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2-Methyl-1-(pyrrolidinium-2-ylmethyl)-pyridinium dibromide

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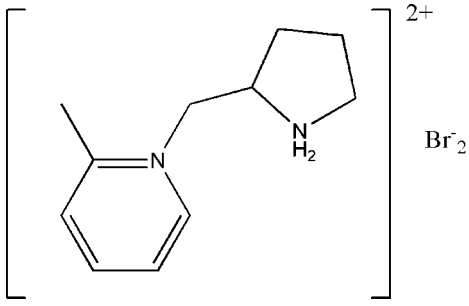
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.008 Å; R factor = 0.045; wR factor = 0.139; data-to-parameter ratio = 23.2.

In the title compound, $C_{11}H_{18}N_2^{2+}\cdot 2Br^-$, whose cation represents the product of racemization of an L-proline derivative under basic conditions, the pyrrolidinium ring has a distorted envelope conformation with the N atom deviating by 0.533 (6) Å from the mean plane of the remaining four atoms of the ring. The methylene C atom which connects the pyrrolidinium ring and the 2-methylpyridine group is displaced from the plane of the four pyrrolidinium C atoms by 0.625 (8) Å in the same direction as the N atom. The cation and anions are linked by N—H···Br hydrogen bonds.

Related literature

See Ishii *et al.* (2004) and Andrey *et al.* (2004) for the catalytic properties of L-proline. The synthesis of (*S*)-(+)-2-bromomethylpyrrolidine hydrobromide is described by Xu *et al.* (2006). Details of the racemization of amino acids under basic conditions are given by Ebbers *et al.* (1997). For the method used for the extinction correction, see: Larson (1970).



Experimental

Crystal data

$C_{11}H_{18}N_2^{2+}\cdot 2Br^-$
M_r = 338.08
Monoclinic, $P2_1/c$
a = 12.588 (3) Å
b = 10.023 (4) Å
c = 12.461 (4) Å
β = 117.617 (13)°
V = 1393.1 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 5.81 mm^{-1}
T = 298 (1) K
0.26 × 0.19 × 0.17 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.225, T_{max} = 0.372
13165 measured reflections
3178 independent reflections
2192 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.139
S = 1.01
3178 reflections
137 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.88 e Å^{-3}
$\Delta\rho_{min}$ = −0.69 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N21—H211···Br1	0.95	2.24	3.186 (3)	176
N21—H212···Br2	0.90	2.35	3.233 (3)	169

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC & Rigaku, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure*.

We acknowledge the help of Professor Jian-Ming Gu of Zhejiang University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: YA2056).

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supplementary materials

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2-Methyl-1-(pyrrolidinium-2-ylmethyl)pyridinium dibromide

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Comment

There has been growing interest (Ishii *et al.*, 2004; Andrey *et al.*, 2004) in the studies of catalytic properties of proline and its derivatives. The title compound (I), a quaternary ammonium salt obtained from *L*-proline, can act as organocatalyst in several important processes such as the Michael reaction, the Mannich reaction and others. When this compound was used as a catalyst of the Michael addition of cyclohexanone to nitroolefins, the products were obtained in good yields, however the reactions showed poor enantioselectivities. In order to establish the structure of (I) unambiguously, as well as to investigate the reason for the above mentioned lack of enantioselectivity, the X-ray analysis of (I) was undertaken. The structure of (I) is shown in Fig. 1.

It came as a surprise, that the crystal of (I) turned out to be racemic and crystallize in centrosymmetric space group, even though it was prepared from the chiral *L*-proline derivative. It is known however that in basic conditions under heating *L*-proline and its derivatives may undergo racemization (Ebbers *et al.*, 1997).

The crystal of (I) is built of pyrrolidinium dications and bromide anions. The N21 atom of the pyrrolidinium ring and the C5 atom are displaced from the mean plane of C1, C2, C3, C4 in the same direction by 0.533 (6) and 0.625 (8) Å. Thanks to two N—H···Br bonds (Table 2) the dications and anions form "ion-pairs" in crystal of (I).

