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Stabilization of caesium ions by simple organic molecules: crystal structures of Cs(OXL) (OXL = oxalurate anion), and CsOH/cyanuric acid co-crystal $Cs_3(CYH_3)_4(OH)_3$ (CYH_3 = cyanuric acid)

Francesco Isaia,*[a] Alessandra Garau,[a] Carlo Castellano,[b] Francesco Demartin,[b] M. Carla Aragoni,[a] Massimiliano Arca,[a] Claudia Caltagirone,[a] Vito Lippolis,[a] Tiziana Pivetta[a]

[a]Dipartimento di Scienze Chimiche e Geologiche, Università degli Studi di Cagliari, Cittadella Universitaria, Monserrato CA, 09042, Italy

[b]Dipartimento di Chimica, Università degli Studi di Milano, via Golgi 19, Milano, 20133, Italy.

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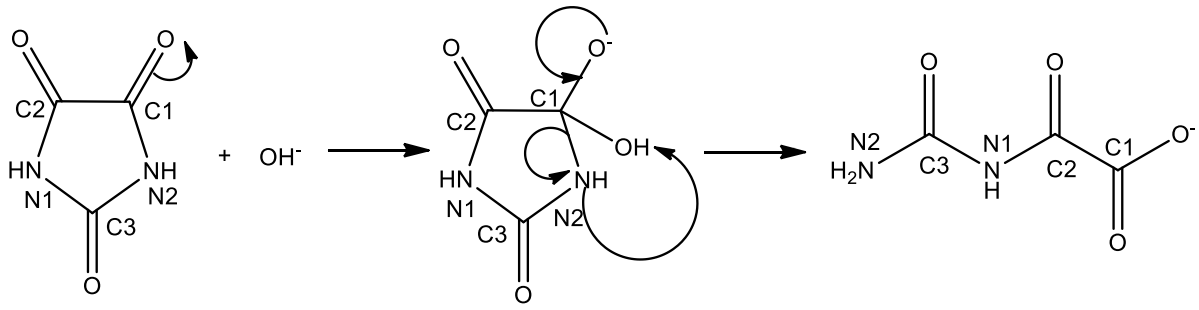


Scheme S1. The parabanic acid undergoes the basic hydrolysis of the imide bond, the attack of OH^- occurs either on C4 or C5 as they are more positive than C2 because they are bound together. Consequently, the break of the carbon-nitrogen bond will occur between the atoms N3-C4 or N1-C5 leading to the oxalurate anion formation.[1]

Table S1. Crystallographic data and structure refinement details

Compound	CsOXL(**1**)	$Cs_3(CYH_3)_4(OH)_3$ (**2**)
Formula	$C_3H_3CsN_2O_4$	$C_4HCsN_3O_5$
Crystal system	triclinic	triclinic
Space group	*P*-1 (no. 2)	*P*-1 (no. 2)
M.W.	263.98	966.09
a / Å	7.8313(4)	10.506(1)
b / Å	8.4529(4)	10.536(1)
c / Å	10.3855(5)	13.657(2)
α / °	71.08(1)	98.13(2)
β / °	83.49(1)	103.99(2)
γ / °	81.22(1)	111.54(2)
V / Å^3	641.22(5)	1319.5(3)
Z	4	2
D_c /g/cm^{-3}	2.734	2.432
μ/ mm^{-1}	5.730	4.215
Measured reflections	8153	13917
Unique reflections, R_{int}	3188, 0.030	7891, 0.054
Observed reflections [$I > 2\sigma(I)$]	2503	5787
Absorption correction	*SADABS*	*SADABS*
T_{min}, T_{max}	0.554, 1.000	0.583, 1.000
R	0.0299	0.087
*wR*2 [all data]	0.0750	0.267
GOF	0.959	1.069

$R = \Sigma||Fo|-|Fc||/\Sigma|Fo|$; $wR2 = \{\Sigma[w(Fo^2-Fc^2)^2]/\Sigma[w(Fo^2)^2]\}^{1/2}$;
$GOF = \{\Sigma[w(Fo^2-Fc^2)]/(n-p)\}^{1/2}$ where n is the number of reflections and p is the number of refined parameters.

