

Crystalline peroxosolvates: nature of the coformer, hydrogen-bonded networks and clusters, intermolecular interactions

Alexander G. Medvedev,[†] Andrei V. Churakov,[†] Petr V. Prikhodchenko,[†] Ovadia Lev,^{§,*} Mikhail V. Vener^{†,‡,*}

[†]*Kurnakov Institute of General and Inorganic Chemistry, Russian Academy of Sciences, Leninskii prosp. 31, Moscow 119991, Russia*

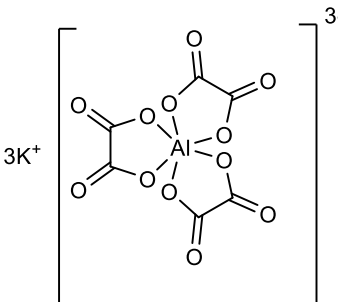
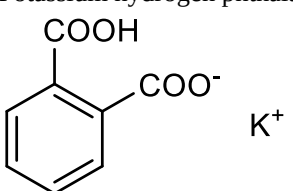
[‡]*Department of Quantum Chemistry, Mendeleev University of Chemical Technology, Miusskaya Square 9, Moscow 125047, Russia*

[§]*The Casali Center of Applied Chemistry, The Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem 91904, Israel.*

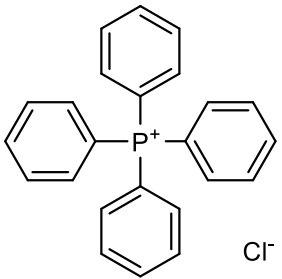
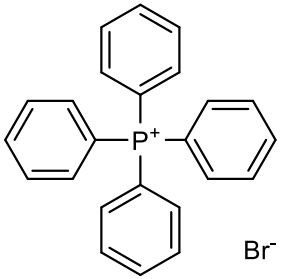
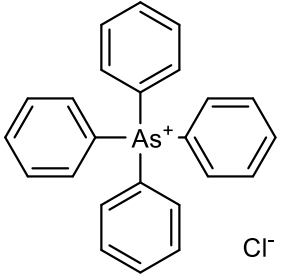
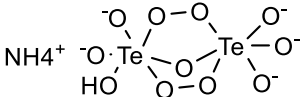
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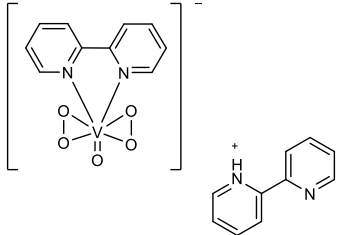
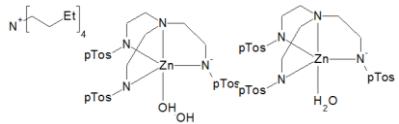
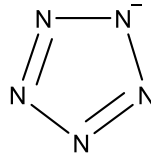
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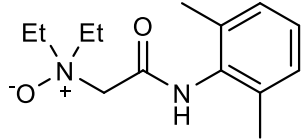
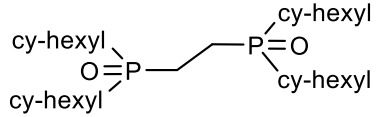
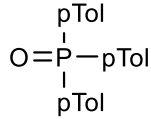
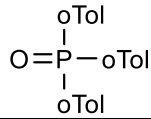
Table S1. Structure features of peroxosolvates with localized protons.

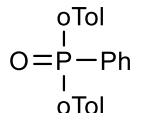
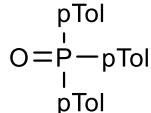
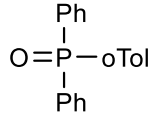
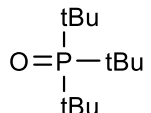
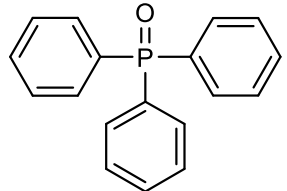
	Coformer (Cof)	Refcode ^{a)}	Stoichiometry	X, Y ^{c)}	n(H ₂ O ₂) ^{d)}	N ₁ ^{e)}	N ₂ ^{f)}	Contact Me-O _p , Å	Ref
Salts of inorganic and carboxylic acids									
1	Ammonium oxalate, (NH ₄) ₂ C ₂ O ₄ ,	AMOXPH10	Cof•(0.94H ₂ O ₂ •0.06H ₂ O) ^{b)}	O,O	1	2	2		[1]
2	Lithium oxalate, Li ₂ C ₂ O ₄	LIOXPH	Cof•H ₂ O ₂	O,O	1	2	0	(Li): 2.088; 2.284	[2]
3	Sodium oxalate, Na ₂ C ₂ O ₄	NAOXAP	Cof•H ₂ O ₂	O,O	1	2	0	(Na): 2.423; 2.435	[3]
		NAOXAP11=246301 ^{g)} , NAOXAP01	Cof•H ₂ O ₂	--/--	--/--	--/--	--/--	(Na): 2.388; 2.425	[4]
4	Potassium oxalate, K ₂ C ₂ O ₄	KOXPHY11, (KXPHY10=246300) ^{g)} KXPHY01	Cof•H ₂ O ₂	O,O	1	2	0	(K): 2.856 - 3.240	[5,6]
5	Tripotassium tris(oxalato-κ ² O,O')-aluminate 	GADMUU, 170728	Cof•H ₂ O ₂ •(0.75H ₂ O ₂ •0.25H ₂ O)	O,O	2	2; 2	1; 1	(K): 2.776 - 3.370	[7]
6	Guanidinium sulfate, (CN ₃ H ₆) ₂ SO ₄	BOHLOC	Cof•H ₂ O ₂	O,O	1	2	1		[8]
7	Ammonium succinate, (NH ₄) ₂ C ₄ H ₄ O ₄	BAMXAR	Cof•2H ₂ O ₂	O,O	1	2	0		[9]
8	Potassium hydrogen phthalate, 	YUHTAW	Cof•0.5H ₂ O ₂	O,O	1	2	0	(K): 2.798 - 3.482	[10]

