is a mirror image of the Cl(*D*) atom. Root-mean-square displacement of the Zn atom is almost isotropic, 0·102 ±0·003 Å. The Zn—Cl(*B*) bond length is longer by 0·028 (1) Å than the other Zn—Cl distances. It may be due to the weak hydrogen bond of Cl(*B*)···H(N22$^{\rm iii}$)—N(2$^{\rm iii}$) (symmetry code is given in Table 2). An averaged deformation density of the $ZnCl_2$ plane assuming T_d symmetry is presented in Fig. 2. The charge distribution around the Zn atom is not perfectly isotropic. On the Zn—Cl bond axis a negative trough of −0·42 (7) e Å^{-3} is observed at 0·4 Å from the Zn nucleus. A postive peak of 0·29 (10) Å^{-3} lies on the bisector of the Cl—Zn—Cl angle and 0·7 Å from the Zn atom. The asphericity around the Zn atom agrees qualitatively with that observed around the Co atom in $CoAl_2O_4$ (Toriumi, Ozima, Akaogi & Saito, 1978). It suggests that the electron configuration of the Zn^{2+} ion is $(3d\text{-}e)^4(3d\text{-}t_2)^{6-x}(4s)^x$ with $0 < x < 2$. However, there is some noise in the deformation density. Investigations including theoretical calculations should be continued to exclude the possibility of anharmonic thermal vibration conclusively.

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Structures of Cadmium Nitrite Dihydrate and Cadmium Dipotassium Tetranitrite

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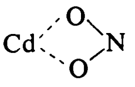
Abstract. $Cd(NO_2)_2.2H_2O$ (I), $M_r = 240{\cdot}4$, orthorhombic, *Pbcn*, $a = 7{\cdot}4446$ (4), $b = 7{\cdot}8889$ (5), $c = 9{\cdot}5992$ (7) Å, $V = 563{\cdot}8$ (1) Å^3, $Z = 4$, $D_m(C_2H_2Br_4/CCl_4) = 2{\cdot}71$ (2), $D_x = 2{\cdot}83$ Mg m^{-3}, Mo $K\alpha_1$, $\lambda = 0{\cdot}70930$ Å, $\mu = 3{\cdot}83$ mm^{-1}, $F(000) = 452{\cdot}2$, $T = 299$ (1) K, final $R = 0{\cdot}042$ for 716 observed unique reflections. $Cd(NO_2)_2.2KNO_2$ (II), $M_r = 374{\cdot}7$, orthorhombic, *Pnma*, $a = 12{\cdot}1935$ (5), $b = 11{\cdot}7154$ (8), $c = 6{\cdot}5520$ (4) Å, $V = 936{\cdot}0$ (1) Å^3, $Z = 4$, $D_m = 2{\cdot}64$ (2), $D_x = 2{\cdot}66$ Mg m^{-3}, Mo $K\alpha_1$, $\mu = 3{\cdot}25$ mm^{-1}, $F(000) = 710{\cdot}3$, $T = 296$ (1) K, final $R = 0{\cdot}024$ for 1844 reflections. In (I) the Cd atom lies on a twofold axis and is octacoordinated by two nitrite N atoms, four nitrite O atoms and two water O atoms. The Cd atom in (II) lies on a mirror plane and is surrounded by eight O atoms of four NO_2^- ions. Each nitrite ion in both (I) and (II) forms a nearly coplanar  unit with Cd···O distances 2·357 (3) to 2·581 (4) Å.

Introduction. Coloration of nitrite ion is caused by certain post-transition-metal cations (McGlynn, Azumi & Kumar, 1981). The arrangement of post-transition-metal cations around NO_2^- has been studied in crystals of $K_3[Hg(NO_2)_4]NO_3$ (Power, King & Moore, 1976), $K_2Pb(NO_2)_3(NO_3).H_2O$ (Nardelli & Pelizzi, 1980), $AgNO_2$ (Ohba & Saito, 1981), $TlBa_2(NO_2)_5$ (Gasparri, Nardelli & Fermi, 1984), $Pb(NO_2)_2.H_2O$ (Ohba, Nosé & Saito, 1985), and $Hg_2(NO_2)_2$ and $Ag_2Li(NO_2)_3$ (Ohba, Matsumoto, Ishihara & Saito, 1986). Structures of the title Cd$^{\rm II}$ salts have been determined to study further the relation between the color and the structure.

