

SUPPORTING INFORMATION

Oxamate-Based Potassium-Organic Assembly With the Uncommon Binodal (6,12)-Coordinated alb Topology.

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[†]To the beloved memory of Prof. Miguel Julve.

Table S1- Some details of the metal complexes with H₄mpba; H₄opba, H₄ppba, and H₄edpba as ligands in the last two decades (2000-2023).

Oxamate-derivate compound	CSD code	Salt	Acid/ester	Building block	Reference
Na ₄ [Cu ₂ (mpba) ₂]·10H ₂ O	VODXUH	-	Et ₂ H ₂ mpba/ NaOH	-	¹
Na ₈ [Ni ₂ (mpba) ₃]·10H ₂ O	-	-	H ₄ mpba/ NaOH	-	²
{[Ni ₂ (mpba) ₃][Ni(dpt)(H ₂ O)] ₆ }(ClO ₄) ₄ ·12.5H ₂ O	FAJFIG	-	-	Na ₈ [Ni ₂ (mpba) ₃]·10H ₂ O	²
{[Cu ₂ (mpba) ₂][Cu(tmen)] ₄ }(ClO ₄) ₄ ·6H ₂ O	-	-	-	Na ₄ [Cu ₂ (mpba) ₂]·10H ₂ O	³
[Co ₂ Cu ₂ (mpba) ₂ (H ₂ O) ₆]·6H ₂ O	EVUCED	-	-	Na ₄ [Cu ₂ (mpba) ₂]·10H ₂ O	⁴
Li ₅ [Li ₃ Co ₂ (mpba) ₃ (H ₂ O) ₆]·31H ₂ O	POBNEA	-	Et ₂ H ₂ mpba/ LiOH	-	⁵
Li ₂ [Mn ₃ Co ₂ (mpba) ₃ (H ₂ O) ₆]·22H ₂ O	-	-	-	Li ₅ [Li ₃ Co ₂ (mpba) ₃ (H ₂ O) ₆]· 31H ₂ O	⁵
Na{[M ₂ (mpba) ₃ [Cu(Me ₅ dien)] ₆ }(ClO ₄) ₆ ·12H ₂ O M= Cu ^{II} ; Ni ^{II}	EXEDUG/FA JFIG	-	Et ₂ H ₂ mpba/ NaOH	-	⁶
[Na(H ₂ O) ₄] ₄ [Mn ₄ {Cu ₂ (mpba) ₂ (H ₂ O) ₄ } ₃]·56·5H ₂ O	DAPXID	-	-	Na ₄ [Cu(mpb) ₂]·10H ₂ O	⁷
Na ₈ [M ^{II} ₂ (mpba) ₃]·15H ₂ O	VEHNED/ VEHNIH	-	Et ₂ H ₂ mpba/ NaOH	-	⁸
M= Ni ^{III} ; x= 15H ₂ O; Co ^{II} ; x=17 H ₂ O					
TBA ₂ [Co ₂ (H ₂ mpba) ₃]·2DMF·5H ₂ O	KEVKON		Et ₂ H ₂ mpba/ TBAOH	-	⁹
(HNEt ₃) ₂ [Co ₂ (H ₂ mpba) ₃]·6DMF·5H ₂ O	KEVKUT		H ₄ mpba·3H ₂ O / NEt ₃	-	⁹
Mn ₄ (H ₂ mpba) ₄ (H ₂ O) ₁₂ {[Mn ₈ Cu ₈ (mpba) ₈ (H ₂ O) ₂₄]}· 29.5H ₂ O	QEJSEF	-	-	Na ₄ [Cu ₂ (mpba) ₂]·10H ₂ O	¹⁰