Experimental

The title compound was synthesized by treating of 2-methylpyridine (1.10 g, 11 mmol) with (*S*)-(+)-2-bromomethylpyrrolidine hydrobromide (2.50 g, 10 mmol; see Xu *et al.*, 2006 for the synthesis of the latter) in MeCN (30 ml) under stirring at 353 K for 24 h (yield 95%). The reaction is accompanied by racemization of the *L*-proline derivative. Suitable crystals of the title compound were obtained by slow evaporation of ethanol solution at room temperature (m.p. 421 K).

Refinement

The H211 and H212 atoms were located in a difference Fourier map; all carbon-bound H atoms were placed in calculated position with C—H = 0.98 Å (*sp*), C—H = 0.97 Å (sp2), C—H = 0.96 Å (sp3), C—H = 0.93 Å (aromatic). All H atoms included in the final cycles of refinement in the riding motion approximation, with U_{iso}(H) = 1.2U_{eq} of the carrier atoms.

Figures

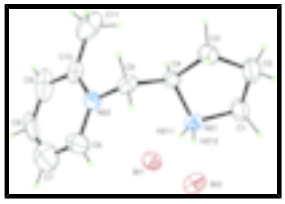
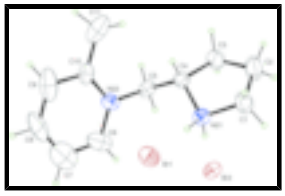


Fig. 1. The asymmetric unit of the structure of the title compound, with the atomic labeling scheme. Displacement ellipsoids are drawn at the 40% probability level. Atomic labels are shown only for those H atoms which participate in the H-bonding.



2-Methyl-1-(pyrrolidinium-2-ylmethyl)pyridinium dibromide

Crystal data

$C_{11}H_{18}N_2^{2+}\cdot 2Br^-$	F_{000} = 672.00
M_r = 338.08	D_x = 1.612 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 148 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71075 Å
a = 12.588 (3) Å	Cell parameters from 9608 reflections
b = 10.023 (4) Å	θ = 3.1–27.5º
c = 12.461 (4) Å	μ = 5.81 mm^{-1}
β = 117.617 (13)º	T = 298 (1) K
V = 1393.1 (8) Å^3	Block, yellow
Z = 4	0.26 × 0.19 × 0.17 mm

Data collection

Rigaku R-AXIS RAPID diffractometer	2192 reflections with $I > 2\sigma(I)$
Detector resolution: 10.00 pixels mm^{-1}	R_{int} = 0.032
ω scans	θ_{max} = 27.5º
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	h = −16→16
T_{min} = 0.225, T_{max} = 0.372	k = −12→13
13165 measured reflections	l = −14→16
3178 independent reflections	

Refinement

Refinement on F^2	$w = 1/[0.0017F_o^2 + 1.0\sigma(F_o^2)]/(4F_o^2)$
$R[F^2 > 2\sigma(F^2)]$ = 0.045	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.139	$\Delta\rho_{max}$ = 0.88 e Å^{-3}
S = 1.01	$\Delta\rho_{min}$ = −0.69 e Å^{-3}
3178 reflections	Extinction correction: Larson (1970)
137 parameters	Extinction coefficient: 28 (2)
H-atom parameters constrained	

