 3186	62786, 10716, 5935	23067, 4443, 3359	17981, 2640, 2024
R_{int}	0.030	0.061	0.038	0.028
(sin θ/λ)$_{max}$ (Å^{-1})	0.770	0.772	0.770	0.770
Refinement				
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.043, 0.134, 1.04	0.057, 0.189, 1.04	0.045, 0.136, 1.01	0.050, 0.169, 1.25
No. of reflections	4211	10716	4443	2640
No. of parameters	163	509	183	163
No. of restraints	n.a.	649	n.a.	n.a.
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H-atom parameters constrained	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.41, −0.25	0.48, −0.34	0.46, −0.23	0.41, −0.25
Special remarks	The 1,2-bis(4-pyridyl)ethane component lies about an inversion centre.	The asymmetric unit contains two 4-nitrobenzoic acid molecules, one 1,2-di(4-pyridyl)ethylene molecule and half of a 1,2-di(4-pyridyl)ethylene, unequally disordered over two adjacent sites and lying about an inversion centre.	The 1,2-di(4-pyridyl)ethylene component lies about an inversion centre.	The asymmetric unit contains half of a malonic acid component lying about a twofold axis and two half 1,2-di(4-pyridyl)ethylene molecules lying disordered about an inversion centre.

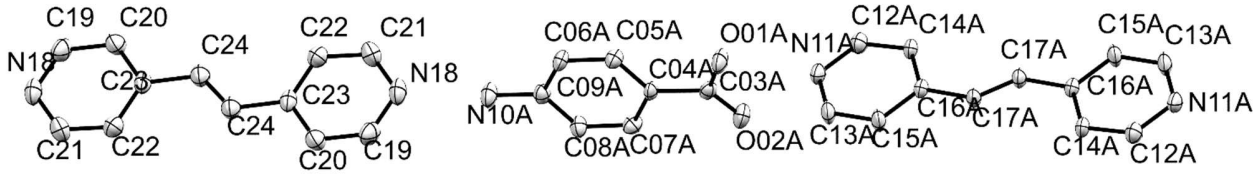
Labeled ORTEP plots and H-bonding details

a) 4,4'-bipyridine + resorcinol (p1812d)



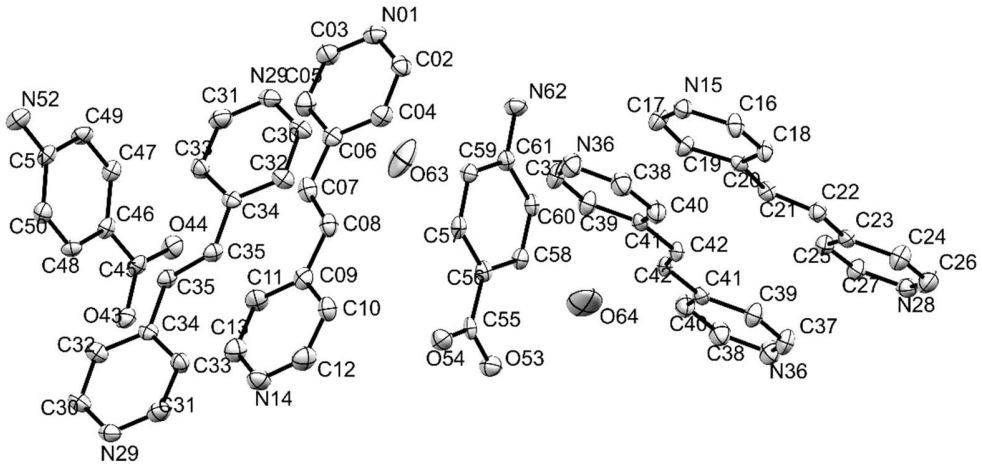
Nr	Res	Donor	--- H....	Acceptor	[ARU]	D - H	H...A	D...A	D - H...A
1	3	O01	--H01	..N06	[1555.01]	0.93(4)	1.83(4)	2.755(3)	172(4)
2	4	O02	--H02	..N05	[1555.01]	0.95(4)	1.87(4)	2.820(3)	177(4)
3	3	O03	--H03	..N07	[1555.02]	0.92(4)	1.92(4)	2.844(3)	178(4)
4	4	O04	--H04	..N09	[1555.02]	0.92(4)	1.83(4)	2.748(3)	172(3)
5	4	C10	--H10	..N05	[1555.01]	0.95	2.51	3.243(3)	134
6	3	C12	--H12	..N07	[1555.02]	0.95	2.58	3.313(3)	134
7	1	C30	--H30	..O04	[1445.04]	0.95	2.48	3.396(4)	163

b) 1,2-di(4-pyridyl)ethylene + 4-aminobenzoic acid (p1823c)



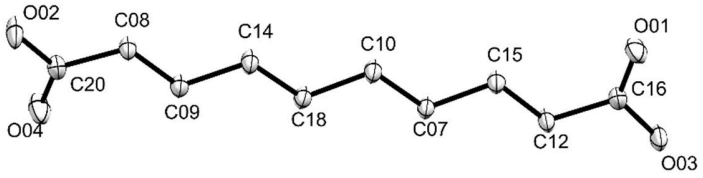
Nr	Typ	Res	Donor	--- H....	Acceptor	[ARU]	D - H	H...A	D...A	D - H...A
1		4>O01A	--H01A	..N11A	[1555.02]	0.84	1.83	2.642(3)	163
2		4>O01A	--H01A	..N11B	[1555.03]	0.84	1.96	2.734(18)	152
3		4>N10A	--H10A	..O02A	[1565.04]	0.86(5)	2.16(4)	3.007(3)	167(4)
4		4>N10A	--H10B	..N18	[1555.01]	0.89(3)	2.54(4)	3.141(3)	125(3)
5		2>C12A	--H12A	..O02B	[2667.05]	0.95	2.41	3.20(2)	142
6		1 C20	--H20	..O02B	[2676.05]	0.95	2.44	3.202(18)	137