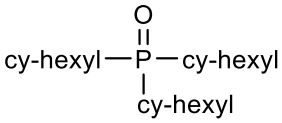
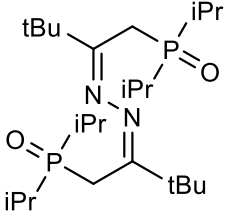
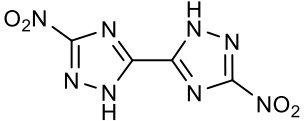
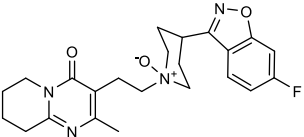
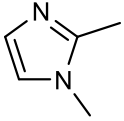
	Coformer (Cof)	Refcode ^{a)}	Stoichiometry	X,Y ^{c)}	n(H ₂ O ₂) ^{d)}	N ₁ ^{e)}	N ₂ ^{f)}	Contact Me-O _p , Å	Ref
9	Potassium fluoride, KF	22365, 22366	Cof•2H ₂ O ₂	F,F	2	2; 2	0; 0	(K): 2.785-3.167	[11]
10	Rubidium fluoride, RbF	200383, 200384	Cof•H ₂ O ₂	O,O	1	2	0	(Rb): 2.970-3.097	[12]
11	Ammonium fluoride, NH ₄ F	28552	Cof•H ₂ O ₂	F,F	1	2	2		[13]
12	Nonasodium tetrasulfate chloride, Na ₉ (SO ₄) ₄ Cl	171004, (1715) ^{g)}	Cof•2H ₂ O ₂	O,O	4	2; 2; 2; 2	0; 0; 0; 0	(Na): 2.354 – 2.420	[14]
13	Nonasodium tetrasulfate bromide, Na ₉ (SO ₄) ₄ Br	171005	Cof•H ₂ O ₂	O,O	1	2	0	(Na): 2.379 – 2.391	[14]
14	Guanidinium oxalate, (CN ₃ H ₆) ₂ C ₂ O ₄	GADOXP10	Cof•H ₂ O ₂ •2H ₂ O	O,O	1	2	2		[15]
15	Sodium carbonate, Na ₂ CO ₃	200044, WUTKUT08,(1304) ^{g)}	Cof•1.5H ₂ O ₂	O,O	2	2; 2	0; 0		[16,17]
		281382, WUTKUT	--/--	--/--	--/--	--/--	--/--		[18]
		281383, WUTKUT01	--/--	--/--	--/--	--/--	--/--		
		281384, WUTLEE	--/--	--/--	--/--	--/--	--/--	(Na): 2.401 - 2.504	
		281385, WUTKUT02	--/--	--/--	--/--	--/--	--/--	(Na): 2.388 - 2.511	
		281386, WUTKUT03	--/--	--/--	--/--	--/--	--/--	(Na): 2.377 - 2.497	
		281387, WUTKUT04	--/--	--/--	--/--	--/--	--/--	(Na): 2.371 - 2.492	
		281388, WUTKUT05	--/--	--/--	--/--	--/--	--/--		
		281389, WUTKUT06	--/--	--/--	--/--	--/--	--/--		
		281390, WUTKUT07	--/--	--/--	--/--	--/--	--/--		
16	Ammonium carbonate, (NH ₄) ₂ CO ₃	262530, WUXSIT	Cof•H ₂ O ₂	O,O	2	2; 2	0; 0		[19]
17	Caesium carbonate, Cs ₂ CO ₃	262531, WUXSOZ	Cof•3H ₂ O ₂	O,O	4	2; 2; 2; 2	0; 0; 0; 0	(Cs): 3.056 - 3.467	
18	Potassium hydrogendioxoperoxocarbonate, K(H(O ₂)CO ₂)	407779	Cof•H ₂ O ₂	O,O	1	2	0	(K): 2.747- 2.820	[20]
19	Tetrapotassium bis(hydrogenphosphate), K ₄ (HPO ₄) ₂	418249	Cof•3H ₂ O ₂	O,O	3	2; 2; 2	0; 0; 0	(K): 2.695 – 3.303	[21]
20	Pottasium dioxoperoxocarbonate, K ₂ (O ₂)CO ₂	421906	Cof•3.5H ₂ O ₂	O,O	5	2; 2; 2; 2; 2	0; 0; 0; 0; 0	(K): 2.772 - 3.290	[22]

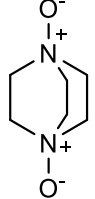
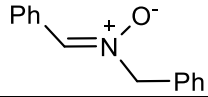
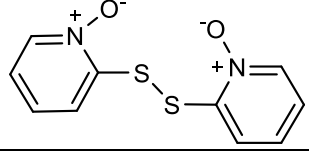
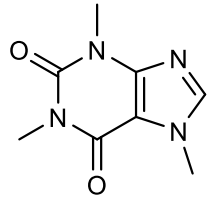
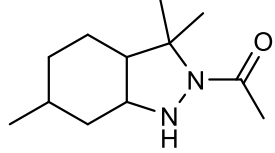
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21	Tetraphenylphosphonium chloride, 	CAZHAN	Cof•H ₂ O ₂ •(0.85H ₂ O ₂ •0.15H ₂ O)	Cl, Cl	2	2; 2	0; 0		[23]
22		CAZHAN01	Cof•H ₂ O ₂ •(0.9H ₂ O ₂ •0.1H ₂ O)	--/--	--/--	--/--	--/--		
23		CAZHAN02	Cof•H ₂ O ₂ •(0.73H ₂ O ₂ •0.27H ₂ O)	--/--	--/--	--/--	--/--		
24	Tetraphenylphosphonium bromide 	CAZHER [s7]	Cof•H ₂ O ₂ •(0.84H ₂ O ₂ •0.16H ₂ O)	Br, Br	2	2; 2	0; 0		
25		CAZHIV [s7]	Cof•H ₂ O ₂ •(0.5H ₂ O ₂ •0.5H ₂ O)	Br, Br	2	2; 2	0; 0		
26	Tetraphenylarsonium chloride 	CAZHOB	Cof•H ₂ O ₂ •(0.85H ₂ O ₂ •0.15H ₂ O)	Cl, Cl	2	2; 2	0; 0		
27		CAZHUH	Cof•1.5H ₂ O ₂	Cl, Cl	2	2; 2	0; 0		
28		CAZJAP	Cof•(0.98H ₂ O ₂ •0.02H ₂ O)	Cl, Cl	2	2; 2	0; 0		
29	Ammonium peroxotellurate, 	196444	Cof•(0.72H ₂ O ₂ •0.28H ₂ O)•H ₂ O	O, O	1	2	1		[24]