Special details

Refinement. Refinement using all reflections. The weighted *R*-factor (*wR*) and goodness of fit (S) are based on F^2. *R*-factor (gt) are based on F. The threshold expression of $F^2 > 2.0$ sigma(F^2) is used only for calculating *R*-factor (gt).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.41438 (4)	0.56892 (5)	0.64583 (4)	0.06054 (16)
Br2	0.08574 (4)	0.16025 (5)	0.45070 (4)	0.05775 (16)
N21	0.3228 (3)	0.3124 (3)	0.4761 (2)	0.0487 (9)
N22	0.1717 (2)	0.5515 (3)	0.3133 (2)	0.0516 (10)
C1	0.4223 (4)	0.2119 (6)	0.5167 (5)	0.0741 (17)
C2	0.4018 (6)	0.1369 (6)	0.4052 (5)	0.094 (2)
C3	0.3048 (5)	0.2097 (5)	0.2990 (4)	0.0762 (18)
C4	0.2946 (3)	0.3451 (4)	0.3492 (3)	0.0481 (12)
C5	0.1739 (4)	0.4108 (4)	0.2777 (3)	0.0511 (12)
C6	0.1146 (4)	0.5837 (6)	0.3801 (4)	0.087 (2)
C7	0.1090 (7)	0.7146 (7)	0.4121 (7)	0.119 (3)
C8	0.1624 (7)	0.8095 (9)	0.3721 (7)	0.106 (3)
C9	0.2193 (5)	0.7798 (4)	0.3032 (5)	0.106 (2)
C10	0.2226 (3)	0.6472 (3)	0.2744 (4)	0.0577 (13)
C11	0.2778 (6)	0.6100 (7)	0.1949 (6)	0.119 (2)
H4	0.3570	0.4043	0.3502	0.058*
H6	0.0792	0.5168	0.4044	0.104*
H7	0.0712	0.7378	0.4582	0.142*
H8	0.1598	0.8982	0.3927	0.127*
H9	0.2539	0.8461	0.2773	0.128*
H101	0.4190	0.1520	0.5763	0.089*
H102	0.4995	0.2563	0.5514	0.089*
H111	0.3484	0.5576	0.2404	0.143*
H112	0.2213	0.5592	0.1271	0.143*
H113	0.2989	0.6896	0.1663	0.143*
H201	0.3764	0.0464	0.4090	0.112*
H202	0.4750	0.1345	0.3974	0.112*
H211	0.3489	0.3871	0.5289	0.057*
H212	0.2604	0.2740	0.4796	0.057*
H301	0.3271	0.2205	0.2347	0.091*
H302	0.2295	0.1617	0.2683	0.091*
H501	0.1534	0.4084	0.1925	0.061*
H502	0.1146	0.3610	0.2905	0.061*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0632 (3)	0.0577 (3)	0.0598 (3)	−0.0061 (2)	0.0278 (2)	−0.0152 (2)
Br2	0.0576 (3)	0.0641 (3)	0.0493 (3)	−0.0091 (2)	0.0228 (2)	0.0049 (2)

N21	0.0508 (19)	0.050 (2)	0.0420 (18)	−0.0043 (16)	0.0184 (15)	−0.0055 (15)
N22	0.0438 (18)	0.064 (2)	0.0402 (18)	0.0065 (17)	0.0138 (14)	−0.0026 (17)
C1	0.071 (3)	0.074 (3)	0.068 (3)	0.024 (2)	0.024 (2)	0.005 (2)
C2	0.125 (5)	0.070 (4)	0.074 (3)	0.039 (3)	0.036 (3)	0.005 (3)
C3	0.112 (4)	0.060 (3)	0.062 (3)	0.015 (3)	0.045 (3)	−0.008 (2)
C4	0.057 (2)	0.043 (2)	0.048 (2)	−0.0016 (19)	0.0284 (19)	−0.0019 (18)
C5	0.056 (2)	0.050 (2)	0.041 (2)	−0.012 (2)	0.0174 (18)	−0.0013 (19)
C6	0.053 (2)	0.147 (6)	0.051 (2)	0.025 (3)	0.017 (2)	−0.004 (3)
C7	0.087 (5)	0.153 (12)	0.079 (5)	0.023 (6)	0.008 (4)	−0.019 (7)
C8	0.081 (7)	0.110 (8)	0.075 (6)	0.067 (6)	−0.007 (4)	−0.012 (5)
C9	0.087 (4)	0.058 (3)	0.107 (5)	0.011 (3)	−0.012 (4)	−0.007 (3)
C10	0.051 (2)	0.044 (2)	0.061 (2)	0.002 (2)	0.011 (2)	0.006 (2)
C11	0.148 (6)	0.089 (5)	0.110 (5)	−0.021 (5)	0.052 (5)	0.030 (4)

Geometric parameters (Å, °)