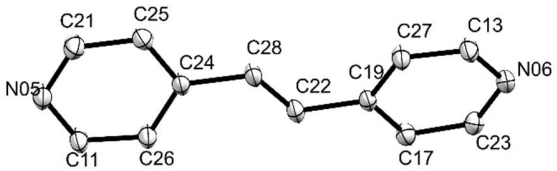
c) 1,2-di(4-pyridyl)ethylene + 4-aminobenzoic acid dihydrate (p1823a)



Nr	Typ	Res	Donor	---	H	....Acceptor	[	ARU	]	D - H	H...A	D...A	D - H...A
1		5	O43	--H43	..	N15	[	1556.02]		0.99(4)	1.66(4)	2.643(4)	173(4)
2		5	N52	--H52A	..	N29	[	2656.03]		0.93(5)	2.15(5)	3.060(5)	165(3)
3		5	N52	--H52B	..	O54	[	2556.06]		0.87(4)	2.16(5)	3.011(4)	166(4)
4		6	O53	--H53	..	N01	[	1455.01]		0.89(5)	1.74(5)	2.622(5)	173(4)
5		6	N62	--H62A	..	N28	[	1545.02]		0.90(4)	2.15(4)	3.020(6)	162(3)
6		6	N62	--H62B	..	O44	[	2666.05]		0.95(4)	2.04(4)	2.956(5)	161(3)
7		1	C11	--H11	..	O44	[	1555.05]		0.95	2.59	3.518(5)	165
8		2	C18	--H18	..	O54	[	2565.06]		0.95	2.60	3.524(4)	165

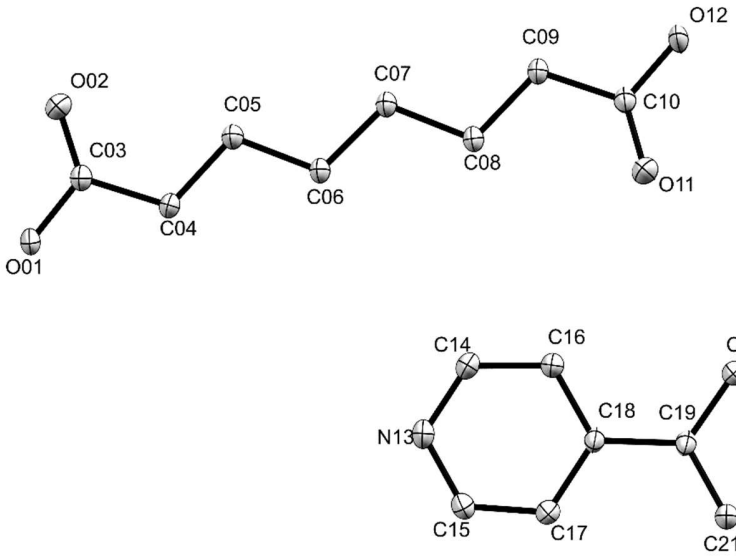
d) 1,2-di(4-pyridyl)ethylene + sebacic acid (p1907a)





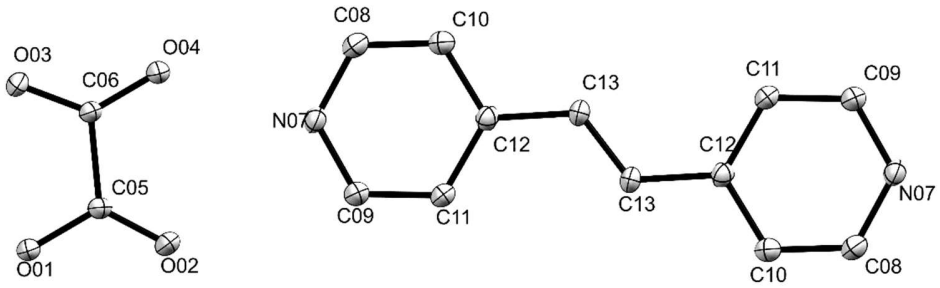
Nr	Typ	Res	Donor	---	H	....Acceptor	[	ARU	]	D - H	H...A	D...A	D - H...A
1		1	O02	--H02	..N05		[	2555.02]		0.915(18)	1.748(18)	2.6516(12)	168.7(14)
2		1	O03	--H03	..N06		[	2876.02]		0.906(17)	1.764(17)	2.6641(12)	172.2(15)
3		1	C08	--H08A	..O01		[	2756.01]		0.99	2.60	3.5371(12)	158
4		2	C17	--H17	..O04		[	2665.01]		0.95	2.60	3.4280(12)	146
5		2	C25	--H25	..O01		[	2766.01]		0.95	2.45	3.3788(13)	165

e) 4,4'-bipyridine + suberic acid (p1818a)



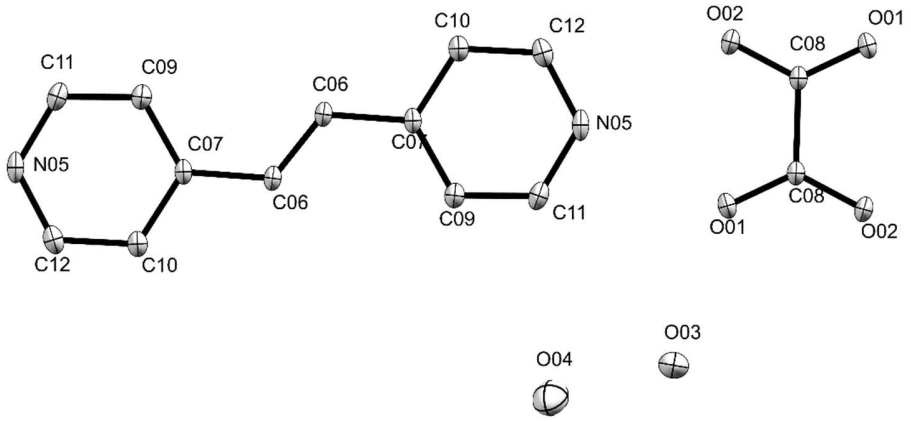
Nr	Typ	Res	Donor	---	H	....Acceptor	[	ARU	]	D - H	H...A	D...A	D - H...A
1		1	O01	--H01	..N24		[	1664.02]		0.969(17)	1.710(18)	2.6607(14)	166.0(17)
2		1	O12	--H12	..N13		[	1455.02]		0.959(17)	1.699(18)	2.6411(14)	166.3(18)
3		1	C09	--H09A	..O02		[	2575.01]		0.99	2.59	3.5660(13)	168
4		2	C16	--H16	..O11		[	1555.01]		0.95	2.56	3.5045(17)	173
5		2	C17	--H17	..O02		[	1546.01]		0.95	2.55	3.5004(14)	174

f) 1,2-di(4-pyridyl)ethylene + oxalic acid (p1922b)