Table S2. Cs(OXL) (**1**) - Selected interatomic distances (Å) and angles (deg.)

Cs1-O1	3.007(3)	Cs2-O1	3.232(4)
Cs1-O2a	3.180(4)	Cs2-O3b	3.112(3)
Cs1-O3	3.229(3)	Cs2-O4c	3.601(4)
Cs1-O3b	3.228(4)	Cs2-O4b	3.221(3)
Cs1-O4c	3.285(3)	Cs2-O5	2.975(3)
Cs1-O4b	3.306(4)	Cs2-O5e	3.334(4)
Cs1-O6d	3.184(4)	Cs2-O6e	3.433(4)
Cs1-O7b	3.036(3)	Cs2-O7	3.183(3)
Cs1-O8b	3.068(3)	Cs2-O8c	3.150(3)
O1-C1	1.241(5)	O5-C4	1.234(6)
O2-C1	1.255(5)	O6-C4	1.258(5)
O3-C2	1.219(5)	O7-C5	1.218(5)
O4-C3	1.226(5)	O8-C6	1.223(5)
N1-C2	1.356(6)	N3-C5	1.369(6)
N1-C3	1.403(6)	N3-C6	1.420(6)
N2-C3	1.328(6)	N4-C6	1.327(6)
C1-C2	1.556(6)	C4-C5	1.567(6)
Hydrogen bonds			
N1···O2	2.648(5)	N1-H1···O2	101.1(3)
N3···O6	2.650(5)	N3-H3···O6	108.2(3)
N2···O6f	2.902(5)	N2-H2B··O6f	156.1(3)
N1···O6f	2.972(5)	N1-H1···O6f	155.6(3)
N3···O2f	2.895(6)	N3-H3···O2f	153.4(3)
N4···O2f	2.875(5)	N4-H4B···O2f	153.0(3)
N4-O5g	2.849(6)	N4-H4A···O5g	171.7(3)
N2-O1g	2.878(6)	N2-H2A···O1g	170.9(3)

Symmetry codes: a = 1- x,1-y,1-z; b = -x, 1-y,1-z; c = x, 1+y, z; d = x, y, z+1; e = -x, 2-y, -z; f = 1-x, 1-y, -z; g = x, y-1, z.

TABLE S3. $Cs_3(CYH_3)_4(OH)_3$ (**2**) - Selected interatomic distances (Å) and angles (deg.)

Cs1-O1	3.095(9)	Cs2-O1	3.404(11)
Cs1-O2e	3.169(10)	Cs2-O2h	3.114(8)
Cs1-O9f	3.583(11)	Cs2-O3c	3.007(9)
Cs1-O11a	3.271(11)	Cs2-O5h	3.478(12)
Cs1-O11g	3.307(13)	Cs2-O8g	3.651(12)
Cs1-O12f	3.166(9)	Cs2-O10i	3.072(8)
Cs1-OH1	3.295(15)	Cs2-O11g	3.156(10)
Cs1-OH2	3.149(13)	Cs2-OH2j	3.648(14)
Cs1-O4	3.823(13)	Cs2-OH3	3.281(12)
Cs3-O4	3.297(11)	Cs3-O9d	3.580(11)
Cs3-O5a	3.332(10)	Cs3-OH1	3.448(15)
Cs3-O6d	3.192(9)	Cs3-OH1d	3.336(14)
Cs3-O7	3.209(9)	Cs3-OH2	3.161(14)
Cs3-O8e	3.333(10)	Cs3-OH3e	3.653(17)
C1-O1	1.248(13)	C4-O4	1.234(13)
C1-N1	1.391(15)	C4-N4	1.408(15)
C1-N3	1.340(14)	C4-N6	1.356(15)
C2-O2	1.251(15)	C5-O5	1.219(15)
C2-N1	1.384(14)	C5-N4	1.348(13)
C2-N2	1.368(14)	C5-N5	1.367(14)
C3-O3	1.250(14)	C6-O6	1.231(14)
C3-N2	1.386(15)	C6-N5	1.415(15)
C3-N3	1.357(13)	C6-N6	1.341(15)
C7-O7	1.224(13)	C10-O10	1.237(13)
C7-N7	1.369(15)	C10-N10	1.411(14)
C7-N9	1.380(14)	C10-N12	1.365(14)
C8-O8	1.234(16)	C11-O11	1.236(15)
C8-N7	1.391(15)	C11-N10	1.375(13)
C8-N8	1.369(15)	C11-N11	1.361(14)
C9-O9	1.232(14)	C12-O12	1.251(13)
C9-N8	1.361(15)	C12-N11	1.384(14)
C9-N9	1.365(13)	C12-N12	1.355(13)

