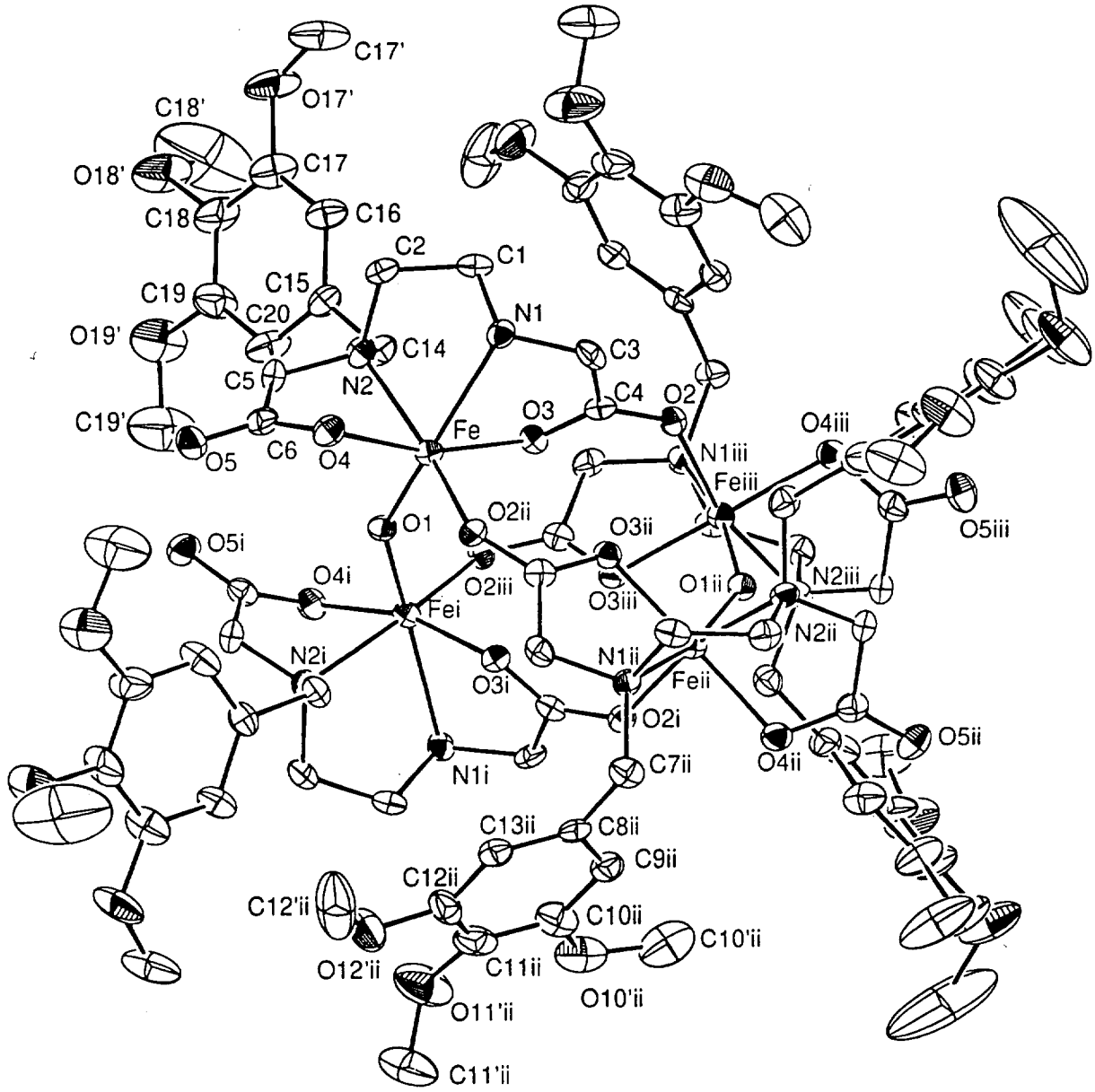

Table S1 . Crystallographic experimental details

I.Crystal data

Formula: $[Fe_4\ (\mu\text{-}O)_2(C_{26}H_{34}N_2O_{10})_4]\ 10\ H_2O$
Fw: 2563.68
Crystal system: tetragonal — Space group: $I4_1/a$
a= 21.006(16)Å — V= 13203(17)Å^3
b= 21.006(16)Å — Z(units/cell)=4
c= 29.923(22)Å — D_x= 1.285 g/cm^3
Cell parameters from 23 reflections — θ = 10-15°
F(000)=5384
Linear absorption factor(λMoKα): — μ=0.518 mm^{-1}
Morphology: — Octahedron, dark red
Crystal dimensions: — 0.20x 0.20X 0.30 mm