Experimental. (I): Colorless tabular (010) crystals grown from filtrate of a mixture of $CdCl_2$ and $AgNO_2$ aqueous solutions, hygroscopic. A rectangular crystal of 0·12 × 0·32 × 0·55 mm sealed in a glass capillary. Rigaku AFC-5 four-circle diffractometer with graphite-monochromatized Mo *Kα* radiation. Laue group *mmm*, systematic absences *hk*0 with *h*+*k* odd, *h*0*l* with *l* odd and 0*kl* with *k* odd; cell parameters refined by least

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squares for 20 2θ values ($58 < 2\theta < 60°$), intensity measurement performed up to $2\theta = 60°$ (h $-10 \rightarrow 10$, k $-11 \rightarrow 11$, l $0 \rightarrow 13$), θ–2θ scan, scan speed 6° min^{-1} in θ. Variation of four standard reflections, $0{\cdot}96 \le |F_o|/|F_o|_{\rm initial} \le 1{\cdot}00$. 3082 reflections measured, 2439 observed reflections with $|F_o| > 3\sigma(|F_o|)$, 716 unique ($R_{\rm int} = 0{\cdot}010$) after absorption correction ($0{\cdot}334 < A < 0{\cdot}635$). Since $Z = 4$, Cd atoms are required to lie on a twofold axis or on a center of symmetry. Structure solved by Patterson and Fourier methods. Coordinates and anisotropic thermal parameters refined. No water H atoms located on difference synthesis. $\sum w||F_o| - |F_c||^2$ minimized, $w^{-1} = \sigma^2(|F_o|) + (0{\cdot}015|F_o|)^2$, final $R = 0{\cdot}042$, $wR = 0{\cdot}066$, $S = 3{\cdot}63$ for 716 unique reflections.* Reflection/parameter ratio 17·1, $\Delta/\sigma < 0{\cdot}33$, $-0{\cdot}36 \le \Delta\rho \le 0{\cdot}11$ e Å^{-3}. Complex neutral-atom scattering factors from *International Tables for X-ray Crystallography* (1974). *UNICS*-III program system (Sakurai & Kobayashi, 1979), Facom M-380R computer of this university.

(II): Pale yellow prisms grown from filtrate of a mixture of $CdCl_2$, $AgNO_2$ and KNO_2 (Cd/Ag/K = 1/2/2). Spherical crystal of diameter 0·70 (1) mm ground with sandpaper. Laue group *mmm*, systematic absences $0kl$ with $k+l$ odd and $hk0$ with h odd; cell parameters refined by least squares for 20 2θ values ($60 < 2\theta < 70°$), intensity measurement performed to $2\theta = 70°$ (h $-19 \rightarrow 19$, k $0 \rightarrow 18$, l $-10 \rightarrow 10$), θ–2θ scan. Variation of five standard reflections, $0{\cdot}96 < |F_o|/|F_o|_{\rm initial} < 1{\cdot}07$, 8139 reflections measured, 6552 observed reflections with $|F_o| > 3\sigma(|F_o|)$, 1844 unique ($R_{\rm int} = 0{\cdot}019$). Absorption correction ($\mu r = 1{\cdot}14$, $0{\cdot}203 < A < 0{\cdot}228$). The Laue group and systematic absences showed that the space group is *Pnma* or $Pn2_1a$. D_m and V suggested the chemical formula $Cd(NO_2)_2.2KNO_2$ with $Z = 4$. If the space group is assumed to be *Pnma*, the y coordinate of the Cd atom is required to be $\frac{1}{4}$. This was indeed verified by inspecting the Patterson function. Other atoms were located by Fourier synthesis. The Cd, N(2) and N(3) atoms lie on a mirror plane perpendicular to **b** (see Fig. 2*a*). Reduction of R from 0·095 to 0·024 achieved by introducing an isotropic secondary-extinction-correction parameter (Zachariasen, 1967), $g = 4{\cdot}94\,(11) \times 10^{-4}$, $wR = 0{\cdot}034$, $S = 1{\cdot}94$ for 1844 unique reflections.* Smallest extinction-correction factor (F_o^2/F_c^2) 0·15 for 420. Reflection/parameter ratio 24·9, $\Delta/\sigma \le 0{\cdot}2$, $-0{\cdot}16 < \Delta\rho < 0{\cdot}05$ e Å^{-3}. Full-matrix least-squares program *RADIEL* (Coppens, Guru Row, Leung, Stevens, Becker & Yang, 1979).