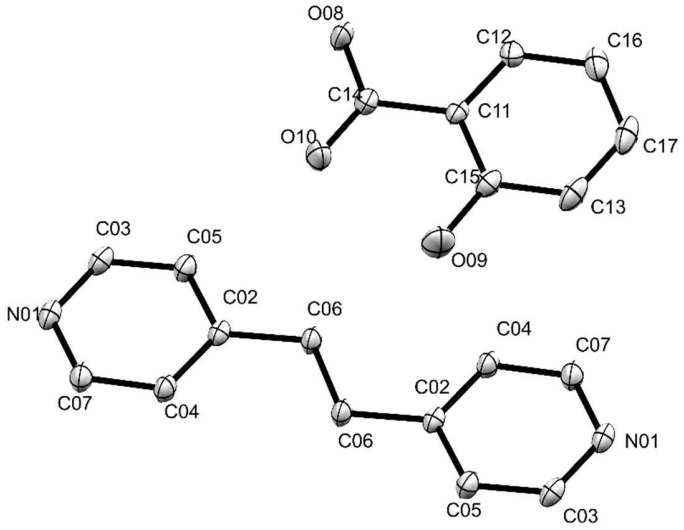
Nr	Typ	Res	Donor	---	H....Acceptor	[ARU]	D - H	H...A	D...A	D - H...A
1	Intra	2	O01	--H01	..O03	[ ]	0.86(3)	2.14(3)	2.682(3)	120.1(18)
2		2	O01	--H01	..O03	[2565.02]	0.86(3)	1.93(2)	2.669(3)	142(2)
3		1	N07	--H07	..O02	[1555.02]	1.00(2)	2.39(2)	3.076(3)	125.1(16)
4		1	N07	--H07	..O04	[1555.02]	1.00(2)	1.69(2)	2.613(3)	150.7(19)
5		1	C08	--H08	..O04	[2566.02]	0.95	2.37	3.239(3)	153
6		1	C09	--H09	..O02	[1555.02]	0.95	2.54	3.128(3)	120
7		1	C10	--H10	..O03	[2566.02]	0.95	2.52	3.237(4)	133

g) 1,2-di(4-pyridyl)ethylene + oxalic acid dihydrate (p1914b)



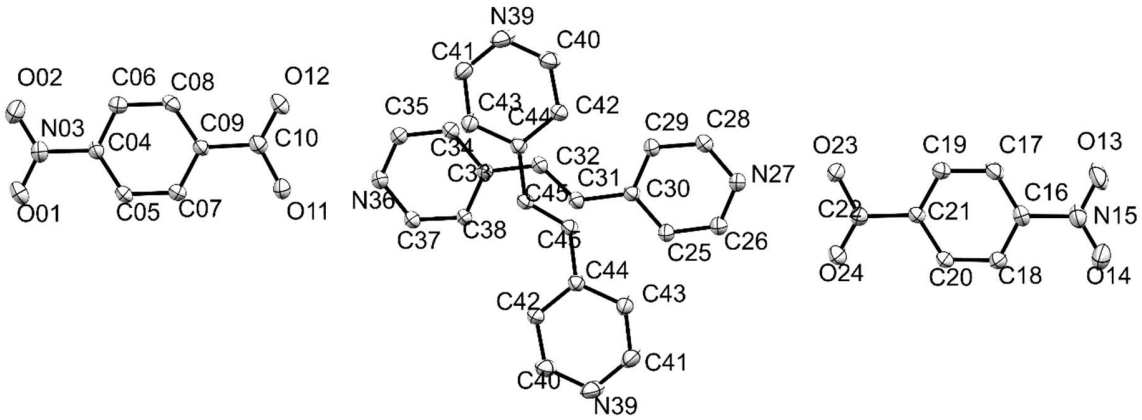
Nr	Typ	Res	Donor	---	H....Acceptor	[ARU]	D - H	H...A	D...A	D - H...A
1		3	O03	--H03A	..O01	[1555.02]	0.90(3)	1.86(3)	2.7491(14)	167(3)
2		3	O03	--H03B	..O04	[1555.04]	0.81(4)	1.97(4)	2.7385(16)	159(3)
3		4	O04	--H04A	..O02	[6657.02]	0.89(3)	1.95(3)	2.8245(11)	167(3)
5		4	O04	--H04B	..O03	[1555.03]	0.84(2)	2.04(4)	2.7385(16)	141(3)
6		1	N05	--H05	..O01	[1555.02]	0.98(3)	1.92(2)	2.7395(17)	138.6(14)
7		1	N05	--H05	..O02	[2656.02]	0.98(3)	2.02(2)	2.8069(17)	135.8(13)
8		1	C10	--H10	..O03	[1554.03]	0.95	2.34	3.2659(18)	164

i) 1,2-bis(4-pyridyl)ethane + salicylic acid (p1908a)