[Mn ₄ Cu ₄ (mpba) ₄ (H ₂ O) ₉]·14H ₂ O	QEJSIJ	-	-	Na ₄ [Cu ₂ (mpba) ₂]·10H ₂ O	10
[Cu(bipy)(H ₂ mpba)] ₂ ·2H ₂ O	QIQYOG	K ₂ H ₂ mpba	-	-	11
[Cu(bipy)(H ₂ mpba)]·dmsO	QIQYUM	K ₂ H ₂ mpba	-	-	11
{[K ₄ (H ₂ O)(dmsO)][Pd ₂ (mpba) ₂]}	BUBGIQ	-	-	K ₄ [Pd ₂ (mpba) ₂]·4H ₂ O	12
{[Cu(bpca)] ₄ [Pd ₂ (mpba) ₂]}·6H ₂ O	BUBJOZ	-	-	K ₄ [Pd ₂ (mpba) ₂]·4H ₂ O	12
[EDAP{Li ₆ (H ₂ O) ₈ [(Cu ₂ (μ-mpba) ₂ (H ₂ O) ₂]}] _n	CEBZIW	-	Et ₂ H ₂ mpba/ LiOH	-	13
[(EDAP) ₂ {K(H ₂ O) ₄ [Cu ₂ (μ-mpba) ₂ (H ₂ O) ₂]}Cl·2H ₂ O] _n	CEBZUI	-	Et ₂ H ₂ mpba/ KOH	-	13
{[K ₂ (dmf) ₂ (H ₂ O) ₂][Co ₂ (H ₂ mpba) ₃]·2H ₂ O} _n	GUDHUL	K ₂ H ₂ mpba	-	-	14
{[K ₂ (dmf) ₂ (H ₂ O) ₂][Ni ₂ (H ₂ mpba) ₃]·2H ₂ O} _n	GUDJAT	K ₂ H ₂ mpba	-	-	14
[Co(tppz) ₂][Co ₂ (H ₂ mpba) ₃]·9H ₂ O	GUDHOF	K ₂ H ₂ mpba	-	-	14
[Ni(tppz) ₂][Ni ₂ (H ₂ mpba) ₃]·9H ₂ O	GUDHIZ	K ₂ H ₂ mpba	-	-	14
[Co(H ₂ O) ₆][Co ₂ (H ₂ mpba) ₃]·2H ₂ O·0.5dmsO	UYIQOL	K ₂ H ₂ mpba	-	-	15
[Co(H ₂ O) ₆][Co ₂ (H ₂ mpba) ₃]·3H ₂ O·0.5dpss	UYIQUR	K ₂ H ₂ mpba	-	-	15
[Co ₂ (H ₂ mpba) ₂ (H ₂ O) ₄] _n ·4nH ₂ O	UYIQEB	K ₂ H ₂ mpba	-	-	15
[Co ₂ (H ₂ mpba) ₂ (CH ₃ OH) ₂ (H ₂ O) ₂] _n ·0.5nH ₂ O·2ndpss	UYIQIF	K ₂ H ₂ mpba	-	-	15
{[K ₂ (dmsO) ₂ (H ₂ O) ₂][Ni ₂ (H ₂ mpba) ₃]·2H ₂ O} _n	-	K ₂ H ₂ mpba			16
[Ni ₂ (H ₂ mpba) ₃][Ni(H ₂ O) ₆]	-	K ₂ H ₂ mpba			16
Oxamate-derivate compound	CSD code	Salt	Acid/ester	Building block	Reference
Na ₄ [Cu ₂ (ppba) ₂ (H ₂ O) ₂]·10H ₂ O	OLEMIB	-	-	Li ₄ [Cu ₂ (ppba) ₂]·10H ₂ O	17
{[Cu ₂ (ppba) ₂][Cu(pmdien)] ₄ }(ClO ₄) ₄	IYAVUZ	-	-	Li ₄ [Cu ₂ (ppba) ₂]·10H ₂ O	3
(Bu ₄ N) ₄ [Cu ₂ (ppba)]·2CH ₃ OH	PIJPEF	-	H ₂ Et ₂ ppba/ nBu ₄ NOH	-	18
[{Cu(bpca)} ₂ (H ₂ ppba)]·dmsO	EQAQIY	-	H ₄ ppba/ [Cu(bpca)]	-	19

[{Cu(bpca)} ₂ (H ₂ ppba)]·6H ₂ O	EQAQOE	K ₂ H ₂ ppba	(H ₂ O) ₂]NO ₃ · 2H ₂ O	-	19
(Bu ₄ N) ₄ [Pd ₂ (ppba) ₂]	-	-	H ₂ Et ₂ ppba/ nBu ₄ NOH	-	20