An attempt to determine the structure of cadmium potassium trinitrite failed owing to poor quality of the crystals. $Cd(NO_2)_2.KNO_2$, colorless plate-like crystals, cubic, $Pa\bar{3}$ (No. 205), $a = 10{\cdot}6679\,(7)$ Å, $V = 1214{\cdot}1\,(1)$ Å^3, $Z = 8$, $D_m = 3{\cdot}16\,(2)$, $D_x =$

Table 1. *Positional parameters* (× 10^4; *for* Cd *and* K × 10^5) *and equivalent isotropic temperature factors* (*Hamilton*, 1959)

	x	y	z	$B_{\rm eq}$(Å^2) × 10
Compound (I)				
Cd	0	26270 (6)	25000	13
N	2745 (5)	5261 (6)	2300 (4)	17
O(1)	2693 (4)	4009 (5)	3112 (4)	22
O(2)	1487 (4)	5294 (5)	1454 (3)	25
O(*W*)	−214 (4)	1950 (7)	177 (4)	23
Compound (II)				
Cd	1693 (1)	25000	−1228 (2)	21
K	14641 (3)	−451 (3)	41012 (6)	26
N(1)	−1237 (1)	687 (1)	1329 (2)	28
O(11)	−385 (1)	1026 (1)	2146 (2)	33
O(12)	−1456 (2)	1169 (2)	−305 (2)	36
N(2)	620 (3)	2500	−4417 (4)	34
O(2)	471 (1)	1614 (1)	−3401 (2)	39
N(3)	2493 (2)	2500	760 (5)	38
O(3)	1927 (2)	1609 (1)	634 (3)	42

Table 2. *Interatomic distances* (Å) *and angles* (°)

Compound (I)			
N–O(1)	1·259 (6)	Cd···N^{ii}	2·518 (4)
N–O(2)	1·240 (5)	Cd···N^{iii}	2·518 (4)
O(1)–N–O(2)	113·5 (4)	Cd···O(2)	2·581 (4)
Cd···O(*W*)	2·298 (4)	Cd···O(2^{i})	2·581 (4)
Cd···O(*W*^{i})	2·298 (4)	Cd···O(1)–N	103·6 (3)
Cd···O(1)	2·357 (3)	Cd···O(2)–N	93·0 (3)
Cd···O(1^{i})	2·357 (3)	O(1)–N···Cd^{iv}	123·7 (3)
		O(2)–N···Cd^{iv}	122·5 (3)
		N–O(1)···O(*W*^{v})	128·5 (3)

Symmetry code: (i) $-x, y, -z+\frac{1}{2}$; (ii) $x-\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (iii) $-x+\frac{1}{2}, y-\frac{1}{2}, z$; (iv) $x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (v) $-x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$