II. Intensity measurements

Temperature: — 293K
Diffractometer: — 4 circle Nicolet XRD
Monochromator: — graphite (220)
Radiation: — λ(MoKa)=0.71073Å
Scan mode: — ω scan
Scan width: — 1.2°
Data collection limits: — 3°≤ 2θ ≤50°
(0≤h≤25, 0≤k≤25, 0≤l≤35)

5689 mesured reflections — 5666 independent reflections
3 standard reflections — monotored every 200 reflections

III.Structure determination and refinement:

Solved by Patterson procedure — SHELXS-86
Refinement on F^2 — SHELXL-93
R(F)=0.109[for 2171 F> 4 σ(F)] — $(\Delta/\sigma)_{max}$ = 0.063
$wR(F^2)$=0.292 — $\Delta\rho_{max}$ = 0.52 e.Å^{-3}
S=1.152 — $\Delta\rho_{max}$ = -0.32 e.Å^{-3}
Number of reflections: 5666 — Refined parameters: 382

Calculated weights: $w = 1/[\sigma^2(Fo^2) + (0.035P)^2 + 221.077P]$
where $P = (Fo^2 + 2\ Fc^2)/3$

Table S2 :

Atomic positions and equivalent thermal parameters U_{eq} ($Å^2$) for non-hydrogen atoms with their estimated standard deviations.

Atoms	x	y	z	U_{eq}	s.o.f.
Fe	0.57982(8)	0.26158(8)	0.29688(6)	0.0360(5)	
O1	0.5000	0.2500	0.2778(4)	0.039(3)	0.5
N1	0.6723(4)	0.3074(5)	0.3256(3)	0.039(2)	
C1	0.6725(5)	0.3722(5)	0.3046(4)	0.043(3)	
C2	0.6548(6)	0.3679(6)	0.2560(4)	0.044(3)	
N2	0.5880(4)	0.3436(5)	0.2510(3)	0.040(3)	
C3	0.6595(5)	0.3137(6)	0.3741(4)	0.042(3)	
C4	0.5896(6)	0.3253(5)	0.3821(4)	0.039(3)	
O2	0.5728(4)	0.3401(3)	0.4209(3)	0.038(2)	
O3	0.5522(4)	0.3173(3)	0.3492(3)	0.037(2)	
C5	0.5794(6)	0.3134(6)	0.2074(4)	0.044(3)	
C6	0.6022(6)	0.2445(6)	0.2073(5)	0.043(3)	
O4	0.6259(4)	0.2239(4)	0.2441(3)	0.046(2)	
O5	0.5994(4)	0.2136(4)	0.1722(3)	0.057(3)	
C7	0.7377(5)	0.2787(6)	0.3171(4)	0.047(3)	
C8	0.7488(6)	0.2160(7)	0.3404(5)	0.049(3)	
C9	0.7274(6)	0.1586(7)	0.3218(5)	0.053(4)	
C10	0.7365(7)	0.1017(8)	0.3447(6)	0.063(4)	
O10'	0.7151(6)	0.0438(6)	0.3305(5)	0.095(4)	
C10'	0.6878(9)	0.0410(8)	0.2868(7)	0.107(7)	
C11	0.7709(7)	0.1006(9)	0.3851(6)	0.073(5)	
O11'	0.7746(6)	0.0460(6)	0.4095(5)	0.130(6)	
C11'	0.8330(10)	0.0164(10)	0.4099(8)	0.155(10)	
C12	0.7952(7)	0.1586(9)	0.4022(5)	0.069(5)	
O12'	0.8280(6)	0.1543(7)	0.4408(4)	0.102(4)	
C12'	0.8598(9)	0.2111(12)	0.4577(7)	0.144(10)	
C13	0.7832(6)	0.2150(7)	0.3794(5)	0.059(4)	
C14	0.5390(6)	0.3940(6)	0.2593(4)	0.047(3)	
C15	0.5300(6)	0.4429(6)	0.2244(4)	0.049(3)	
C16	0.5717(6)	0.4936(6)	0.2177(5)	0.058(4)	
C17	0.5614(7)	0.5385(7)	0.1848(6)	0.069(5)	
O17'	0.6004(6)	0.5888(5)	0.1765(4)	0.098(4)	
C17'	0.6614(8)	0.5902(7)	0.1980(7)	0.108(7)	
C18	0.5081(8)	0.5333(7)	0.1577(6)	0.075(5)	
O18'	0.4963(6)	0.5777(6)	0.1242(5)	0.117(5)	
C18'	0.4584(18)	0.6352(13)	0.1431(14)	0.347(30)	
C19	0.4661(8)	0.4834(8)	0.1646(6)	0.080(5)	
O19'	0.4114(6)	0.4846(6)	0.1371(5)	0.116(5)	
C19'	0.3623(10)	0.4410(10)	0.1467(8)	0.166(12)	
C20	0.4750(7)	0.4382(7)	0.1975(5)	0.067(4)	