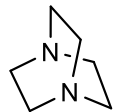
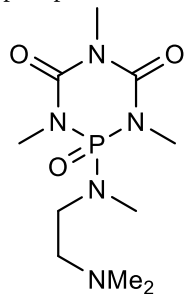
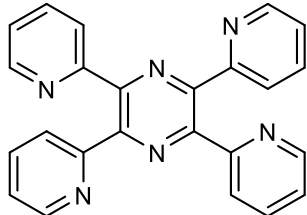
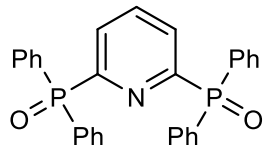
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30	Caesium tetracyanoplatinate, Cs ₂ (Pt(CN) ₄)	418911	Cof•H ₂ O ₂	N,N	1	2	0	(Cs): 3.115 - 3.180	[25]
31	Rubidium tetracyanoplatinate, Rb ₂ (Pt(CN) ₄)	418912	Cof•H ₂ O ₂	N,N	1	2	0	(Rb): 2.980 -3.000	
32	Potassium tetracyanoplatinate, K ₂ (Pt(CN) ₄)	418913	Cof•H ₂ O ₂	N,N	1	2	0	(K): 2.843 - 2.918	
33	2,2'-Bipyridinium (2,2'-bipyridine)- oxo-diperoxo-vanadium 	CEYXUZ	Cof•3.4H ₂ O ₂ •1.6H ₂ O	O,O	3	2; 2; 2	0; 2; 2		[26]
34	Tetra-n-butylammonium ((hydrogen peroxide)-(N,N,N- tris(2-((4-methylbenzene-1- sulfonyl)amino)ethyl)amine)-zinc aqua-(N,N,N-tris(2-((4- methylbenzene-1- sulfonyl)amino)ethyl)amine)- zinc) 	BABGUJ	Cof•(0.52H ₂ O ₂ •0.48H ₂ O)	O,O	1	2	0	(Zn): 2.172	[27]
35	Ammonium cyclopentazolate, NH ₄ ⁺ 	ZUWCIG	Cof•0.5H ₂ O ₂	N,N	1	2	2		[28]
		ZUWCIG01	Cof•0.5H ₂ O ₂	N,N	1	2	2		

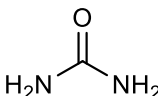
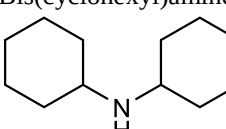
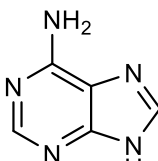
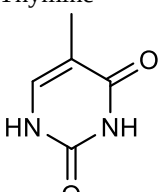
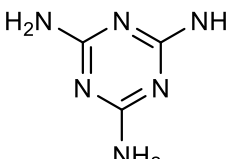
	Coformer (Cof)	Refcode ^{a)}	Stoichiometry	X, Y ^{c)}	n(H ₂ O ₂) ^{d)}	N ₁ ^{e)}	N ₂ ^{f)}	Contact Me-O _p , Å	Ref
Molecular organic compounds with a lone electron pair on nitrogen and/or oxygen atoms									
36	Lidocaine N-oxide 	KELXEH	Cof•3H ₂ O ₂	O,O	4	2; 2; 2; 2	0; 0; 2; 2		[29]
37	bis(dicyclohexylphosphino)ethane dioxide 	TOYTEJ	Cof•H ₂ O ₂	O,O	1	2	0		[30]
38	tris(4-methylphenyl)(oxo)- phosphine 	POMQEQ	Cof•H ₂ O ₂	O,O	1	2	0		[31]
39	tris(2-methylphenyl)(oxo)- phosphine 	POMQIU	Cof•H ₂ O ₂	O,O	1	2	0		

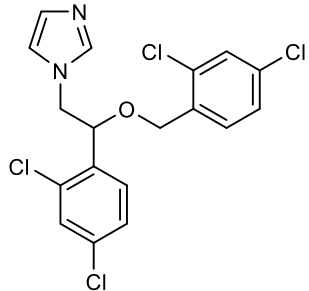
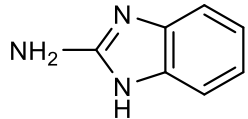
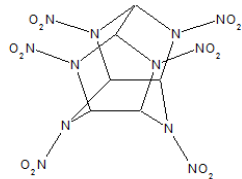
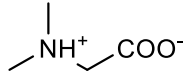
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40	bis(2-methylphenyl)(oxo)phenylphosphine 	POMQOA	Cof•H ₂ O ₂	O,O	1	2	0		
41	bis(tris(4-methylphenyl)(oxo)phosphine) 	POMQUG	Cof•0.5H ₂ O ₂	O,O	1	2	0		
42	(2-methylphenyl)(oxo)diphenylphosphine 	POMRAN	Cof•0.5H ₂ O ₂	O,O	1	2	0		
43	Tri-t-butylphosphine oxide 	BAFGOH	Cof•H ₂ O ₂	O,O	1	2	0		[32]
44	Triphenylphosphine oxide 	BAFJUQ, (TPPOPH) ^{g)}	Cof•1.5H ₂ O ₂	O,O	2	2; 2	0; 1		[32,33]

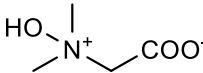
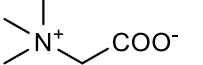
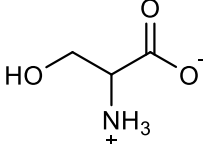
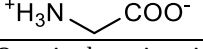
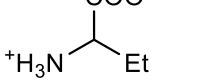
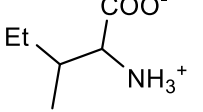
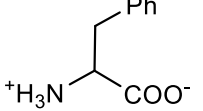
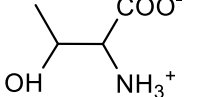
	Coformer (Cof)	Refcode ^{a)}	Stoichiometry	X,Y ^{c)}	n(H ₂ O ₂) ^{d)}	N ₁ ^{e)}	N ₂ ^{f)}	Contact Me-O _p , Å	Ref
45	Tricyclohexylphosphine oxide 	VANVOX	Cof•H ₂ O ₂	O,O	1	2	0		[34]
46	3,6-Di- <i>t</i> -butyl-1,8-dioxo-1,8-diphospha-1,1,8,8-tetra- <i>i</i> -propyl-4,5-diazaocta-3,5-diene 	XETSUK	Cof•2H ₂ O ₂	O,O	2	2; 2	0; 0		[35]
47	5,5'-dinitro-2H,2'H-3,3'-bi-1,2,4-triazole 	TUBNUC	Cof•0.4H ₂ O ₂ •0.2H ₂ O	N,N	1	2	2		[36]
48		TUBPOY	Cof•0.5H ₂ O ₂	N,N	1	2	2		
49	Risperidone N-oxide 	DATHIQ	Cof•H ₂ O ₂ •MeOH	O,O	1	2	0		[37]
50	1,2-dimethylimidazole 	DOJMIZ	Cof•0.5H ₂ O ₂	N,N	1	2	0		[38]