Compound (II)			
N(1)–O(11)	1·234 (2)	Cd···O(3)–N(3)	98·1 (1)
N(1)–O(12)	1·239 (2)	Cd···N(1)	2·891 (1)
O(11)–N–O(12)	114·2 (1)	Cd···N(2)	2·867 (3)
N(2)–O(2)	1·246 (2)	Cd···N(3)	2·892 (2)
O(2)–N(2)–O(2^{i})	112·8 (2)	N(1)···Cd···N(1^{i})	94·6 (1)
N(3)–O(3)	1·254 (2)	N(1)···Cd···N(2)	115·9 (1)
O(3)–N(3)–O(3^{i})	112·7 (2)	N(1)···Cd···N(3)	121·0 (1)
Cd···O(11)	2·377 (1)	N(2)···Cd···N(3)	90·5 (1)
Cd···O(11^{i})	2·377 (1)	K···O(12^{ii})	2·814 (2)
Cd···O(2)	2·414 (1)	K···O(2^{iii})	2·815 (1)
Cd···O(2^{i})	2·414 (1)	K···O(3^{iv})	2·866 (2)
Cd···O(3)	2·435 (2)	K···O(11)	2·881 (1)
Cd···O(3^{i})	2·435 (2)	K···N(1^{v})	2·945 (1)
Cd···O(12)	2·525 (2)	K···O(12^{v})	3·013 (2)
Cd···O(12^{i})	2·525 (2)	K···O(11^{vi})	3·016 (1)
Cd···O(11)–N(1)	101·6 (1)	K···O(2^{ii})	3·026 (1)
Cd···O(12)–N(1)	94·1 (1)	K···O(3)	3·039 (2)
Cd···O(2)–N(2)	98·0 (1)	K···N(1^{vi})	3·100 (1)

Symmetry code: (i) $x, -y+\frac{1}{2}, z$; (ii) $-x, -y, -z$; (iii) $x, y, z+1$; (iv) $-x+\frac{1}{2}, -y, z+\frac{1}{2}$; (v) $x+\frac{1}{2}, y, -z+\frac{1}{2}$; (vi) $-x, -y, -z+1$; (vii) $-x, y-\frac{1}{2}, z+\frac{1}{2}$; (viii) $-x, y-\frac{1}{2}, -z$; (ix) $x, -y+\frac{1}{2}, z+1$

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* Lists of structure factors, anisotropic thermal parameters for compounds (I) and (II) and some experimental details for $CdK(NO_2)_3$ have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43381 (24 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

$3{\cdot}17$ Mg m^{-3}, $\mu(\mathrm{Mo}\,K\alpha) = 4{\cdot}26$ mm^{-1}, $T = 296$ (1) K. The Cd atoms are at (000) and ($\frac{1}{2}\frac{1}{2}\frac{1}{2}$), and the K atom at ($xxx$) with $x = 0{\cdot}2366$ (1). $R = 0{\cdot}21$ for 524 unique reflections.* The difference synthesis showed several possible positions of NO_2^-, suggesting disorder.

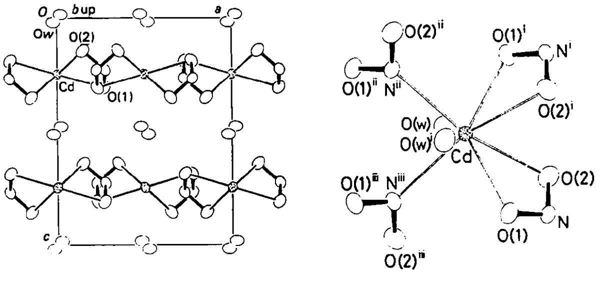

Fig. 1. (*a*) Projection of crystal structure of (I) along **b** and (*b*) environment of Cd^{2+} ions. The symmetry code is given in Table 2.