Table S3 :

Atomic positions, isotropic thermal parameters U_{iso} ($Å^2$) for hydrogen atoms with their estimated standard deviations. The hydrogens were calculed and refined with a riding model for the positional parameters and with isotropic thermal parameters ($U(H)=1.5U_{eq}$ (C) for the methyl hydrogen atoms and $U(H) = 1.2U_{eq}$ (C) for the aromatic hydrogen atoms and methylene hydrogen atoms).

Atoms	x	y	z	Uiso
H1A	0.7144(5)	0.3910(5)	0.3074(4)	0.052
H1B	0.6424(5)	0.3995(5)	0.3200(4)	0.052
H2A	0.6582(6)	0.4097(6)	0.2424(4)	0.053
H2B	0.6840(6)	0.3395(6)	0.2408(4)	0.053
H3A	0.6840(5)	0.3489(6)	0.3861(4)	0.050
H3B	0.6725(5)	0.2751(6)	0.3893(4)	0.050
H5A	0.6028(6)	0.3372(6)	0.1850(4)	0.052
H5B	0.5346(6)	0.3146(6)	0.1994(4)	0.052
H7A	0.7431(5)	0.2727(6)	0.2852(4)	0.056
H7B	0.7699(5)	0.3088(6)	0.3270(4)	0.056
H9	0.7071(6)	0.1586(7)	0.2942(5)	0.063
H10A	0.6746(9)	-0.0018(8)	0.2806(7)	0.160
H10B	0.7189(9)	0.0541(8)	0.2652(7)	0.160
H10C	0.6517(9)	0.0688(8)	0.2854(7)	0.160
H11A	0.8307(10)	-0.0213(10)	0.4279(8)	0.232
H11B	0.8643(10)	0.0448(10)	0.4221(8)	0.232
H11C	0.8447(10)	0.0052(10)	0.3799(8)	0.232
H12A	0.8811(9)	0.2012(12)	0.4852(7)	0.217
H12B	0.8289(9)	0.2439(12)	0.4629(7)	0.217
H12C	0.8904(9)	0.2257(12)	0.4362(7)	0.217
H13	0.7989(6)	0.2531(7)	0.3908(5)	0.071
H14A	0.4985(6)	0.3731(6)	0.2642(4)	0.056
H14B	0.5501(6)	0.4157(6)	0.2869(4)	0.056
H16	0.6074(6)	0.4973(6)	0.2359(5)	0.069
H17A	0.6839(8)	0.6281(7)	0.1892(7)	0.162
H17B	0.6855(8)	0.5534(7)	0.1893(7)	0.162
H17C	0.6557(8)	0.5901(7)	0.2298(7)	0.162
H18A	0.4506(18)	0.6654(13)	0.1197(14)	0.521
H18B	0.4825(18)	0.6552(13)	0.1665(14)	0.521
H18C	0.4185(18)	0.6206(13)	0.1550(14)	0.521
H19A	0.3281(10)	0.4467(10)	0.1258(8)	0.249
H19B	0.3468(10)	0.4482(10)	0.1765(8)	0.249
H19C	0.3784(10)	0.3984(10)	0.1444(8)	0.249
H20	0.4456(7)	0.4057(7)	0.2019(5)	0.080