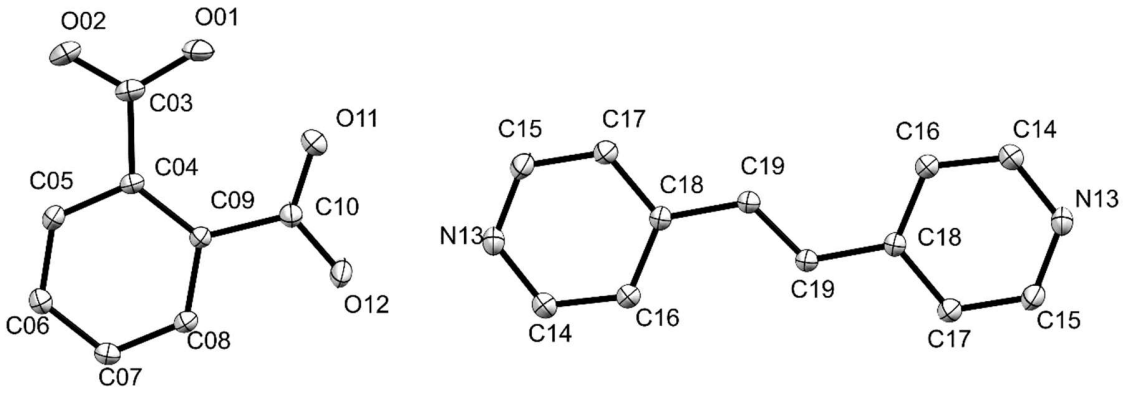
Nr	Typ	Res	Donor	---	H....Acceptor	[ARU]	D - H	H...A	D...A	D - H...A
1		1	N01	--H01	..O08	[1665.02]	1.09(3)	1.45(3)	2.5333(10)	176(2)
2		1	N01	--H01	..O10	[1665.02]	1.09(3)	2.52(3)	3.2433(10)	122.7(17)
3	Intra	2	O09	--H09	..O10	[ ]	0.966(14)	1.633(14)	2.5383(10)	154.3(14)
4		1	C04	--H04	..O09	[1555.02]	0.95	2.47	3.3581(12)	155
5		2	C16	--H16	..O08	[2455.02]	0.95	2.57	3.3087(12)	134

j) 1,2-di(4-pyridyl)ethylene + 4-nitrobenzoic acid (p1926b)



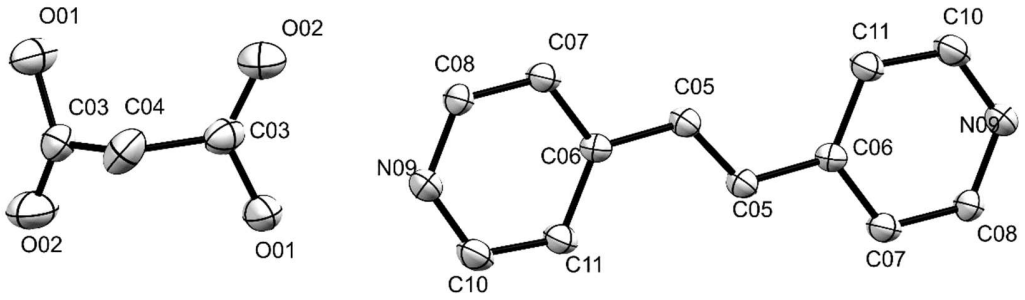
Nr	Typ	Res	Donor	---	H....Acceptor	[	ARU	]	D - H	H...A	D...A	D - H...A
1		4	O11	--H11	..N36	[	1555.01]		0.84	1.77	2.6044(15)	174
2		4	O11	--H11	..N36B	[	1555.03]		0.84	2.13	2.934(14)	161
3		5	O23	--H23	..N27	[	1555.01]		0.84	1.78	2.6213(16)	177
4		5	O23	--H23	..N27B	[	1555.03]		0.84	2.11	2.890(14)	154
5		5	C20	--H20	..O24	[	2777.05]		0.95	2.56	3.2267(19)	127
6		1>C26		--H26	..O24	[	1555.05]		0.95	2.55	3.196(2)	126
7		1>C28		--H28	..O12	[	2566.04]		0.95	2.46	3.341(2)	154
8		1>C37		--H37	..O01	[	2665.04]		0.95	2.57	3.469(2)	157
9		1>C38		--H38	..N39	[	1655.02]		0.95	2.50	3.377(2)	154
10		2	C41	--H41	..O01	[	2565.04]		0.95	2.55	3.4916(19)	171
11		2	C42	--H42	..O13	[	2677.05]		0.95	2.58	3.5245(18)	176
12		2	C45	--H45	..O13	[	1554.05]		0.95	2.57	3.5054(18)	167

k) 1,2-di(4-pyridyl)ethylene + phthalic acid (p1910a)



Nr	Typ	Res	Donor	---	H....Acceptor	[	ARU	]	D - H	H...A	D...A	D - H...A
1	Intra	2	O01	--H01	..O11	[		]	1.05(2)	1.36(2)	2.4049(14)	175(2)
3		1	N13	--H13	..O12	[	1555.02]		0.94(2)	1.61(2)	2.5505(13)	174.9(19)
4	Intra	2	C05	--H05	..O02	[		]	0.95	2.30	2.6851(14)	103
5		2	C07	--H07	..O12	[	2655.02]		0.95	2.44	3.2773(14)	147
6	Intra	2	C08	--H08	..O12	[		]	0.95	2.27	2.6493(14)	103
7		1	C19	--H19	..O01	[	2535.02]		0.95	2.44	3.3066(14)	152
8		1	C19	--H19	..O02	[	2535.02]		0.95	2.58	3.4030(13)	146

l) 1,2-di(4-pyridyl)ethylene + malonic acid (p1913a)

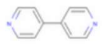
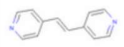
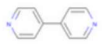
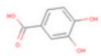
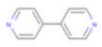
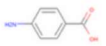
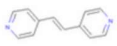
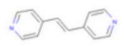
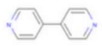
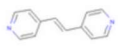
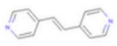
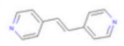
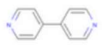
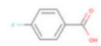
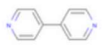
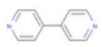
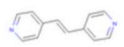
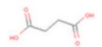
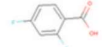
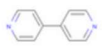
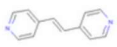
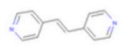
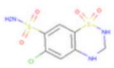
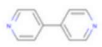
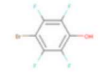
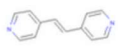


Nr	Typ	Res	Donor	---	H....Acceptor	[ARU]	D - H	H...A	D...A	D - H...A
1	3	O01	--H01		..N09	[1555.01]	1.071(15)	1.520(17)	2.580(8)	169.4(14)
2	3	O01	--H01		..N16	[1555.02]	1.071(15)	1.49(2)	2.53(2)	164.4(16)
3	1>C05		--H05		..O02	[2665.03]	0.95	2.50	3.4005(15)	159
4	1>C08		--H08		..O02	[1555.03]	0.95	2.56	3.240(4)	129
5	1>C10		--H10		..O01	[3756.03]	0.95	2.53	3.428(6)	157

S3 - Top 100 predictions of the scoring method

In Table S3, the algorithm's top 100 predictions are presented in descending order of score value.