Oxamate-derivate compound	CSD code	Salt	Acid/ester	Building block	Reference
[Bu ₄ N] [Mn ₂ {Cu(opba)} ₃ ·4DMF·5H ₂ O]	-	-	-	(Bu ₄ N) ₂ [Cu(opba)]	21
[Bu ₄ N] [Co ₂ {Cu(opba)} ₃ ·DMF·H ₂ O]	-	-	-	(Bu ₄ N) ₂ [Cu(opba)]	21
Na ₂ [Co ₂ {Cu(opba)} ₃]·2DMSO·6H ₂ O	-	-	-	Na ₂ [Cu(opba)]·H ₂ O	22
[CoCu(opba)(DMSO) ₃]	JEBLAE/ JEBLAE01	-	-	Na ₂ [Cu(opba)]·3H ₂ O	23
[CoCu(opba)]·4H ₂ O} <i>n</i>	-	-	-	Na ₂ [Cu(opba)]·3H ₂ O	24
(PPh ₄) ₂ [Pd(opba)]·2H ₂ O	KEMGIU	-	-	K ₂ [Pd(opba)]·2H ₂ O	25
{[Co(H ₂ O) ₂ Pd(opba)]·dmso} <i>n</i>	KEMGOA/ KEMGOA01	-	-	K ₂ [Pd(opba)]·2H ₂ O	25
{[Cu(bpca)] ₂ [Cu(opba)(H ₂ O)]}·H ₂ O	REZFUZ	-	-	(Bu ₄ N) ₂ [Cu(opba)]	26
{[Cu(bpca)] ₂ (H ₂ opba)} ₂ ·6H ₂ O	REZFOT	-	Et ₂ H ₂ opba	Me ₄ N[Mn(opba)(H ₂ O) ₂]	26
[Cu(bpca)(EtH ₂ opba)] _n	REZFIN	-	Et ₂ H ₂ opba	-	26
(Bu ₄ N) ₂ [Mn ₂ {Cu(opba)} ₂ ox] _n	IDIGUZ	-	-	(Bu ₄ N) ₂ [Cu(opba)]	27
[Pd(NH ₃) ₄][Pd(opba)]	JOHTEH	-	-	K ₂ [Pd(opba)]·2H ₂ O	28
{[Cu(bpca)] ₂ [Pd(opba)]}·1.75dmso·0.25H ₂ O	BUBHOX	-	-	K ₂ [Pd(opba)]·2H ₂ O	12
{[Cu(bpca)] ₂ [Pd(opba)]} <i>n</i> ndmso	BUBHIR	-	-	K ₂ [Pd(opba)]·2H ₂ O	12
[Ni(tpa)Cu(opba)] ₂ ·6H ₂ O	YEQNOA	-	-	(Bu ₄ N) ₂ [Cu(opba)]	29
[{Cu(opba)(H ₂ O) _{1.2} } {Cu(dmphen)(SCN)} ₂]·dmf	GOJHOF	-	-	(Bu ₄ N) ₂ [Cu(opba)]	30
[{Cu(opba)} ₂ {Cu(dmphen)Cl} ₄]·1.5dmf·2.5dmso	GOJHUL	-	-	(Bu ₄ N) ₂ [Cu(opba)]	30
{Cu(opba)} ₂ {Cu(dmphen)Br} ₄]·dmf·2.3dmso	GOJJAT	-	-	(Bu ₄ N) ₂ [Cu(opba)]	30
[{Cu(opba)} {Cu(dmphen)(dca)} ₂] _n	GOJJEX	-	-	(Bu ₄ N) ₂ [Cu(opba)]	30