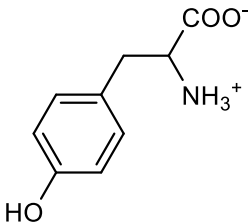
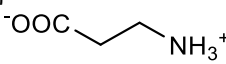
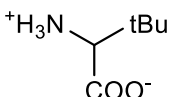
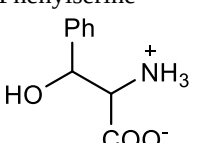
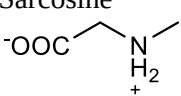
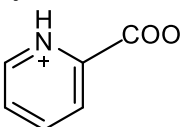
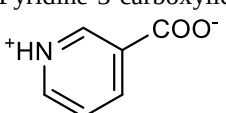
	Coformer (Cof)	Refcode ^{a)}	Stoichiometry	X, Y ^{c)}	n(H ₂ O ₂) ^{d)}	N ₁ ^{e)}	N ₂ ^{f)}	Contact Me-O _p , Å	Ref
51	1,4-Diazabicyclo(2.2.2)octane N,N'-dioxide 	FURFIH	Cof•3H ₂ O ₂	O,O	2	2; 2	0; 0		[39]
52	(Z)-N-benzylidene-1-phenylmethanamine oxide 	JELQOJ	Cof•H ₂ O ₂	O,O	1	2	0		[40]
53	2,2'-Disulfanediylbis(pyridine N-oxide) 	JESXEN	Cof•H ₂ O ₂	O,O	1	2	0		[41]
54	Caffeine 	KUMRER	Cof•0.5H ₂ O ₂	N,N	1	2	0		^{h)}
55	(3aS,6R,7aS)-2-Acetyl-3,3,6-trimethyloctahydro-indazole 	MUXHIX	Cof•H ₂ O ₂	N,O	1	2	0		[42]

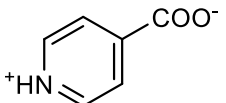
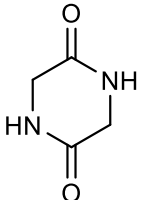
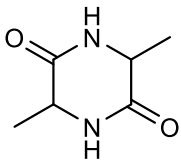
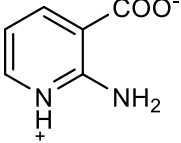
	Coformer (Cof)	Refcode ^{a)}	Stoichiometry	X, Y ^{c)}	n(H ₂ O ₂) ^{d)}	N ₁ ^{e)}	N ₂ ^{f)}	Contact Me-O _p , Å	Ref
56	1,4-diazabicyclo-(2.2.2)-octane 	QOHXUH	Cof•2H ₂ O ₂	N,O	1	2	1		[43]
57	2-(2-(Dimethylamino)-ethylmethylamino)-1,3,5-trimethyl-1,3,5-triaza-2-oxo-2λ ⁵ -phosphorinane-4,6-dione 	RIKJAW	Cof•H ₂ O ₂	N,O	1	2	0		[44]
58	2,3,5,6-tetrakis(pyridin-2-yl)pyrazine 	SEM XIU	Cof•4.75H ₂ O ₂	O,O	6	2; 2; 2; 2; 2; 2	0; 0; 0; 1; 2; 2		[45]
59	2,6-bis-(Diphenyl-phosphoryl)-pyridine 	UKEFEV	Cof•H ₂ O ₂	O,O	1	2	0		[46]

	Coformer (Cof)	Refcode ^{a)}	Stoichiometry	X,Y ^{c)}	n(H ₂ O ₂) ^{d)}	N ₁ ^{e)}	N ₂ ^{f)}	Contact Me-O _p , Å	Ref
60	Urea, 	UREXPO11, 26444 (UREXPO) ^{g)} UREXPO01	Cof•H ₂ O ₂	O,O	1	2	4		[47,48]
61	Bis(cyclohexyl)amine 	VAYGUY	Cof•0.5H ₂ O ₂	N,N	1	2	0		^{h)}
		VAYGUY01	--/--	--/--	--/--	--/--	--/--		[49]
62	Adenine 	JOZZED	Cof•H ₂ O ₂	N,N	1	2	2		[50]
63	Thymine 	WINSAO	Cof•(0.55H ₂ O ₂ •0.45H ₂ O)	O,O	1	2	1		[51]
64		WINSAO01	Cof•(0.78H ₂ O ₂ •0.22H ₂ O)	--/--	--/--	--/--	--/--	--/--	[52]
65		YAFGEU	Cof•H ₂ O ₂	--/--	--/--	--/--	--/--		
66	Melamine 	YAFFUJ	Cof•H ₂ O ₂	N,N	1	2	4		

	Coformer (Cof)	Refcode ^{a)}	Stoichiometry	X, Y ^{c)}	n(H ₂ O ₂) ^{d)}	N ₁ ^{e)}	N ₂ ^{f)}	Contact Me-O _p , Å	Ref
67	1-{2-(2,4-dichlorophenyl)-2-[(2,4-dichlorophenyl)methoxy]ethyl}-1H-imidazole 	UDUROD	Cof•0.5H ₂ O ₂	N,N	1	2	0		[53]
68	2-aminobenzimidazole 	OHIJEX	2Cof•H ₂ O ₂	N,N	1	2	4		[54]
69	2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane 	AZACIP, AZAMIZ, AZAMIZ01	Cof•0.5H ₂ O ₂	O,O	1	2	0		[55]
Amino acids, peptides and related zwitterions									
70	N,N-dimethylglycine 	BONGES	Cof•H ₂ O ₂	O,O	1	2	0		[56]