Hydrogen bonds

N4···O7a	2.765(14)	N4-H4···O7a	173(1)
N1···O10a	2.841(13)	N1-H1···O10a	179(1)
N7···O4a	2.838(14)	N7-H7···O4a	174(1)
N10···O1a	2.867(14)	N10-H10···O1a	175(1)
N5-O9b	2.906(15)	N5-H5···O9b	173(1)
N8···O6b	2.751(15)	N8-H8···O6b	177(1)
N2-O12b	2.846(15)	N2-H2···O12b	170(1)
N11-O3b	2.808(15)	N11-H11···O3b	177(1)
N3···OH3c	2.875(21)	N3-H3···OH3c	132(1)
N9-OH1d	2.671(22)	N9-H9···OH1d	157(1)
N12-OH3e	2.793(21)	N12-H12···OH3e	161(1)

Symmetry codes: a = -x, -y, -z; b = 1-x, 1-y, -z; c = -x, 1-y, -1-z; d = -x, 1-y, -z; e = x,y, 1+z; e = x-1, y, z; f = -x, 1-y, -z; g = x-1, y, z-1; h = -x, -y, -1-z; i = x,y,z-1; j = -1-x,-y,-1-z;

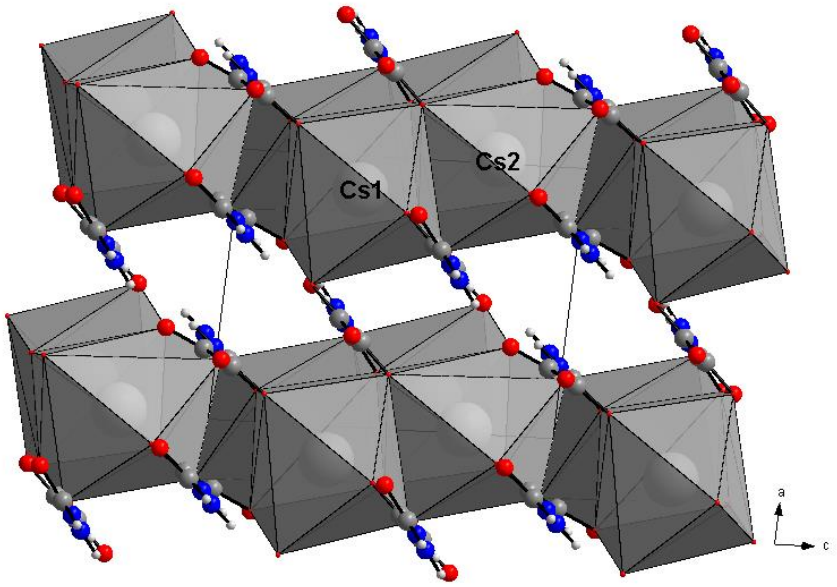


Figure S1. Perspective view of the Cs(OXL) (**1**) structure showing the alignment of the ribbons made by the oxalurate anions along [010].