Table S4 : Anisotropic thermal parameters of non-hydrogen atoms

Atoms	U11	U22	U33	U23	U13	U12
Fe	0.0331(10)	0.0354(11)	0.0396(9)	0.0017(9)	0.0029(9)	-0.0015(8)
O1	0.030(6)	0.045(7)	0.041(7)	0.000	0.000	-0.003(5)
N1	0.030(6)	0.050(7)	0.038(6)	0.002(5)	0.005(5)	0.001(5)
C1	0.031(7)	0.035(7)	0.064(10)	0.005(7)	0.003(7)	-0.005(5)
C2	0.043(8)	0.040(8)	0.050(8)	0.007(6)	0.013(7)	-0.006(6)
N2	0.037(6)	0.043(6)	0.040(6)	-0.001(5)	0.007(5)	0.006(5)
C3	0.039(8)	0.039(7)	0.046(8)	-0.004(6)	-0.018(6)	-0.005(6)
C4	0.036(8)	0.031(7)	0.048(9)	0.005(6)	0.006(7)	-0.006(6)
O2	0.042(5)	0.037(5)	0.036(5)	-0.006(4)	0.002(4)	-0.002(4)
O3	0.037(5)	0.034(5)	0.040(5)	-0.002(4)	-0.004(4)	0.002(4)
C5	0.052(8)	0.052(8)	0.027(7)	-0.001(6)	0.001(6)	0.002(6)
C6	0.036(7)	0.046(8)	0.048(8)	0.002(8)	0.010(7)	-0.004(6)
O4	0.044(5)	0.046(5)	0.048(6)	0.005(4)	0.006(5)	0.005(4)
O5	0.063(6)	0.058(6)	0.051(6)	-0.017(5)	0.006(5)	-0.009(5)
C7	0.027(7)	0.053(8)	0.061(9)	0.009(7)	0.006(6)	-0.003(6)
C8	0.031(7)	0.067(10)	0.050(9)	-0.007(8)	0.012(7)	0.017(7)
C9	0.049(9)	0.058(9)	0.051(9)	0.002(8)	0.012(7)	0.009(7)
C10	0.043(9)	0.059(11)	0.087(13)	0.014(10)	0.007(9)	-0.003(8)
O10'	0.081(9)	0.074(9)	0.130(11)	0.005(9)	0.021(8)	0.010(7)
C10'	0.115(17)	0.069(13)	0.137(19)	-0.025(13)	0.037(15)	-0.028(11)
C11	0.045(10)	0.078(13)	0.096(14)	0.023(11)	0.023(10)	0.017(9)
O11'	0.109(11)	0.104(10)	0.177(14)	0.082(10)	0.035(10)	0.031(8)
C11'	0.152(21)	0.131(20)	0.181(25)	0.025(18)	-0.007(19)	0.085(18)
C12	0.039(9)	0.112(15)	0.056(10)	0.032(11)	0.009(8)	0.022(9)
O12'	0.085(9)	0.148(13)	0.073(9)	0.022(8)	-0.012(7)	0.031(9)
C12'	0.086(15)	0.262(31)	0.086(15)	0.030(19)	-0.027(13)	-0.049(18)
C13	0.049(9)	0.074(11)	0.055(10)	0.003(8)	0.014(8)	0.022(8)
C14	0.055(9)	0.040(8)	0.044(8)	0.005(7)	0.013(7)	-0.002(6)
C15	0.053(9)	0.044(8)	0.049(8)	0.013(7)	0.005(7)	0.005(7)
C16	0.050(9)	0.040(8)	0.083(11)	0.007(8)	0.016(8)	0.000(7)
C17	0.053(10)	0.050(9)	0.105(14)	0.030(9)	0.000(9)	0.014(8)
O17'	0.087(9)	0.064(7)	0.145(11)	0.056(7)	-0.001(8)	-0.023(7)
C17'	0.080(13)	0.061(11)	0.183(21)	0.035(13)	-0.004(14)	-0.023(10)
C18	0.081(12)	0.053(10)	0.091(13)	0.044(9)	-0.011(10)	0.002(9)
O18'	0.111(10)	0.081(9)	0.160(13)	0.078(9)	-0.041(9)	-0.014(8)
C18'	0.409(57)	0.135(26)	0.498(66)	0.168(36)	-0.293(53)	-0.064(33)
C19	0.070(11)	0.073(12)	0.097(14)	0.024(10)	-0.036(10)	-0.014(9)
O19'	0.108(10)	0.091(9)	0.149(12)	0.063(9)	-0.063(9)	-0.012(8)
C19'	0.119(19)	0.147(21)	0.230(29)	0.098(21)	-0.100(19)	-0.042(17)
C20	0.052(9)	0.058(9)	0.091(12)	0.028(9)	0.009(9)	-0.002(7)
O6	0.079(33)	0.211(50)	0.090(15)	-0.048(27)	0.029(19)	-0.094(22)