	Coformer (Cof)	Refcode ^{a)}	Stoichiometry	X, Y ^{c)}	n(H ₂ O ₂) ^{d)}	N ₁ ^{e)}	N ₂ ^{f)}	Contact Me-O _p , Å	Ref
71	N,N,N-hydroxy-dimethylglycine 	BONGIW	Cof•H ₂ O ₂	O,O	1	2	0		
72	N,N,N-trimethylglycine (betaine) 	MEXTIU	Cof•(0.76H ₂ O ₂ •0.24H ₂ O)	O,O	1	2	0	100 K	[57]
		MEXTIU01	Cof•(0.77H ₂ O ₂ •0.23H ₂ O)	--/--	--/--	--/--	--/--	295 K	
73	L-serine 	KULMOU, KULMOU01	Cof•H ₂ O ₂	O,O	1	2	1		[58,59]
74		UDUWEX	Cof•(0.91H ₂ O ₂ •0.09H ₂ O)	--/--	--/--	--/--	--/--		^{h)}
75	Glycine 	KULMUA, KULMUA01	Cof•1.5H ₂ O ₂	O,O	3	2; 2; 2	1; 2; 2		[58,59]
76	2-aminobutyric acid 	TANCAO	Cof•1.5H ₂ O ₂	O,O	3	2; 2; 2	1; 1; 2		[59]
77	L-isoleucine 	TANCES	Cof•H ₂ O ₂ •0.5H ₂ O	O,O	1	2	2		
78		TANDET	Cof•H ₂ O ₂	O,O	1	2	1-bifur		
79	L-phenylalanine 	TANCIW	Cof•H ₂ O ₂ •0.5H ₂ O	O,O	1	2	2		
80		UDUWIB	Cof•H ₂ O ₂ •(0.43H ₂ O ₂ •0.07H ₂ O)	O,O	2	2; 2	0; 2		^{h)}
81	L-threonine 	TANCOC	Cof•H ₂ O ₂	O,O	1	2	3		[59]

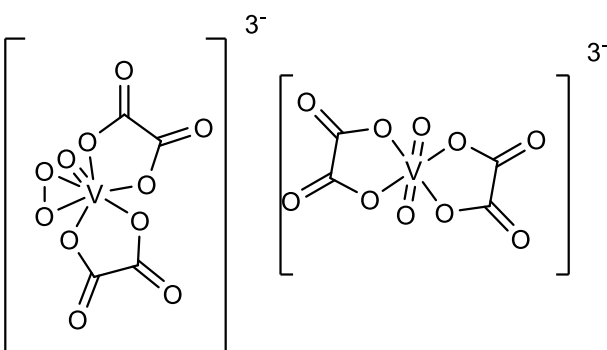
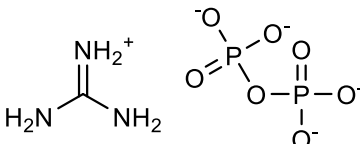
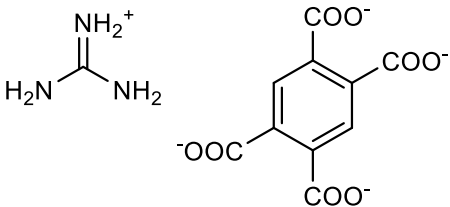
	Coformer (Cof)	Refcode ^{a)}	Stoichiometry	X, Y ^{c)}	n(H ₂ O ₂) ^{d)}	N ₁ ^{e)}	N ₂ ^{f)}	Contact Me-O _p , Å	Ref
82	L-tyrosine 	TANCUI	Cof•2H ₂ O ₂	O,O	2	2; 2	0; 1		
83	β-alanine 	TANDAP	Cof•2H ₂ O ₂	O,O	2	2; 2	0; 2		
84	L-tert-Leucine 	OJOCOH	Cof•H ₂ O ₂ •0.5H ₂ O	O,O	1	2	2		
85	Phenylserine 	VILGAB	Cof•H ₂ O ₂	O,O	1	2	2	H ₂ O ₂ chains	[60]
86	Sarcosine 	VILFUU	Cof•H ₂ O ₂	O,O	3	2; 2; 2	1; 1; 1		
87	Pyridine-2-carboxylic acid 	ANINES	Cof•H ₂ O ₂	O,O	1	2	1		[61]
88	Pyridine-3-carboxylic acid 	ANINAO	Cof•H ₂ O ₂	O,O	1	2	0		

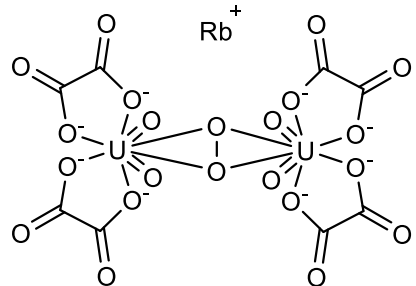
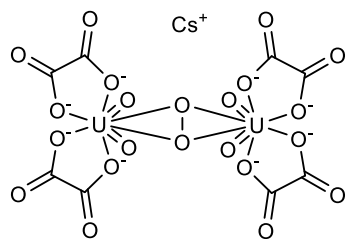
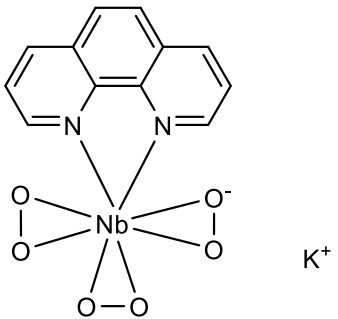
	Coformer (Cof)	Refcode ^{a)}	Stoichiometry	X, Y ^{c)}	n(H ₂ O ₂) ^{d)}	N ₁ ^{e)}	N ₂ ^{f)}	Contact Me-O _p , Å	Ref
89	Pyridine-4-carboxylic acid 	ANIMUH	Cof•2H ₂ O ₂	O,O	2	2; 2	0; 1		
90	Cyclo-diglycine, 	HOQRUD	Cof•1.786H ₂ O ₂ •0.214H ₂ O	O,O	1	2	1-bifur		[62]
91		HOQSAK	Cof•2H ₂ O ₂	O,O	1	2	1-bifur		
92		HOQSEO	Cof•H ₂ O ₂	O,O	1	2	0		
93	Cyclo-dialanine, 	HOQSIG	Cof•2H ₂ O ₂	O,O	2	2; 2	1; 1		
94	2- aminonicotinic acid, 	KELXAD	Cof•1.5H ₂ O ₂	O,O	6	2; 2; 2; 2; 2; 2	1; 1; 1; 1; 1- bifur; 2		[29]

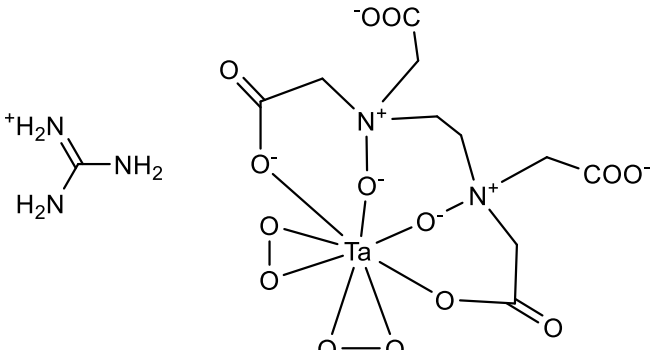
^{a)} Alphanumeric refcodes corresponds to Cambridge Structural Database (CSD); numeric refcodes corresponds to Inorganic Crystal Structure Database (ICSD).