Table S5 The RA scoring algorithm's top 100 predictions

1	75.359764			**8**	47.668949			**15**	41.426933			**22**	40.245972		
2	59.823074			**9**	45.430702			**16**	41.426933			**23**	40.050869		
3	54.224815			**10**	45.075985			**17**	41.370590			**24**	39.820210		
4	52.733902			**11**	42.923214			**18**	41.049618			**25**	39.506470		
5	49.512886			**12**	41.780567			**19**	41.023731			**26**	38.456535		
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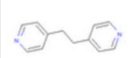
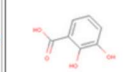
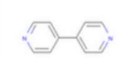
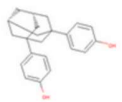
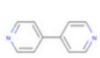
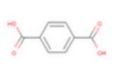
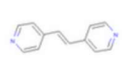
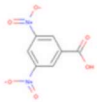
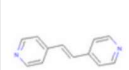
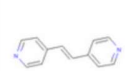
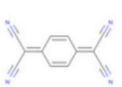
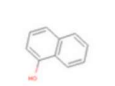
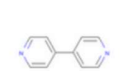
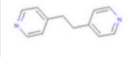
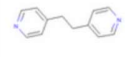
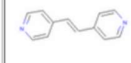
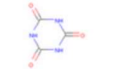
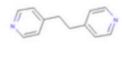
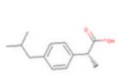
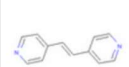
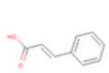
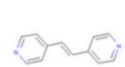
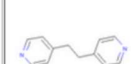
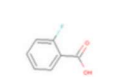
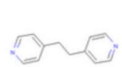
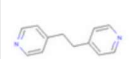
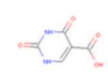
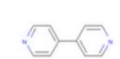
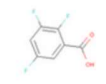
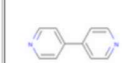
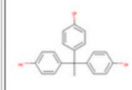
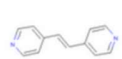
29	37.516613			**36**	36.070789			**43**	34.253639			**50**	33.198208		
30	36.885445			**37**	35.655060			**44**	34.156055			**51**	33.198059		
31	36.777348			**38**	35.386303			**45**	34.035328			**52**	33.038921		
32	36.582294			**39**	35.384716			**46**	33.963779			**53**	32.792377		
33	36.524605			**40**	35.317924			**47**	33.961014			**54**	32.706879		
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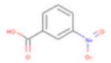
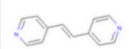
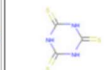
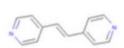
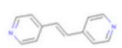
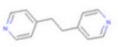
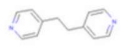
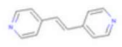
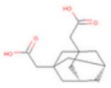
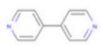
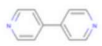
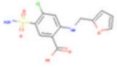
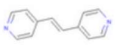
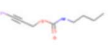
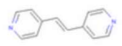
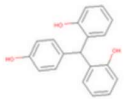
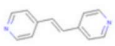
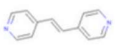
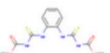
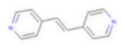
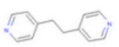
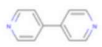
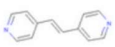
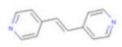
57	32.494797			**64**	31.322908			**71**	30.965084			**78**	30.338097		
58	32.215023			**65**	31.270685			**72**	30.806206			**79**	30.240723		
59	32.040550			**66**	31.185358			**73**	30.685154			**80**	30.240723		
60	31.682217			**67**	31.094425			**74**	30.533785			**81**	30.240723		
61	31.538536			**68**	31.082464			**75**	30.509993			**82**	30.240723		
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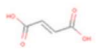
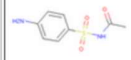
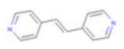
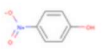
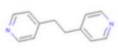
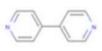
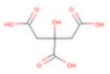
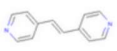
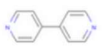
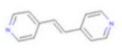
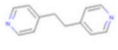
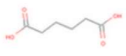
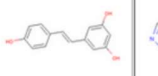
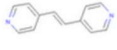
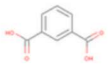
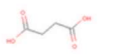
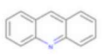
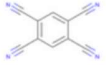
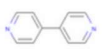
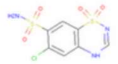
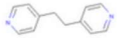
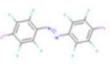
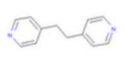
85	29.917561			**92**	28.502075			**99**	27.877150		
86	29.893450			**93**	28.420525			**100**	27.852009		
87	29.461119			**94**	28.368240						
88	29.225071			**95**	28.301092						
89	28.745815			**96**	28.239725						
90	28.710207			**97**	28.196133						
91	28.688921			**98**	28.131899						

S4 – Predefined lists of common solvents and gases

Solvents and gases are indicated with their chemical names or SMILES code when the former is missing.

Solvents:

```
1,2-dichlorobenzene
triethylamine
perfluorobenzene
perdeuterocyclohexanone
1-nitropropane
2,3-butanedione
1,3-dichlorobenzene
cyclohexanol
bromoform
heptan-1-ol
ethanethiol
cyclooctane
ethanol
aniline
1,3-dibromobenzene
2-methyl-2-propanol
cycloheptane
1,2,3-trichloropropane
benzyl alcohol
p-xylene
(.+-.)-limonene
cyclobutanone
2-ethoxyethyl acetate
1,4-dioxane
diethyl sulfide
n,n'-dimethylpiperazine
1-phenyldecane
heavy water
perdeuteronitromethane
dodecane
butan-2-ol
pentanol
1,3,5-trifluorobenzene
butan-1-ol
benzonitrile
hexane
2,2,2-trifluoroethanol
n-pentane
triethyl orthoformate
4-methylpyridine
dibromo-dideuteromethane
propionic acid
furan
tetradeutero-acetic acid
trifluoroacetic acid
1,1-dichloroethane
cyclooctanamine
cyclopentanone
methyl acrylate
1-bromobutane
acrylic acid
```