N21—C1	1.500 (6)	C1—H101	0.970
N21—C4	1.488 (6)	C1—H102	0.970
N22—C5	1.483 (5)	C2—H201	0.970
N22—C6	1.367 (7)	C2—H202	0.970
N22—C10	1.361 (6)	C3—H301	0.970
C1—C2	1.494 (9)	C3—H302	0.970
C2—C3	1.509 (7)	C4—H4	0.980
C3—C4	1.524 (7)	C5—H501	0.970
C4—C5	1.511 (5)	C5—H502	0.970
C6—C7	1.383 (10)	C6—H6	0.930
C7—C8	1.384 (13)	C7—H7	0.930
C8—C9	1.382 (13)	C8—H8	0.930
C9—C10	1.382 (6)	C9—H9	0.930
C10—C11	1.496 (11)	C11—H111	0.960
N21—H211	0.949	C11—H112	0.960
N21—H212	0.895	C11—H113	0.960
Br1···N21	3.186 (3)	H101···H201^{ix}	3.192
Br2···N21	3.234 (4)	H101···H202^{ix}	3.119
Br2···N22^{i}	3.554 (2)	H101···H301^{vi}	2.998
Br2···C10^{i}	3.586 (3)	H102···Br1^{iii}	3.571
N21···Br1	3.186 (3)	H102···C9^{iii}	3.161
N21···Br2	3.234 (4)	H102···C10^{iii}	3.293
N22···Br2^{ii}	3.554 (2)	H102···C11^{iii}	3.381
C10···Br2^{ii}	3.586 (3)	H102···H9^{iii}	3.017
Br1···H4^{iii}	2.868	H102···H111^{iii}	3.045
Br1···H9^{iv}	3.250	H102···H113^{iii}	3.292
Br1···H101^{v}	3.217	H102···H201^{ix}	3.343
Br1···H102^{iii}	3.571	H111···Br1^{iii}	2.934
Br1···H111^{iii}	2.934	H111···H101^{xiii}	3.326
Br1···H113^{iv}	2.895	H111···H102^{iii}	3.045

Br1···H202^{iii}	3.429	H111···H202^{xiv}	3.467
Br1···H202^{vi}	3.514	H111···H211^{iii}	3.596
Br1···H211	2.239	H112···Br2^{xiii}	3.018
Br1···H301^{iii}	3.574	H112···C7^{xi}	3.288
Br1···H301^{vi}	3.461	H112···C8^{xi}	3.193
Br2···H7^{vii}	2.883	H112···H7^{xi}	2.908
Br2···H8^{viii}	2.986	H112···H8^{xi}	2.686
Br2···H112^{vi}	3.018	H112···H101^{xiii}	3.540
Br2···H212	2.351	H113···Br1^{xi}	2.895
Br2···H302	3.501	H113···C7^{xi}	3.106
Br2···H501^{vi}	2.810	H113···C8^{xi}	3.248
Br2···H502	2.973	H113···H7^{xi}	2.929
N21···H301^{vi}	3.215	H113···H8^{xi}	3.150
C1···H201^{ix}	3.437	H113···H102^{iii}	3.292
C1···H301^{vi}	3.505	H113···H202^{xiv}	3.336
C2···H9^{viii}	3.428	H201···C1^{ix}	3.437
C2···H201^{ix}	3.246	H201···C2^{ix}	3.246
C2···H202^{ix}	3.510	H201···C8^{viii}	3.458
C5···H7^{i}	3.572	H201···C9^{viii}	3.221
C7···H112^{iv}	3.288	H201···H8^{viii}	3.027
C7···H113^{iv}	3.106	H201···H9^{viii}	2.600
C7···H501^{ii}	3.520	H201···H101^{ix}	3.192
C7···H502^{ii}	3.141	H201···H102^{ix}	3.343
C8···H112^{iv}	3.193	H201···H201^{ix}	3.026
C8···H113^{iv}	3.248	H201···H202^{ix}	2.903
C8···H201^{x}	3.458	H202···Br1^{iii}	3.429
C8···H502^{ii}	3.160	H202···Br1^{xiii}	3.514
C9···H102^{iii}	3.161	H202···C2^{ix}	3.510
C9···H201^{x}	3.221	H202···H101^{ix}	3.119
C10···H102^{iii}	3.293	H202···H111^{xv}	3.467
C11···H7^{xi}	3.268	H202···H113^{xv}	3.336
C11···H8^{xi}	3.348	H202···H201^{ix}	2.903
C11···H102^{iii}	3.381	H202···H202^{ix}	3.566
H4···Br1^{iii}	2.868	H211···Br1	2.239
H7···Br2^{vii}	2.883	H211···H111^{iii}	3.596
H7···C5^{ii}	3.572	H211···H301^{vi}	2.910
H7···C11^{iv}	3.268	H212···Br2	2.351
H7···H112^{iv}	2.908	H212···H301^{vi}	2.888
H7···H113^{iv}	2.929	H301···Br1^{iii}	3.574
H7···H501^{ii}	3.086	H301···Br1^{xiii}	3.461
H7···H502^{ii}	3.144	H301···N21^{xiii}	3.215