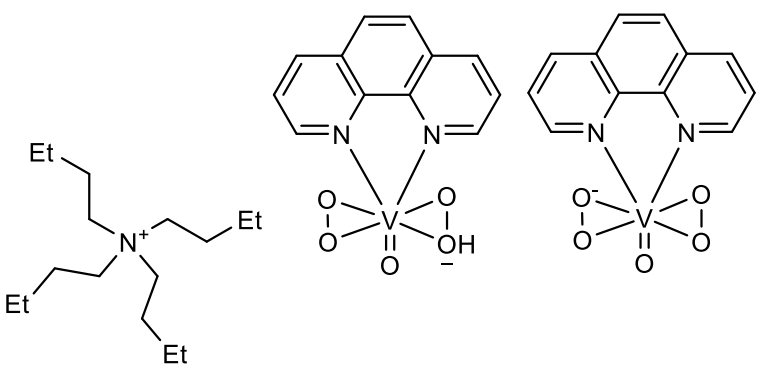
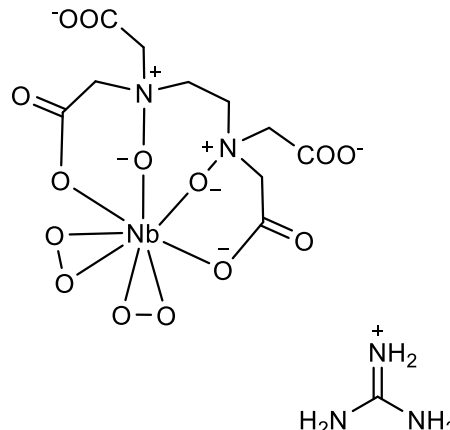
- b) Parenthesis denotes one crystallographical position occupied by both H_2O_2 and H_2O .
- c) X and Y are atoms with electron lone pair in $\text{X}\cdots\text{HOOH}\cdots\text{Y}$ fragment.
- d) Number of crystallographically independent H_2O_2 molecules.
- e) Number of H-bonds formed by H_2O_2 molecule as proton donor. If there are two or more crystallographically independent H_2O_2 molecules, than values are separated by commas.
- f) Number of H-bonds formed by H_2O_2 molecule as proton acceptor. If there are two or more crystallographically independent H_2O_2 molecules, than values are separated by commas.
- g) This structure has duplicate without localized protons.
- h) CSD Communication (Private communication).

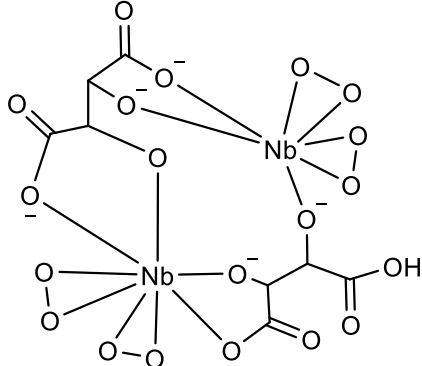
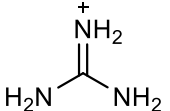
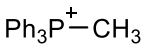
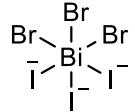
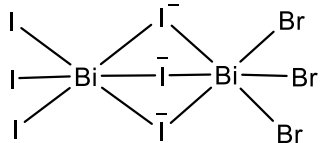
Table S2. Refcodes of proton disordered peroxosolvates.

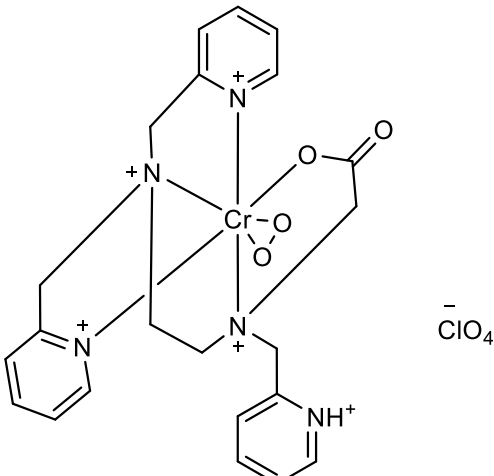
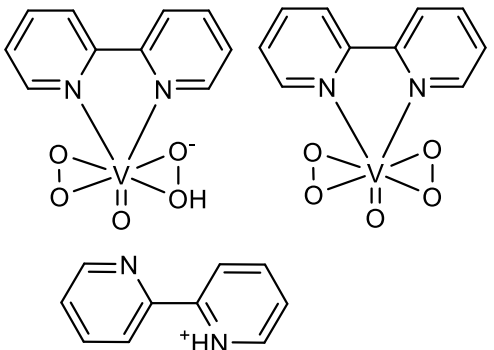
	Coformer (Cof)	Refcode ^{a)}	Stoichiometry	Comments	Ref
Salts of inorganic and carboxylic acids					
1	Potassium bis(oxalato)peroxo-vanadate(V), K^+ 	FAPJEL, 109697	Cof•(0.1H ₂ O ₂ •0.4H ₂ O)	Not localized ^{b)}	[63]
2	Guanidinium diphosphate, 	GUOPYQ, 2247	Cof•H ₂ O ₂ •1.5H ₂ O	Not localized	[64]
3	Guanidinium pyromellitate, 	GUPMEL	Cof•3H ₂ O ₂	Not localized	[65]
4		GUPYML	Cof•H ₂ O ₂ •3H ₂ O	Not localized	[66]