ethyl formate
glycerol
formamide
trans-1,2-dichloroethene
1,2-difluorobenzene
cyclohexanone
diethylamine
hydrogen peroxide
n-butyric acid
acrylonitrile
1,4-pentadiene
adiponitrile
perdeuterotoluene
2-methylheptane
pentan-2-one
2,4-lutidine
dioxolane
n-hexylamine
octafluorotoluene
hexamethyl-disiloxane
2-methylpyrazine
octadeuterofuran
dichloromethane
benzene-d6
2-bromo-2-methylpropane
tert-butylacetat
1,2-dibromobenzene
1,3-propanediol
methyl propanoate
hexafluoroisopropanol
2,2,3-trimethylbutane
O=S1(=O)CCCC1
2-methyltetrahydrofuran
diiodomethane
nitromethane
1,3-dimethyl-2-imidazolidinone
cyclopentane
butyronitrile
1,1,2,2-tetrachloroethane
1,2-bis(dimethylphosphino)ethane
nitric acid
dodecadeuterocyclohexane
tert-amyl alcohol
dimethylformamide
cis-1,2-dichloroethene
3-picoline
CC(CC(=O)C)C
hexanol
1,5-pentanediol
perfluoromethylcyclohexane
thionyl chloride
ClC(=C)Cl
1,1,1-trichloroethane
piperidine
dideutero-formic acid
pyridine
antimony pentafluoride
toluene

perdeuteroaniline
n-hexadecane
1,4-cyclohexadiene
nitrobenzene
quinoline
1,3,3-trimethyl-2-oxabicyclo(2.2.2)octane
cis-cyclooctene
diethyldiglycol
dimethyl sulfide
dimethyl carbonate
1,2,3,4-tetrafluorobenzene
n,n-dimethylacetamide
cyclopentene
tetramethyldiarsane
diethyl ether
anisole
pyrimidine
fluorobenzene
1,1,2-trichloroethane
2-hexanone
water
heptane
2,2-dimethylbutane
2-chloro-2-methylpropane
sulfuric acid
perchloric acid
1,2-dichloroethane
m-xylene
perfluorohexane
trifluoroethanol
formic acid
2,5-dimethylpyrazine
perdeuteropyridine
dimethoxymethane
butanone
n-nonylamine
3,5-dimethylpyridine
decane
allylamine
2,6-xylidine
acetonitrile
isobutyl acetate
trans-1,4-dimethylcyclohexane
2-cyanopropene
2-nitropropane
iodobenzene
2-aminopropane
pyrrole
tetradeutero-methanol
cis-stilbene
trimethyl orthoformate
carbon tetrachloride
propionitrile
cyclohexane
3,4-lutidine
1,2-dimethoxyethane
ethylcyclohexane
acetophenone

undecane
methyl formate
ethyl acetate
tetraethylene glycol dimethyl ether
diisopropyl ether
pivalonitrile
hydrazine
mesitylene
1-methyl-2-pyrrolidinone
methyl methacrylate
ethyl propionate
ethynylbenzene
heptanoic acid
2-methylbut-2-ene
valeric acid
n-methylformamide
2-picoline
1-octanol
hexamethylphosphoramide
tmeda
1,3-propanediamine
methylcyclohexane
n-pentylamine
methyl iodide
CC(c1ccccc1)C
ClC=C(Cl)Cl
pent-1-ene
tetrahydropyran
dichloromethane (disordered C
benzene
n-butylamine
tetrahydrothiophene
benzoyl chloride
methyl acetate
diethylzinc
2-phenylacetonitrile
1-methylnaphthalene
methyl nitrate
styrene
nitroethane
pentyl acetate
ethylbenzene
pyridazine
butyl acetate
1,3-bis(trifluoromethyl)benzene
hexamethyldisilane
carbon disulfide
tetramethylsilane
methylpyrrolidine
butyrolactone
bromochloromethane
monochlorobenzene
1,3,5-triethylbenzene
hexanoic acid
furfuranol
propylene carbonate
isobutanol
1,2,4,5-tetrafluorobenzene

propyl acetate
pentafluorobenzonitrile
decalin
diacetone alcohol
deutero-bromoform
methyl tert-butyl ether
perdeutero-p-xylene
isopropyl cyclohexane
morpholine
diglyme
benzaldehyde
3-methylbutan-2-one
trifluoromethanesulfonic acid
cyclohexene
2,2,4-trimethylpentane
isopropanol
ethane-1,2-diol
2-ethoxy-2-methylpropane
n,n,n',n',n''-pentamethyldiethylenetriamine
methyl benzoate
dicyclohexylamine
2,4,6-collidine
methanol
but-2-yne
1,3-difluorobenzene
bromobenzene
pentafluorobenzene
1,2-diaminoethane
2-pentanol
perdeuterodimethylsulfoxide
1,5-pentanediamine
dibutyl ether
hexamethyldisilazane
1-bromo-2,4,6-trifluorobenzene
cyclo-octatetraene
o-xylene
tetramethylurea
azetidine
1,3-dioxolane
chlorotrimethylsilane
tetrahydrofuran
1,1,1,2,2-pentachloroethane
C1CCc2c(C1)cccc2
ethanoic anhydride
perdeutero-4-methylpyridine
peg-4
pyrrolidine
isohexane
thiophene
2,2-dimethoxypropane
isopropyl acetate
2-(2-methoxyethoxy)ethanol
2-chloroaniline
nonanoic acid
methylimidazole
2-ethoxyethanol
perdeutero-m-xylene
acetic acid

m-cresol
diethylenetriamine
monomethylhydrazine
acetone
COCCO
1-propanol
n-propylamine
n-octane
chloroform-d
propyl ether
isopentane
perdeutero-acetone
tetradecane
2-ethylhexanol
chloroform
3-pentanone
oxetane
3-methylbutan-1-ol
vinyl acetate
octanoic acid
n-nonane
3,3-dimethylbutan-2-one
decanoic acid
dimethyl sulfoxide
methylcyclopentane
perdeutero-o-xylene
2,2-dimethylbutanoic acid
triethylborane
2-nonanone
oxacycloheptane
n-octylamine