Atomic positions, equivalent thermal parameters U_{eq} ($Å^2$) or isotropic thermal parameters U_{iso} ($Å^2$) and site occupaction factors (s.o.f.) for water molecule solvents with their estimated standard deviations.

Atoms	**x**	**y**	**z**	**U_{eq}**	**s.o.f.**
O6	0.5088(30)	0.2600(40)	0.1108(7)	0.126(15)	0.5
Atoms	**x**	**y**	**z**	**U_{iso}**	**s.o.f.**
O7	0.4230(62)	0.4168(58)	0.0221(43)	0.546(80)	0.5
O8	0.3745(33)	0.3954(31)	0.0146(22)	0.309(31)	0.5
O9	0.5149(44)	0.5404(43)	0.0475(33)	0.517(52)	0.5
O10	0.4822(34)	0.3792(32)	0.0504(23)	0.360(33)	0.5

Table S5 : Bond distances (Å) and their e.s.d

Fe	Fe^{i}	3.389(4)	O1	Fe^{i}	1.788(4)
Fe	Fe^{ii}	5.253(5)	O2	Fe^{iii}	2.028(8)
Fe	Fe^{iii}	5.253(5)	N1	C3	1.482(14)
Fe	O1	1.788(4)	N1	C1	1.500(14)
Fe	O4	2.014(8)	N1	C7	1.522(13)
Fe	$O2^{ii}$	2.028(8)	C1	C2	1.50(2)
Fe	O3	2.039(8)	C2	N2	1.500(14)
Fe	N2	2.209(10)	N2	C5	1.463(14)
Fe	N1	2.331(10)	N2	C14	1.498(14)
C3	C4	1.51(2)	C5	C6	1.52(2)
C4	O2	1.254(13)	C6	O4	1.284(14)
C4	O3	1.270(13)	C6	O5	1.236(14)
C7	C8	1.51(2)	C14	C15	1.48(2)
C8	C13	1.37(2)	C15	C16	1.39(2)
C8	C9	1.40(2)	C15	C20	1.41(2)
C9	C10	1.39(2)	C16	C17	1.38(2)
C10	O10'	1.36(2)	C17	O17'	1.36(2)
C10	C11	1.41(2)	C17	C18	1.39(2)
O10'	C10'	1.43(2)	O17'	C17'	1.43(2)
C11	O11'	1.36(2)	C18	C19	1.38(2)
C11	C12	1.42(2)	C18	O18'	1.39(2)
O11'	C11'	1.37(2)	O18'	C18'	1.55(4)
C12	O12'	1.35(2)	C19	C20	1.38(2)
C12	C13	1.39(2)	C19	O19'	1.41(2)
O12'	C12'	1.46(2)	O19'	C19'	1.41(2)

symmetry equivalent positions:

i) 1-x, 1/2-y, z ii) 1/4+y, 3/4-x, 3/4-z iii) 3/4-y, x-1/4, 3/4-z

Selected non-bonding distances (Å)