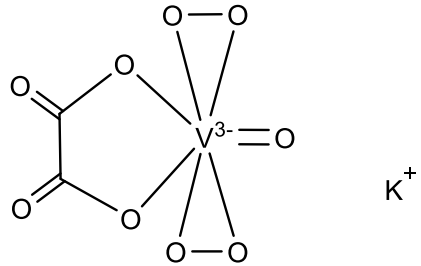
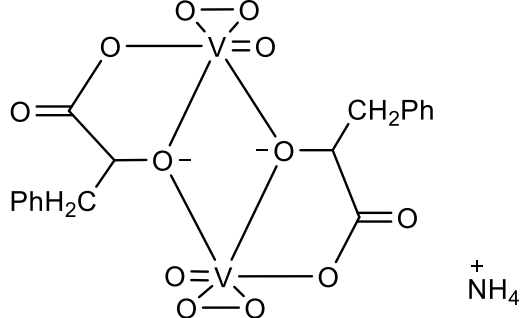
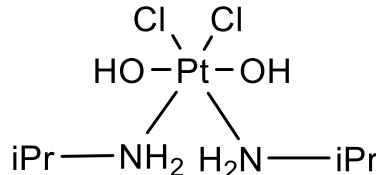
	Coformer (Cof)	Refcode ^{a)}	Stoichiometry	Comments	Ref
5	Hexarubidium (μ_2 -peroxo)-tetrakis(oxalato-O,O')-tetraoxo-diuranium(VI), 	IGIHU	Cof•3H ₂ O ₂ •4H ₂ O	Not localized	[67]
6	Hexacaesium (μ_2 -peroxo)-tetrakis(oxalato-O,O')-tetraoxo-diuranium(VI), 	IGIJAL	Cof•3H ₂ O ₂ •4H ₂ O	Not localized	
7	Potassium triperoxo-(o-phenanthroline)-niobium(potassium triperoxo-(o-phenanthroline)-niobium(V)) 	OPHENB10	Cof•H ₂ O ₂ •3H ₂ O	Not localized	[68]

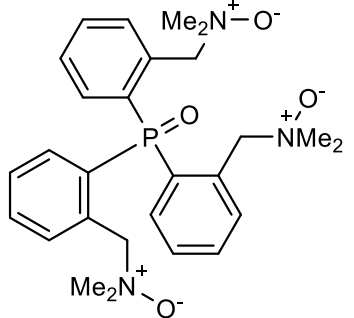
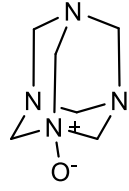
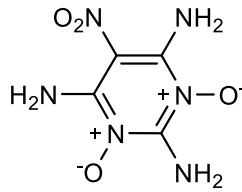
	Coformer (Cof)	Refcode ^{a)}	Stoichiometry	Comments	Ref
8	Rubidium oxalate, $\text{Rb}_2\text{C}_2\text{O}_4$	RBOXPH10	$\text{Cof} \cdot \text{H}_2\text{O}_2$	Not localized	[6]
9	Dirubidium dodecahydroxo-closododecaborate, $\text{Rb}_2(\text{B}_{12}(\text{OH})_{12})$	181873	$\text{Cof} \cdot 2\text{H}_2\text{O}_2$	Short Op-Op distance (1.259 Å)	[69]
10	Trisodium tetraperoxovanadate, $\text{Na}_3(\text{V}(\text{O}_2)_4)$	81292	$\text{Cof} \cdot \text{H}_2\text{O}_2 \cdot 10.5\text{H}_2\text{O}$	Not localized	[70]
11	Dibarium silicododecatungstate, $\text{Ba}_2(\text{SiW}_{12}\text{O}_{40})$	161719	$\text{Cof} \cdot 4\text{H}_2\text{O}_2 \cdot 11\text{H}_2\text{O}$	Not localized	[71]
12	Hexapotassium dodecafluorotriperoxotrizirconate, $\text{K}_6(\text{Zr}_3\text{F}_{12}(\text{O}_2)_3)$	80814	$\text{Cof} \cdot 2\text{H}_2\text{O}_2 \cdot \text{H}_2\text{O}$	Not localized	[72]
13	Potassium octafluorodiperoxodititanate, $\text{K}_4(\text{Ti}_2\text{F}_8(\text{O}_2)_2)$	68668	$\text{Cof} \cdot \text{H}_2\text{O}_2$	Not localized	[73]
14	Strontium peroxide, $\alpha\text{-SrO}_2$	24764	$\text{Cof} \cdot 2\text{H}_2\text{O}_2$	Not localized	[74]
15	Strontium peroxide, $\beta\text{-SrO}_2$	24765	$\text{Cof} \cdot 2\text{H}_2\text{O}_2$	Not localized	
16	Barium peroxide, $\alpha\text{-BaO}_2$	24776	$\text{Cof} \cdot 2\text{H}_2\text{O}_2$	Not localized	[75]
17	Barium peroxide, $\beta\text{-BaO}_2$	24777	$\text{Cof} \cdot 2\text{H}_2\text{O}_2$	Not localized	
18	Barium peroxide, $\gamma\text{-BaO}_2$	24778	$\text{Cof} \cdot 2\text{H}_2\text{O}_2$	Not localized	
19	Barium peroxide, BaO_2	24779	$\text{Cof} \cdot \text{H}_2\text{O}_2$	Not localized	[76]
20		44406	$\text{Cof} \cdot \text{H}_2\text{O}_2 \cdot 2\text{H}_2\text{O}$	Not localized	[75]
21	tris(Guanidinium) (ethylenediaminetetra-acetato N,N'-dioxide)-bis(peroxo)-tantalum(V) hydrogenperoxide solvate hydrate, 	ABUNUH	$\text{Cof} \cdot (0.68\text{H}_2\text{O}_2 \cdot 0.32\text{H}_2\text{O}) \cdot 2\text{H}_2\text{O}$	Not localized	[77]