Oxamate-derivate compound	CSD code	Salt	Acid/ester	Building block	Reference
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$[\text{Cu}_2(\text{H}_2\text{edpba}^{\text{anti}})_2(\text{EtOH})_2] \cdot 2\text{EtOH}$	AGODIL	-	$\text{Et}_2\text{H}_2\text{edpba}/$ Et_4NOH	-	31
$[\text{n-Bu}_4\text{N}]_4[\text{Cu}_2(\text{edpba}^{\text{gauche}})_2] \cdot 4\text{H}_2\text{O}$	AGODUX	-	$\text{Et}_2\text{H}_2\text{edpba}/$ Bu_4NOH	-	31
$[\text{Ni}(\text{bipy})(\text{H}_2\text{edpba})] \cdot \text{dmsO}$	DOVKIK	$\text{K}_2(\text{H}_2\text{edpba})$	-	-	32
$[\text{Cu}(\text{bipy})(\text{H}_2\text{edpba})]_n \cdot 3n\text{H}_2\text{O} \cdot n\text{dmsO}$	DOVKEG	-	-	$[\text{Ni}(\text{bipy})(\text{H}_2\text{edpba})] \cdot \text{dmsO}$	32
$[\text{Cu}(\text{bipy})(\text{H}_2\text{edpba})]_n \cdot 1.5n\text{H}_2\text{O}$	DOVQOK	$\text{K}_2(\text{H}_2\text{edpba})$	-	-	32
$[\text{Mn}_5\text{Cu}_5(\text{edpba})_5(\text{dmsO})_7(\text{H}_2\text{O})_7] \cdot 4\text{dmsO} \cdot 2\text{H}_2\text{O}$	WUHCAF	-	-	$(\text{Bu}_4\text{N})_4[\text{Cu}_2(\text{edpba})_2] \cdot 4\text{H}_2\text{O}$	33
$\{\text{Mn}(\text{H}_2\text{edpba})(\text{H}_2\text{O})_2\}_2$	NIDDAI	$\text{K}_2(\text{H}_2\text{edpba})$	-	-	34
$[\text{Mn}(\text{H}_2\text{edpba})(\text{dmsO})_2] \cdot \text{dmsO} \cdot \text{CH}_3\text{COCH}_3 \cdot \text{H}_2\text{O}$	NIDDEM	-	-	$\{\text{Mn}(\text{H}_2\text{edpba})(\text{H}_2\text{O})_2\}_2$	34
$[\text{Fe}(\text{H}_2\text{edpba})(\text{H}_2\text{O})_2]\text{Cl}$	-	-	$\text{H}_4\text{edpba}/$ Et_4NOH	-	35
$\{\text{Fe}(\text{H}_2\text{edpba})(\text{dmsO})\}_2(\mu\text{-O}) \cdot \text{dmsO} \cdot \text{H}_2\text{O}$	CIWVUD	-	-	$[\text{Fe}(\text{H}_2\text{edpba})(\text{H}_2\text{O})_2]\text{Cl}$	35

Abbreviations: H_4mpba = *N,N'*-1,3-phenylenebis(oxamic acid); $\text{Et}_2\text{H}_2\text{mpba}$ = diethyl ester of H_4mpba ; dpt = dipropylene triamine; tmen = *N,N,N',N''*-tetramethylethylenediamine; Me_5dien = *N,N,N',N'',N'''*-pentamethyldiethylenetriamine; bipy = 2,2'-bipyridine; EDAP_2^+ = 1,10-ethylenebis(4-aminopyridinium); TBA^+ ; Bu_4N^+ = tetrabutylammonium salt; HNEt_3^+ = triethylammonium salt; tppz = 2,3,5,6-tetrakis(2-pyridyl)pyrazine; dpss = 2,2'-dipyridyldisulfide; pmde = *N,N,N',N'',N'''*-pentamethyldiethylenetriamine; H_4ppba = *N,N'*-1,4-phenylenebis(oxamic acid); Hbpca = bis(2-pyridylcarbonyl)imide; H_4opba = *N,N'*-1,2-phenylenebis(oxamic acid); H_2ox = oxalic acid; PPh_4 = tetraphenylphosphonium cation; EtH_3opba = monoethyl ester derivative of the H_4opba ; dmphen = 2,9-dimethyl-1,10-phenanthroline; dca = dicyanamide anion; tpa = tris(2-pyridylmethyl)amine; H_4edpba = *N,N*-2,2'-ethylenediphenylenebis(oxamic acid).

Table S2. Geometric analysis of the coordination environment of the potassium(I) ion in K_2H_2mpba , showing the site symmetry approximation derived from continuous shape measures (CShM; via SHAPE).³⁶

Label	Symmetry	Shape	CShM*
HP-7	D_{7h}	Heptagon	32.717
HPY-7	C_{6v}	Hexagonal pyramid	19.449
PBPY-7	D_{5h}	Pentagonal bipyramid	5.576
COC-7	C_{3v}	Capped octahedron	5.232
<u>CTPR-7</u>	<u>C_{2v}</u>	<u>Capped trigonal prism</u>	<u>4.261</u>
PBPY-7	D_{5h}	Johnson pentagonal bipyramid J13	8.901
JETPY-7	C_{3v}	Johnson elongated triangular pyramid J7	15.764

*The approach is incorporated into the program SHAPE, which is available for public use.³⁶ The high values of SHAPE measures for polyhedra of K^I in K_2H_2mpba indicate very distorted geometry.