H8···Br2^{x}	2.986	H301···C1^{xiii}	3.505
H8···C11^{iv}	3.348	H301···H101^{xiii}	2.998
H8···H112^{iv}	2.686	H301···H211^{xiii}	2.910
H8···H113^{iv}	3.150	H301···H212^{xiii}	2.888
H8···H201^{x}	3.027	H302···Br2	3.501
H8···H302^{x}	3.378	H302···H8^{viii}	3.378
H8···H501^{ii}	3.578	H302···H9^{viii}	3.175
H8···H502^{ii}	3.159	H501···Br2^{xiii}	2.810
H9···Br1^{xi}	3.250	H501···C7^{i}	3.520
H9···C2^{x}	3.428	H501···H7^{i}	3.086
H9···H102^{iii}	3.017	H501···H8^{i}	3.578
H9···H201^{x}	2.600	H502···Br2	2.973
H9···H302^{x}	3.175	H502···C7^{i}	3.141
H101···Br1^{xii}	3.217	H502···C8^{i}	3.160
H101···H111^{vi}	3.326	H502···H7^{i}	3.144
H101···H112^{vi}	3.540	H502···H8^{i}	3.159
C1—N21—C4	104.9 (4)	C3—C2—H201	110.1
C5—N22—C6	119.6 (4)	C3—C2—H202	110.1
C5—N22—C10	119.1 (4)	H201—C2—H202	109.5
C6—N22—C10	121.2 (4)	C2—C3—H301	110.6
N21—C1—C2	105.5 (4)	C2—C3—H302	110.6
C1—C2—C3	107.0 (5)	C4—C3—H301	110.6
C2—C3—C4	105.0 (4)	C4—C3—H302	110.6
N21—C4—C3	102.5 (3)	H301—C3—H302	109.5
N21—C4—C5	113.7 (4)	N21—C4—H4	109.0
C3—C4—C5	113.5 (3)	C3—C4—H4	109.0
N22—C5—C4	113.0 (3)	C5—C4—H4	109.0
N22—C6—C7	120.7 (6)	N22—C5—H501	108.6
C6—C7—C8	116.8 (9)	N22—C5—H502	108.6
C7—C8—C9	123.6 (8)	C4—C5—H501	108.6
C8—C9—C10	117.1 (6)	C4—C5—H502	108.6
N22—C10—C9	120.6 (5)	H501—C5—H502	109.5
N22—C10—C11	120.0 (4)	N22—C6—H6	119.7
C9—C10—C11	119.3 (5)	C7—C6—H6	119.7
C1—N21—H211	109.2	C6—C7—H7	121.6
C1—N21—H212	108.0	C8—C7—H7	121.6
C4—N21—H211	113.5	C7—C8—H8	118.2
C4—N21—H212	111.3	C9—C8—H8	118.2
H211—N21—H212	109.6	C8—C9—H9	121.5
N21—C1—H101	110.5	C10—C9—H9	121.5
N21—C1—H102	110.5	C10—C11—H111	109.5
C2—C1—H101	110.5	C10—C11—H112	109.5
C2—C1—H102	110.5	C10—C11—H113	109.5
H101—C1—H102	109.5	H111—C11—H112	109.5
C1—C2—H201	110.1	H111—C11—H113	109.5