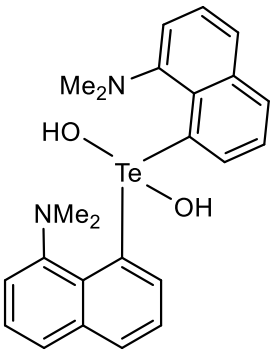
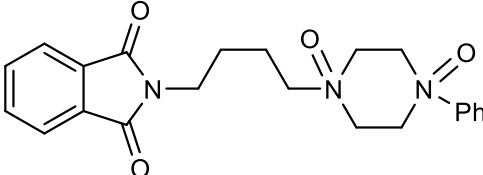
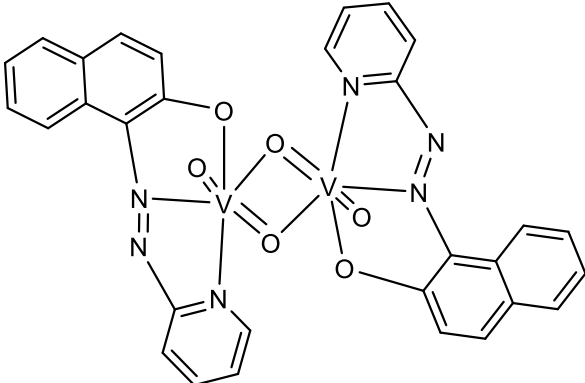
	Coformer (Cof)	Refcode ^{a)}	Stoichiometry	Comments	Ref
22	Tetrabutylammonium (hydrogen peroxo)-(peroxo)-oxo-(1,10-phenanthroline)-vanadium bis(peroxo)-(oxo)-(1,10-phenanthroline)-vanadium, 	CELNIS	Cof•3H ₂ O ₂ •H ₂ O	Short Op-Op distance (1.340 Å, 1.382 Å)	[78]
23	tris(Guanadinium) (N,N'-dioxido-ethylenediaminetetraacetato)-bis(peroxo)-niobium(V), 	XUVRIP	Cof•H ₂ O ₂ •3H ₂ O	Not localized	[79]

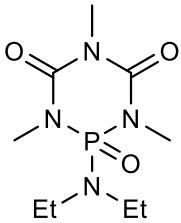
	Coformer (Cof)	Refcode ^{a)}	Stoichiometry	Comments	Ref
24	pentakis(Guanidinium)(μ_2-tartrato)-(μ_2-hydrogen tartrato)-tetrakis(peroxo)-di-niobium(V),  	RASBAP	Cof•H ₂ O ₂ •6H ₂ O	Not localized	[80]
25	hexakis(Triphenyl(methyl)phosphonium) triiodo-tribromo-bismuth tris(μ_2-iodo)-triiodo-tribromo-di-bismuth,   	NAJMES	Cof•H ₂ O ₂	Peroxide H atom positions determined incorrectly.	[81]
26	tris(Tetra-n-butylammonium) (m12-arsenato)-tetracosakis(m2-oxo)-dodecaoxo-dodeca-molybdenum, (C₁₆H₃₆N)₃[AsMo₁₂O₄₀]	LUGSIP	Cof•0.5H ₂ O ₂	Short Op-Op distance (1.292 Å). Peroxide H atom positions determined incorrectly.	[82]

	Coformer (Cof)	Refcode ^{a)}	Stoichiometry	Comments	Ref
27	((2-(bis(Pyridin-2-ylmethyl)amino)ethyl)(pyridinium-2-ylmethyl)amino)acetato)-(peroxo-O,O')-chromium(IV) diperchlorate, 	LUCJEA	Cof•3H ₂ O ₂ •H ₂ O	Angle Op-Op-H=75.5°	[83]
28	2,2'-Bipyridinium bis((2,2'-bipyridine)-oxo-diperoxo-vanadium), 	CEYXOT	Cof•0.5H ₂ O ₂ •5.5H ₂ O	Not localized	[84]

	Coformer (Cof)	Refcode ^{a)}	Stoichiometry	Comments	Ref
29	Tripotassium (oxalato-O,O')-oxo-bis(peroxo)-vanadium perhydrate 	CIBBOE	Cof•2H ₂ O ₂	Not localized	[85]
30	Tetra-ammonium (μ₂-(R)-3-phenyllactato-O,O,O')-(μ₂-(S)-3-phenyllactato-O,O,O')-bis(oxo-(peroxo-O,O')-vanadium(V)) methanol solvate bis(hydrogen peroxide) dihydrate 	YATTIX	Cof•2H ₂ O ₂ •2CH ₃ OH•2H ₂ O	Not localized	[86]
31	cis,trans-Dichloro-dihydroxy-bis(isopropylamine)-platinum(IV), 	CAXCAF	Cof•0.5H ₂ O ₂	Not localized	[87]
32	Trans-diammine-trans-dichloro-trans-dihydroxoplatinum(IV), PtCl₂(NH₃)₂(OH)₂	49991	Cof•H ₂ O ₂	Not localized	[88]

	Coformer (Cof)	Refcode ^{a)}	Stoichiometry	Comments	Ref
Molecular organic compounds with a lone electron pair on nitrogen and/or oxygen atoms					
33	Tris(2-(oxy-N,N-dimethylammoniomethyl)phenyl)phosphine oxide, 	EKULUR	Cof•4H ₂ O ₂ •1.5H ₂ O	Not localized	[89]
34	Hexamethylenetetramine-oxide 	HMTXOH	Cof•H ₂ O ₂ •H ₂ O	Not localized	[90]
35	2,4,6-triamino-5-nitropyrimidine-1,3-dioxide, 	HOJCAN	Cof•0.5H ₂ O ₂	Not localized	[91]

	Coformer (Cof)	Refcode ^{a)}	Stoichiometry	Comments	Ref
36	8,8'-(dihydroxy-tellanediyl)bis(N,N-dimethylnaphthalen-1-amine), 	MAQRIH	Cof•H ₂ O ₂ •H ₂ O	Not localized	[92]
37	1-Phenyl-4-(4-phthalimidobutyl)piperazine-1,4-dioxide, 	ROLPAJ	Cof•H ₂ O ₂ •(0.6H ₂ O ₂ •0.4 H ₂ O)	Not localized	[93]
38	bis((1-(2-Pyridylazo)-2-naphtholato-O,N,N')-(μ₂-oxo)-oxo-vanadium(V)), 	VAYMAJ	Cof•H ₂ O ₂	Not localized	[94]

	Coformer (Cof)	Refcode ^{a)}	Stoichiometry	Comments	Ref
39	2-Diethylamino-1,3,5-trimethyl-1,3,5-triaza-2-oxo-2 λ^5 -phosphinane-4,6-dione, 	YECTOP	Cof•0.5H ₂ O ₂	Not localized	[95]
Others					
40	Water, H ₂ O	24073	2Cof•H ₂ O ₂	Not localized	[96]

^{a)} Alphanumeric refcodes corresponds to Cambridge Structural Database (CSD); numeric refcodes corresponds to Inorganic Crystal Structure Database (ICSD).

^{b)} Peroxide H atom positions were not determined.

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