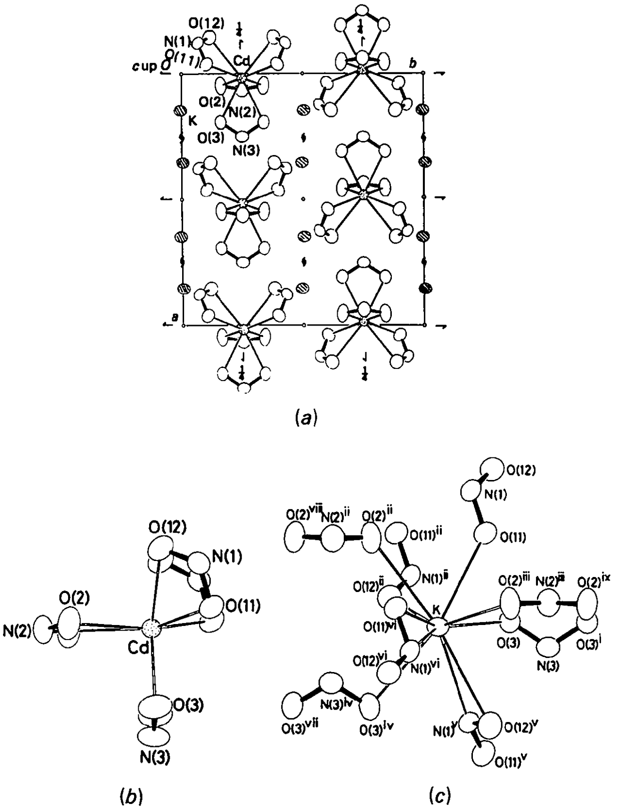

Fig. 2. (*a*) Projection of crystal structure of (II) along **c** and (*b*) environment of Cd^{2+} and (*c*) K$^+$ ions. The symmetry code is given in Table 2.

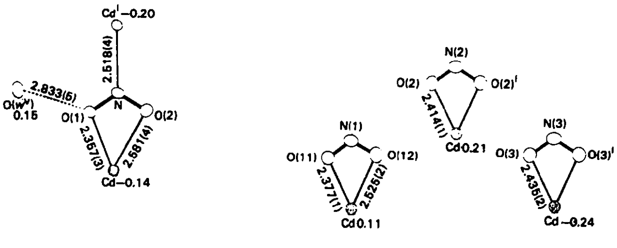

Fig. 3. Arrangement of metal cations and water molecules around the NO_2^- ions in (*a*) (I) and (*b*) (II) with distances from the NO_2 plane less than 0·5 Å, which are indicated by numbers near the atom labels. The symmetry code is given in Table 2. Distances in Å.

Discussion. Final atomic coordinates and interatomic distances and angles are presented in Tables 1 and 2. The crystal structure of (I) is shown in Fig. 1. The Cd^{2+} ion lies on the twofold axis and is surrounded octahedrally by two water molecules and four nitrite ions (hereafter the orientations of the O,O′-bidentate nitrite ions are defined by the O—N—O bisectors). As shown in Fig. 2, the Cd^{2+} ion in (II) lies on the mirror plane and is coordinated to eight O atoms of the four nitrite ions arranged tetrahedrally. The K$^+$ ion is surrounded by eight nitrite ions with distances 2·814 (2) to 3·100 (1) Å. The preferred orientation of the metal cations relative to the nitrite ion coincides with the direction of the lone-pair electrons of the O and N atoms (Ohba, Kikkawa & Saito, 1985; Ohba, Nosé & Saito, 1985). Fig. 3 shows the arrangement of metal cations and water molecules almost lying on an NO_2 plane. The chelated position between two O atoms of each nitrite ion is occupied by a Cd^{2+} ion with Cd···O distances 2·357 (3) to 2·581 (4) Å. Crystals of (I) are colorless, whereas aqueous solutions of (I) and (II) and crystals of (II) are pale yellow. This difference in coloration cannot be explained by the Cd···O distances only. Further study on the structures of double salts containing Cd^{II} nitrite is needed. The absence of coloration in crystals of (I) suggests that the covalency in the Cd···O bond is very weak, as expected from the relatively poor electron affinity of the Cd^{2+} ion (McGlynn, Azumi & Kumar, 1981).

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* See deposition footnote.

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Hydrogénophosphate de Zinc Hydrate

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Abstract. $Zn_3[PO_3(OH)]_3.3H_2O$, $M_r = 538{\cdot}1$, triclinic, $P\bar{1}$, $a = 6{\cdot}429\ (13)$, $b = 7{\cdot}726\ (11)$, $c = 12{\cdot}285\ (16)$ Å, $\alpha = 74{\cdot}11\ (10)$, $\beta = 81{\cdot}35\ (9)$, $\gamma = 80{\cdot}99\ (9)^\circ$, $V = 576{\cdot}0$ Å^3, $D_m = 3{\cdot}10\ (1)$ (by flotation), $D_x = 3{\cdot}103$ Mg m^{-3}, $Z = 2$, Mo $K\alpha$, $\lambda = 0{\cdot}71069$ Å, $\mu = 6{\cdot}855$ mm^{-1}, $F(000) = 528$, room temperature, $R = 0{\cdot}033$ for 2310 reflections. The phase $Zn_3[PO_3(OH)]_3(H_2O)_3$ has been studied by single-crystal X-ray structure analysis with an automatic diffractometer. The structure contains $[ZnO_6]$ and $[ZnO_5]$ polyhedra linked together by $[PO_3(OH)]$ tetrahedra to build complex sheets in the *ab* plane. All these sheets are linked only by hydrogen bonds.