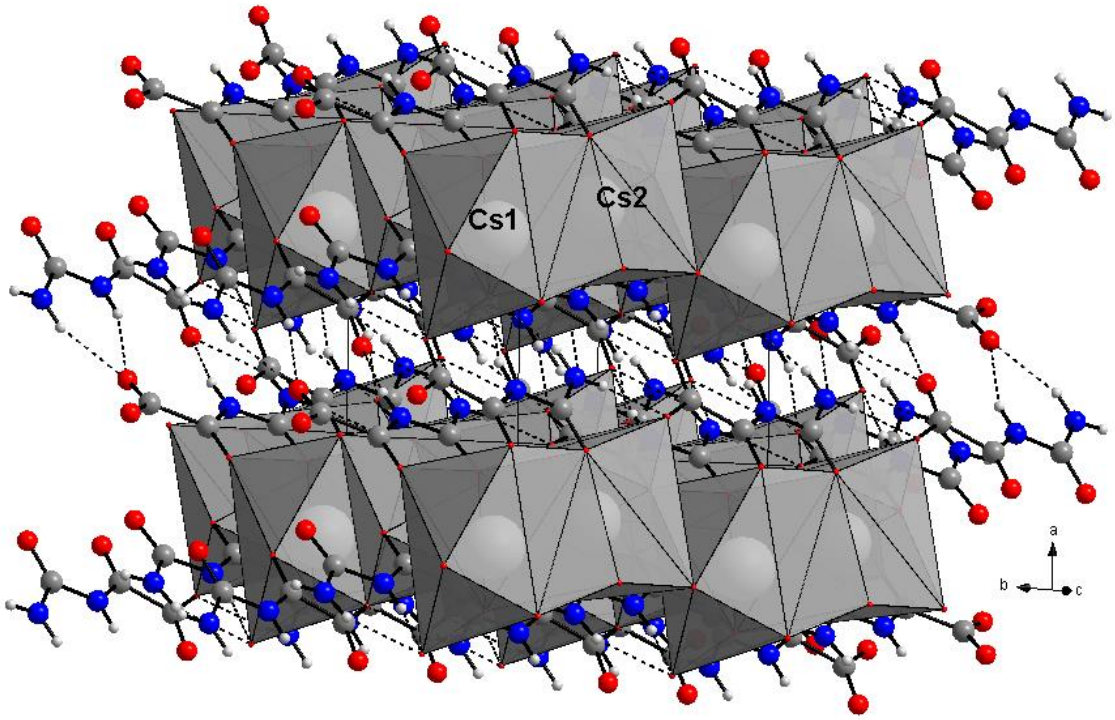
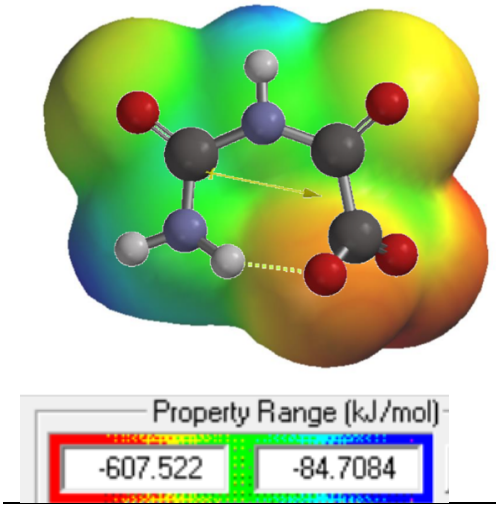


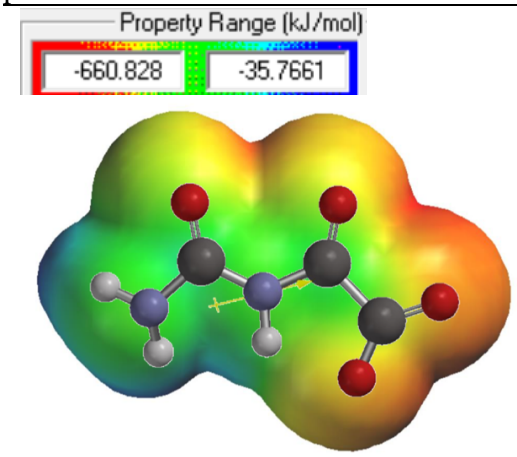
Figure S2. Perspective view of the Cs(OXL) (**1**) structure showing the hydrogen bonds between the layers.

Table S4. Electrostatic potential surface (left), and atoms electrostatic charge (right) of OXL anion, bent form.