Fe	O2	4.065(08)			
Fe	C14	3.120(12)	Fe	C7	3.391(12)
Fe	C15	4.506(13)	Fe	C8	3.900(13)
Fe	C16	5.423(13)	Fe	C9	3.852(13)
Fe	C20	5.240(15)	Fe	C13	5.030(15)

Least-squares planes calculation

Atoms defining the least-square plane	Fe	O3	O2	Fe^{iii}
Distance to the L.S.P (Å)	0.231(3)	-0.405(5)	0.098(3)	0.076(3)
other atom	C4	0.057(15)		

Table S6 : Bond angles (°) and their e.s.d.

O1	Fe	O4	98.4(4)	O4	C6	C5	116.2(12)
O1	Fe	$O2^{ii}$	97.6(3)	C6	O4	Fe	110.7(8)
O4	Fe	O2	88.7(3)	C8	C7	N1	114.2(9)
O1	Fe	O3	93.3(3)	C13	C8	C9	119.6(14)
O4	Fe	O3	164.7(3)	C13	C8	C7	119.1(13)
$O2^{ii}$	Fe	O3	99.6(3)	C9	C8	C7	121.2(13)
O1	Fe	N2	88.9(3)	C10	C9	C8	119.9(14)
O4	Fe	N2	77.4(3)	O10'	C10	C9	124.6(16)
$O2^{ii}$	Fe	N2	165.4(3)	O10'	C10	C11	114.9(16)
O3	Fe	N2	93.0(3)	C9	C10	C11	120.5(16)
O1	Fe	N1	162.7(3)	C10	O10'	C10'	117.0(14)
O4	Fe	N1	92.9(3)	O11'	C11	C10	120.3(18)
$O2^{ii}$	Fe	N1	95.6(3)	O11'	C11	C12	120.6(18)
O3	Fe	N1	73.6(3)	C10	C11	C12	118.7(16)
N2	Fe	N1	80.9(4)	C11	O11'	C11'	115.8(15)
Fe	O1	Fe^{i}	142.7(7)	O12'	C12	C13	124.8(18)
C3	N1	C1	109.3(9)	O12'	C12	C11	115.8(16)
C3	N1	C7	111.2(9)	C13	C12	C11	119.4(16)
C1	N1	C7	106.7(9)	C12	O12'	C12'	118.5(15)
C3	N1	Fe	104.3(6)	C8	C13	C12	121.7(16)
C1	N1	Fe	102.9(7)	C15	C14	N2	117.5(10)
C7	N1	Fe	121.9(7)	C16	C15	C20	119.0(12)
N1	C1	C2	110.5(10)	C16	C15	C14	123.5(13)
N2	C2	C1	110.4(9)	C20	C15	C14	117.5(12)
C5	N2	C14	111.7(9)	C17	C16	C15	121.8(14)
C5	N2	C2	110.7(9)	O17'	C17	C16	124.5(15)
C14	N2	C2	112.6(9)	O17'	C17	C18	116.2(14)
C5	N2	Fe	101.9(7)	C16	C17	C18	119.2(14)
C14	N2	Fe	113.3(7)	C17	O17'	C17'	118.2(12)
C2	N2	Fe	106.1(7)	C19	C18	C17	119.1(14)
N1	C3	C4	110.3(10)	C19	C18	O18'	120.1(15)
O2	C4	O3	125.2(11)	C17	C18	O18'	120.8(14)
O2	C4	C3	117.6(11)	C18	O18'	C18'	110.5(18)
O3	C4	C3	117.2(11)	C20	C19	C18	122.7(15)
C4	O2	Fe^{iii}	131.3(8)	C20	C19	O19'	122.4(14)
C4	O3	Fe	119.7(8)	C18	C19	O19'	114.7(15)
N2	C5	C6	111.9(10)	C19'	O19'	C19	117.8(13)
O5	C6	O4	124.7(12)	C19	C20	C15	118.0(13)
O5	C6	C5	119.0(12)				

symmetry equivalent positions:

i) 1-x, 1/2-y, z

ii) 1/4+y, 3/4-x, 3/4-z

iii) 3/4-y, x-1/4, 3/4-z