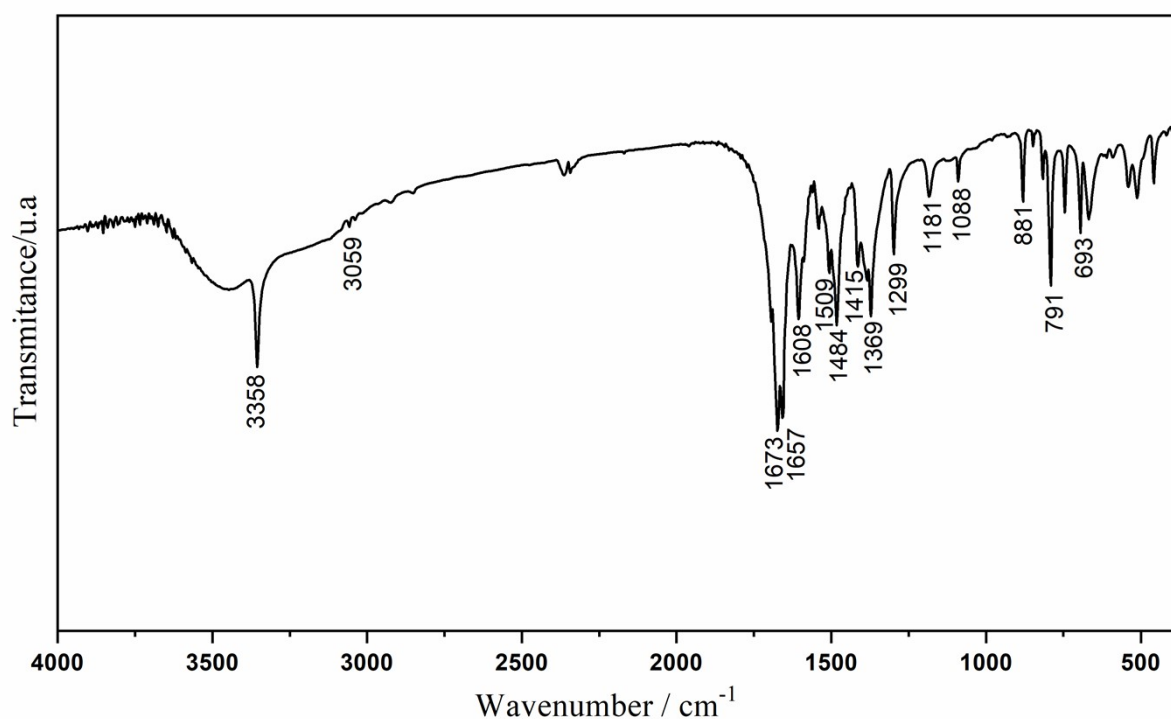


Figure S1. Infrared spectrum for K_2H_2mpba .

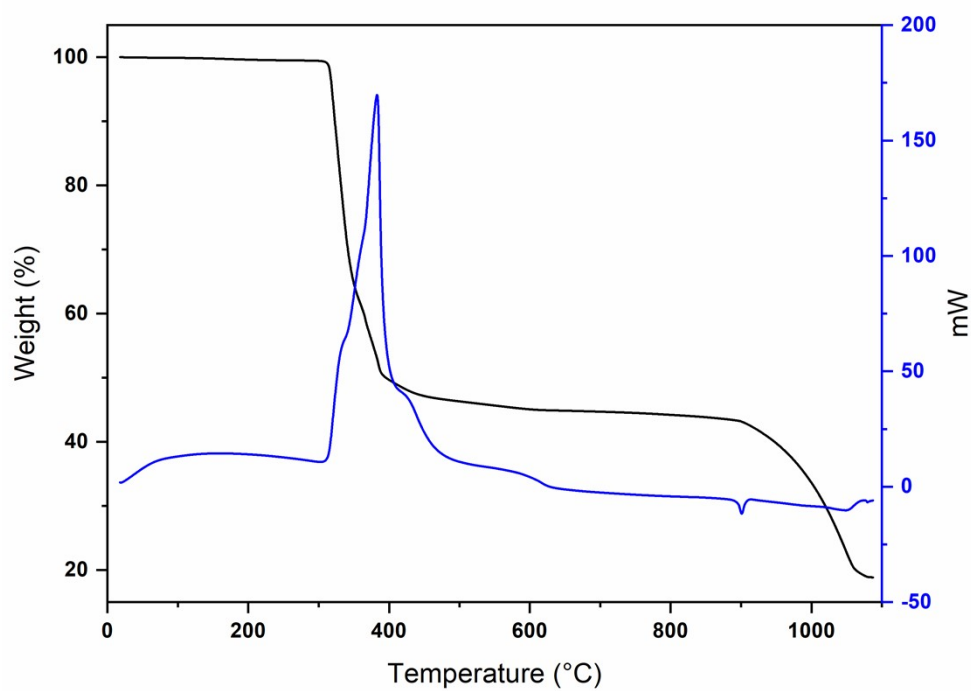


Figure S2. TGA and DTA curves for K_2H_2mpba .