Introduction. De nombreux travaux ont été consacrés à l'étude chimique et structurale des phosphates de zinc. Dans une étude récente du système ternaire $ZnO.P_2O_5.H_2O$ (Cudennec, Lecerf, Riou & Gerault, 1985), comportant un rappel bibliographique des travaux antérieurs, nous avons obtenu par synthèse hydrothermale quelques uns des phosphates déjà cités dans la littérature chimique et présenté un nouvel hydrate de formule $Zn_3(PO_4)_2.H_2O$.

Parmi ces composés on trouve en particulier des hydrogénophosphates de formule $Zn[PO_3(OH)].xH_2O$ qui à notre connaissance n'ont jamais fait l'objet d'études structurales. Seul un mémoire comporte une détermination des paramètres cristallins de $Zn[PO_3(OH)].H_2O$ (Kovarskii, Kozina, Lepilina & Fomina, 1971) mais les résultats sont erronés.

Un isomère de $Zn[PO_3(OH)].H_2O$ présenté sous la formule H_3OZnPO_4 a fait l'objet d'une étude structurale (Sandomirskii, Klientova, Simonov & Belov, 1977), mais les auteurs fournissent peu d'information sur la préparation du cristal étudié. Dans l'étude chimique précédemment citée, nous indiquons les raisons qui permettent d'avancer l'hypothèse que les cristaux étudiés correspondent très probablement à NH_4ZnPO_4 et non à H_3OZnPO_4.

Compte tenu de la diversité des résultats présentés dans les travaux antérieurs et de leurs contradictions, il nous a paru intéressant d'effectuer la détermination structurale complète du composé $Zn[PO_3(OH)].H_2O$ qui est en fait un trimère de formule $Zn_3[PO_3(OH)]_3.3H_2O$. Ce travail est exposé dans ce mémoire.

Partie expérimentale. Cristaux de $Zn_3[PO_3(OH)].3H_2O$ obtenus par une très lente évaporation à 353 K d'un système comprenant 30% de P_2O_5, 17% de ZnO et 53% d'eau. Ces cristaux précipitent sous forme d'aiguilles transparentes parallélépipédiques tronquées. Etudes préliminaires radiocristallographiques menées sur chambres photographiques de Weissenberg et de précession. Paramètres de la maille cristalline affinés par moindres carrés à partir de 25 réflexions optimisées sur diffractomètre automatique. Enregistrement des intensités diffractées sur un diffractomètre automatique (Enraf–Nonius); monochromateur: lame de graphite; distance cristal–détecteur: 173 mm; $1 < \theta < 27^\circ$; balayage: ω–2θ; amplitude de balayage $(1{,}00 + 0{,}35\ \mathrm{tg}\theta)^\circ$; ouveture $(2{,}00 + 0{,}45\ \mathrm{tg}\theta)^\circ$. 2518 réflexions indépendantes mesurées, corrigées du facteur de Lorentz–polarisation mais pas de correction d'absorption; dimensions du cristal: 825 × 125 × 50 µm; pas de variations significatives des trois réflexions de référence; h: −8 à 8; k: −9 à 9; l: 0 à 15. 2310 réflexions avec $I > \sigma(I)$ conservées pour la résolution de la structure. Structure résolue par la méthode de l'atome lourd: positions des atomes de zinc et de phosphore déterminées par déconvolution de la fonction de Patterson tridimensionnelle. Positionnement des atomes d'oxygène appartenant aux groupements phosphates et aux molécules d'eau à l'aide des cartes de

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