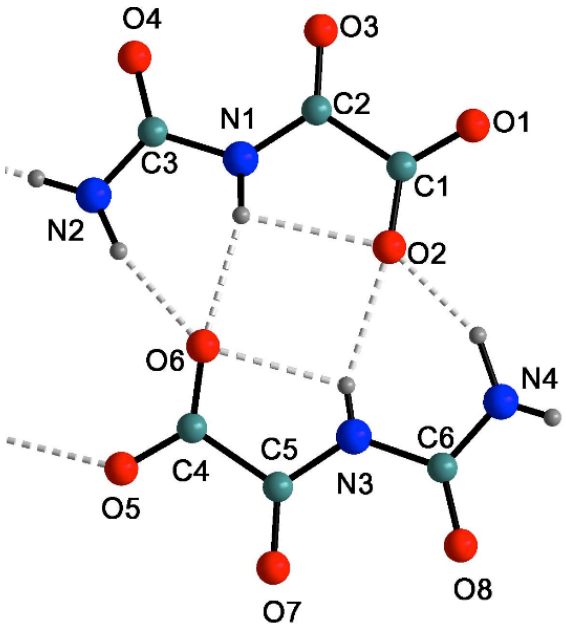
	Charge (e)		
Atom	**Mulliken**	**Electrostatic**	**Natural**
O1	-0.579	-0.598	-0.685
O2	-0.639	-0.671	-0.799
O3	-0.453	-0.479	-0.541
O4	-0.516	-0.587	-0.645
N1	-0.501	-0.684	-0.745
N2	-0.615	-0.899	-0.916
C1	0.514	0.483	0.675
C2	0.412	0.543	0.590
C3	0.591	0.844	0.810
H2 (N2)	0.237	0.343	0.394
H3 (N2)	0.289	0.372	0.436
H4 (N1)	0.262	0.334	0.425

Table S5. Electrostatic potential surface (left), and atoms electrostatic charge (right) of OXL anion, planar form.



	Charge (e)		
Atom	**Mulliken**	**Electrostatic**	**Natural**
O1	-0.678	-0.721	-0.806
O2	-0.774	-0.779	-0.897
O3	-0.554	-0.588	-0.661
O4	-0.611	-0.640	-0.739
N1	-0.810	-0.687	-0.828
N2	-0.765	-1.007	-0.957
C1	0.716	0.698	0.881
C2	0.599	0.592	0.728
C3	0.951	0.974	1.004
H2 (N2)	0.292	0.385	0.409
H3 (N2)	0.288	0.389	0.401
H4 (N1)	0.347	0.353	0.464

Table S6. Atom numbering (left), and atoms electrostatic charge (right) of di-OXL anion.



	Charge (e)		
Atom	**Mulliken**	**Electrostatic**	**Natural**
O1	-0.683	-0.737	-0.810
O2	-0.782	-0.833	-0.920
O3	-0.578	-0.586	-0.683
O4	-0.654	-0.694	-0.779
O5	-0.683	-0.737	-0.810
O6	-0.782	-0.832	-0.920
O7	-0.578	-0.586	-0.683
O8	-0.654	-0.693	-0.779
N1	-0.826	-0.668	-0.817
N2	-0.805	-1.095	-0.968
N3	-0.826	-0.668	-0.817
N4	-0.805	-1.094	-0.968
C1	0.717	0.733	0.892
C2	0.617	0.596	0.732
C3	0.948	1.004	1.002
C4	0.717	0.733	0.895
C5	0.617	0.596	0.732
C6	0.948	1.003	1.002
H1 (N2)	0.272	0.393	0.397
H2 (N4)	0.272	0.392	0.397
H3 (N4-O2)	0.383	0.507	0.469
H4 (N3)	0.391	0.378	0.480
H5 (N2)	0.383	0.507	0.469
H6 (N1)	0.391	0.378	0.480

References.

1 J. March, in Advanced Organic Chemistry (reactions, mechanism and structure); **1992**, Fourth Edition; John Walley & Sons, Page 383. ISBN-10: 0471581488