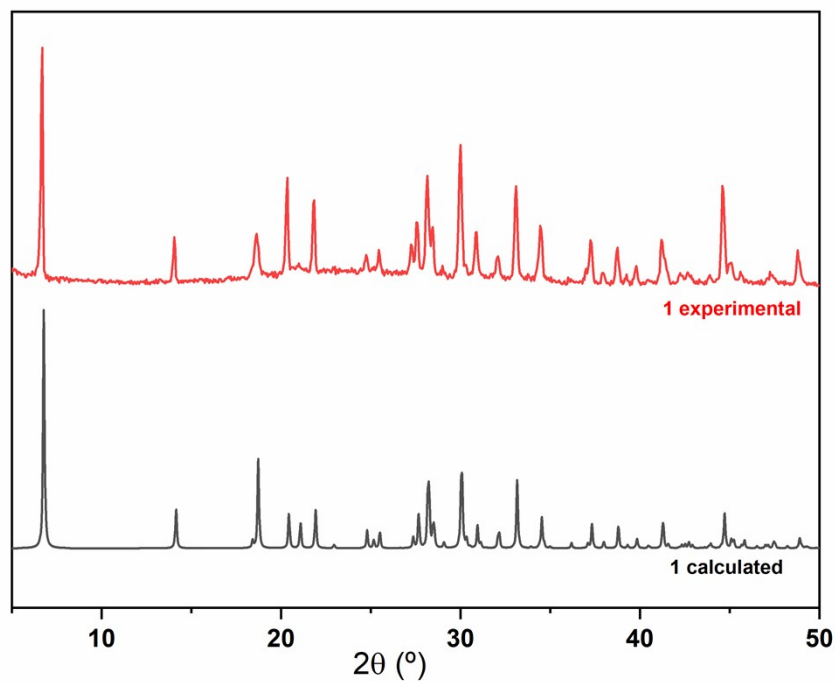


Figure S3. Experimental (red) and calculated (black) PXRD patterns for K_2H_2mpba .

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Coordination sequences

Cum 13 33 117 191 419 583 1027 1317 2049 2501

Cum 7 45 87 233 347 673 895 1473 1839 2741

Vertex symbols for selected sublattice

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symbol:[4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4(2).4(2).4(2).4(2).4(2).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).6(8).6(8).6(8).6(8).6(8).6(8).6(16).6(16).6(16).6(16).6(16).6(16).6(16).6(16).6(16).6(16).6(16).6(16)]
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Extended point symbol:[4.4.4.4.4.4(3).4(3).4(3).4(3).4(3).4(3).4(5).4(5).4(5)]

6,12-c net with stoichiometry $(6-c)_2(12-c)$; 2-nodal net

CRYSTAL

NAME "C5 H3 K N O3"

GROUP P6/mmm

CELL 1.41433 1.41433 1.15451 90.0000 90.0000 120.0000

NODE 1 12 0.00000 0.00000 0.00000

NODE 5 6 0.33333 0.66667 0.50000

EDGE 0.00000 0.00000 0.00000 0.33333 -0.33333 0.50000

EDGE_CENTER 0.16667 -0.16667 0.25000

END

TILING

NAME "C5 H3 K N O3/Systre; PPT 1; [2134]; $2[4^3]+6[4^4]+[4^6] = 2[4b^3]+3[4b^2.4d^2]+3[4d^2.4e^2]+[4e^6]$ "

GROUP P6/mmm

FACES 4

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0.66667 0.33333 -0.50000

0.00000 0.00000 0.00000

0.66667 0.33333 0.50000

FACES 4

1.00000 0.00000 0.00000

0.33333 -0.33333 0.50000

0.00000 0.00000 0.00000

0.66667 0.33333 0.50000

FACES 4

1.00000 0.00000 0.00000

0.33333 -0.33333 0.50000

1.00000 0.00000 1.00000

0.66667 0.33333 0.50000

END

[4.4.4.4.4.4.4(3).4(3).4(3).4(3).4(3).4(3).4(5).4(5).4(5)]

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