C1—C2—H202	110.1	H112—C11—H113	109.5
C1—N21—C4—C3	39.2 (4)	N21—C1—C2—C3	9.6 (7)
C1—N21—C4—C5	162.2 (3)	C1—C2—C3—C4	14.4 (7)
C4—N21—C1—C2	−30.8 (5)	C2—C3—C4—N21	−32.9 (6)
C5—N22—C6—C7	−178.5 (4)	C2—C3—C4—C5	−155.9 (5)
C6—N22—C5—C4	−106.0 (4)	N21—C4—C5—N22	73.6 (5)
C5—N22—C10—C9	178.2 (3)	C3—C4—C5—N22	−169.7 (4)
C5—N22—C10—C11	1.1 (5)	N22—C6—C7—C8	0.7 (7)
C10—N22—C5—C4	76.7 (4)	C6—C7—C8—C9	0.2 (7)
C6—N22—C10—C9	1.0 (5)	C7—C8—C9—C10	−0.4 (9)
C6—N22—C10—C11	−176.2 (3)	C8—C9—C10—N22	−0.1 (5)
C10—N22—C6—C7	−1.3 (6)	C8—C9—C10—C11	177.0 (5)

Symmetry codes: (i) −*x*, *y*−1/2, −*z*+1/2; (ii) −*x*, *y*+1/2, −*z*+1/2; (iii) −*x*+1, −*y*+1, −*z*+1; (iv) *x*, −*y*+3/2, *z*+1/2; (v) −*x*+1, *y*+1/2, −*z*+3/2; (vi) *x*, −*y*+1/2, *z*+1/2; (vii) −*x*, −*y*+1, −*z*+1; (viii) *x*, *y*−1, *z*; (ix) −*x*+1, −*y*, −*z*+1; (x) *x*, *y*+1, *z*; (xi) *x*, −*y*+3/2, *z*−1/2; (xii) −*x*+1, *y*−1/2, −*z*+3/2; (xiii) *x*, −*y*+1/2, *z*−1/2; (xiv) −*x*+1, *y*+1/2, −*z*+1/2; (xv) −*x*+1, *y*−1/2, −*z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N21—H211···Br1	0.95	2.24	3.186 (3)	176
N21—H212···Br2	0.90	2.35	3.233 (3)	169

Fig. 1

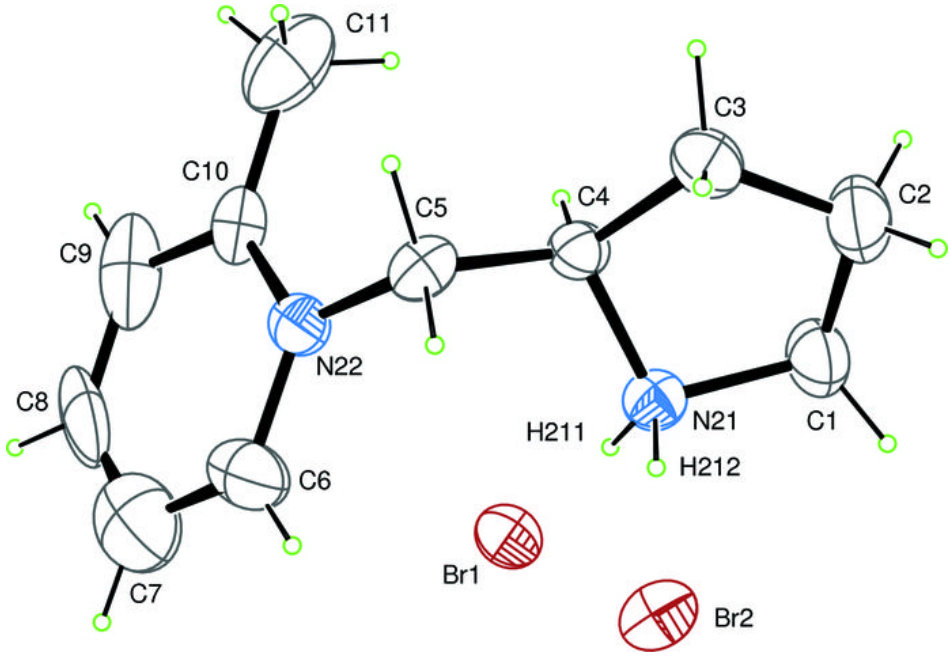


Fig. 2