Gases:

Perfluorobutane
heptafluoro-n-propylÂ isocyanate
Boron trifluoride
Dimethylphosphine
Bromodifluoromethane
Trimethylamine
Argon
1,1-difluoropropene
Dichlorofluoromethane
Perchloryl fluoride
Ethane
Neon
Hexafluorocyclobutene
1,1-Difluoroethene
Tetrafluorosilane
pentafluoroethyl sulfur pentafluoride
Nitrogen tetroxide
Chloropentafluoroethane
Phosphine
Thiothionyl fluoride
1-Butyne
Methyl pentafluoroethyl ether
Vinyl bromide

2-Chloro-2,3,3,3-tetrafluoropropanoyl fluoride
Nitrosyl bromide
1-Buten-3-yne
Dichlorodifluorosilane
Stannane
Sulfur fluoride oxide
3,3,3-Trifluoro-1-propyne
Trifluoromethyl trifluoromethanesulfonate
Perfluoroisobutene
heptafluoroisopropyl hypochlorite
Phosphoryl fluoride
Perfluoro-1-butene
1,3-Butadiyne
1,1,2,3,4,4-Hexafluoro-1,3-butadiene
Chloryl fluoride
1,2-Butadiene
1-chloro-1-fluoroethane
Bromomethane
1,1,2,2-tetrafluoro-1-nitro-2-nitrosoethane
(Trifluoromethyl)silane
Chlorine pentafluoride
1,2-Dichloro-1,1,2,2-tetrafluoroethane
Dimethylsilane
Octafluorocyclopentene
2,2,3,3-tetrafluorobutane
Cyclobutane
tefluraneÂ 2-Bromo-1,1,1,2-tetrafluoroethane
trifluoromethyl fluoroformyl peroxide
Trifluoronitrosomethane
Bismuth hydride
Sulfur hexafluoride
Sulfur bromide pentafluoride
Disiloxane
trifluoromethyl trifluorovinyl ether
HeliumÂ 4
Perfluoro-2-butene
Trifluoromethanesulfonyl fluoride
1,1,1,2,4,4,4-heptafluoro-2-butene
Trifluorosilane
Trifluoroisocyanomethane
Trifluoramine oxide
Isobutene
Difluoromethane
1-Butene
thiocarbonyl fluoride
Hydrogen fluoride
trifluoromethylhypofluorite
Trifluoromethyl 1,1,2,2-tetrafluoroethyl ether
Perfluorodimethoxymethane
trifluoromethyl peroxychloride
difluoromethyl 1,1,2-trifluoroethyl ether
Ethyltrifluorosilane
pentafluoroethyl trifluorovinyl ether
trifluoromethylsulfur pentafluoride
Methylcyclopropane
hexafluorodiazomethaneÂ cis
Difluoromethylborane
trifluoromethyl isocyanate

Neopentane
perfluoro ethyl methyl ether
1,1,1-Trifluoropropane
Disilane
1,1,1,2,3,3,3-Heptafluoropropane
difluoroiodomethane
Bromofluoromethane
Hydrogen selenide
Bromine fluoride
Chlorotrifluorogermane
Propene
1,1-Dichloro-1,2,2,2-tetrafluoroethane
perfluorocyclobutanone
2,2,3,3,4,4,5-heptafluoro oxolane
trans-1,2-Dichloro-1,2-difluoroethene
Fluorine nitrate
monoethylsilane
Methyl trifluoromethyl ether
1,1,1,2-tetrafluoropropane
Trichlorofluorosilane
dimethylchloroborane
Acetaldehyde
Perfluoroisobutane
1,1,1,2,2,3,3,4,4-nonafluorobutane
bis(trifluoromethyl)phosphine
Chlorine trifluoride
Chlorotrifluoroethene
trans-bis(trifluoromethyl)sulfur tetrafluoride
Hexafluorodisilane
Difluoramine
Helium-3
Trifluoroacetyl chloride
2-chloro-1,1,1,2-tetrafluoropropane
1,1,2,2,3,3,3-Heptafluoropropane
Chlorotrifluorosilane
Sulfur dioxide
Chlorine monoxide
pentafluoroguanidine
3-Fluoropropene
Tetrafluorohydrazine
Nitrogen
1-chloro-1,3,3,3-tetrafluoropropene
Hexafluoroethane
difluoro(difluorochloromethyl)amine
trifluoromethyl phosphine
Sulfur chloride pentafluoride
1-Chloro-1,1,2,2-tetrafluoropropane
difluoromethylene dihypofluorite
1-Chloro-1,1,2,2-tetrafluoroethane
trans-2-Butene
1-chloroheptafluoropropane
Perfluoropropane
3,3,3-Trifluoropropene
trifluoromethylsulfonyl hypofluorite
Trifluoroethene
1,1-Dichloro-2,2-difluoroethene
decafluorocyclopentane
1,1-Difluoropropane

2-Fluorobutane
2-chloroheptafluoropropane
difluoroamino carbonyl fluoride
2-Fluoropropene
Trifluoronitromethane
Radon
cis-1-Bromo-1,2-difluoroethylene
Phosphorus(III) dichloride fluoride
Methyl silyl ether
1-bromoheptafluoropropane
Fluorine perchlorate
Perfluorooxetane
Iodine heptafluoride
Diphosphorus tetrafluoride
Methanethio
pentafluoroethyl iminosulfur difluoride
Formyl fluoride
Sulfur fluoride
Carbon dioxide
Fluoroethene
1-Chloro-2,2-difluoroethene
Nitrosyl fluoride
methyl trifluorovinyl ether
Carbon oxysulfide
trans-1-Fluoropropene
Dichlorodifluoromethane
Phosphonium chloride
Pentafluoronitrosoethane
2,2-Difluoropropane
Dichloromethylborane
1,1,1-Trifluoroethane
oxalyl fluoride
Trifluoroacetonitrile
Ozone
2-Chloropropene
Nitrogen trifluoride
2-Chloro-1,1,1,3,3,3-hexafluoropropane
Chloroheptafluorocyclobutane
bis(fluorocarbonyl) peroxide
tetrafluorodiaziridine
1,1,1,3,3,3-Hexafluoropropane
Hexafluoropropene
Nitrogen chloride difluoride
Trifluoromethylcyclopropane
1,1,1,3,3-pentafluorobutane
Bromotrifluoroethene
2,2,2-Trifluorodiazoethane
1,1,1-Trifluoro-2-chloroethane
methoxyacetylene
Trichlorofluoromethane
bromoacetylene
2,3,3,3-tetrafluoropropene
Borirane
Bromotrifluoromethane
Butane
1-Fluoropropane
Acetyl fluoride
Nitrous oxide

Trifluoro(trifluoromethyl)oxirane
2-Fluoro-2-methylpropane
Methyldifluorophosphine
Heptafluoronitrosopropane
Diazomethane
1,1-difluorocyclopropane
Chloroethane
1-Chloro-1-fluoroethene
Thiazyl trifluoride
cis-2-Butene
dibromodifluoromethane
1,1,1,2,2,3-hexaï¬ uoropropane
Selenium dioxydifluoride
pentafluoroiodoethane
Trifluoromethyl phosphorodifluoroperoxoate
Fluorotrimethylsilane
Arsine
1,1,1,2,3-pentafluoropropane
Tetraborane
Cyclobutene
Perfluoroethyldimethylamine
Germanium(IV) fluoride
Hexafluoromethanediamine
Ethylene oxide
Plumbane
Silane
Cyanic acid
Trans-Dimethyldiazene
Vinylsilane
Sulfuryl chloride fluoride
Methane
Trifluoromethyl difluoromethyl ether
Chlorosilane
Formaldehyde
Fluorine monoxide
decafluorodiethyl etherÂ perfluoro ether
Ethylene
Dimethylperoxide
Hydrogen telluride
Chlorine
Sulfur tetrafluoride
PropyneÂ methylacetylene
Cyclopropane
Chlorodifluoromethane
1,1,1,2,2-Pentafluoropropane
Tungsten(VI) fluoride
1,2,2,2-Tetrafluoroethyl difluoromethyl ether
1,1,4,4-tetrafluoro-1,3-butadiene
N,N-difluoroethylamine
Dimethyl ether
Difluorodimethylsilane
Hexafluoroacetone imine
methyltrifluorosilane
Bis(difluoromethyl) ether
Dichlorodifluorogermane
Ethyl methyl ether
Methylarsine
1-Fluoro-2-methylpropane

Methylgermane
Methylamine
1,1-Difluoroethane
Bis(trifluoromethyl)peroxide
Fluoromethane
Ammonia
1-Propen-1-oneÂ methylketene
Carbon monoxide
Methylphosphine
1,1,1-trifluoroacetone
Propadiene
Hydrogen chloride
Ketene
methyl trifluoromethyl sulfide
Nitryl chloride
bis(trifluoromethyl)diazeneÂ trans
bis(Trifluoromethyl)nitroxide
Selenium hexafluoride
Ethyl nitrite
Germane
Carbonyl fluoride
trifluoromethylhypochlorite
1,1,1,3,3-pentafluoropropane
(Difluoroamino)difluoroacetonitrile
Phosphorothioc chloride difluoride
Acetylene
Ethoxytrifluorosilane
Tetrafluoromethane
Tellurium hexafluoride
Hydrogen iodide
Carbonyl fluoride iodide
Hydrogen
Carbon oxyselenide
Formic anhydride
Chloroacetylene
Carbonyl chloride fluoride
cis-1,2-Difluoroethene
Cyanogen chloride
Diborane
Ethyl phosphine
Nitrosyl chloride
Ethylamine
Fluoroethane
Propane
1,1,2-Trifluoroethane
Ethynylsilane
Chloroethene
Chloromethane
Hydrogen bromide
1-Chloro-1,2,2-trifluoroethane
Dichlorosilane
Cyanogen
1-Chloro-1,2,2,2-tetrafluoroethane
2-Chloropentafluoropropene
1,1,1-trifluorobutane
1,1,1,2,3,3-Hexafluoropropane
Perbromyl fluoride
Krypton

Propylsilane
trifluoromethanethiol
Oxygen
Arsenic(V) fluoride
trifluoromethanesulfenylchloride
Difluorine dioxide
Thionyl fluoride
Bromosilane
Trifluoroacetyl fluoride
1,3,3,3-tetrafluoropropene
Nitryl fluoride
Trimethylborane
3-chloropentafluoropropene
Perfluoroazoethane
Bromopentafluoroethane
1,2,2-Trifluoropropane
1,1,1,2-Tetrafluoroethane
Hexafluorobut-2-yne
Stibine
Isobutane
1,1,2,2-Tetrafluoroethane
Phosphorus(III) fluoride
Phosphorus(V) fluoride
Methylstannane
Methylsilane
Sulfuryl fluoride
1,1,2,2-tetrafluoropropane
Phosphorothioc trifluoride
Fluorosilane
Carbonyl chloride
Carbon suboxide
Chlorotrifluoromethane
Cyclopropene
Tetrafluorodiborane
tris(triï¬ uoromethyl)-amine
perfluorodimethylamine
Methyl vinyl ether
N,N-difluoromethanamine
1,3-Butadiene
Methyl nitrite
1-Chloro-1,1-difluoroethane
1-Bromo-2,2-difluoro-ethylene
Tetrafluoroethene
Chloropentafluoroacetone
Difluorosilane
Perfluorocyclobutane
1,1-Dimethylcyclopropane
1-Chloro-1,1,2-trifluoroethane
Trimethylsilane
Xenon tetroxide
Borane carbonyl
Nitric oxide
1-Chloro-2-fluoroethene
Hydrogen sulfide
Trifluoromethyl fluoroformate
1,1,2,2,3,3-hexaï¬ uoropropane
Fluoroacetylene
Cyanogen fluoride

Perfluoroacetone
3-Methyl-1-butene
2-Fluoropropane
heptaï¬ uoroethanamine
1,2-Difluoroethane
Dimethylamine
Trifluoroiodomethane
Pentafluoroethane
methyl chlorosilane
Bromochlorodifluoromethane
Chlorofluoromethane
difluorocyanamide
Chlorine dioxide