

[CN<sub>3</sub>H<sub>6</sub>]<sub>2</sub>[S<sub>2</sub>O<sub>6</sub>]

*hP32*

(186) *P6<sub>3</sub>mc* – c<sup>4</sup>b<sup>3</sup>a

[C(NH<sub>2</sub>)<sub>3</sub>]<sub>2</sub>S<sub>2</sub>O<sub>6</sub> [1]

Structural features: Planar CN<sub>3</sub>H<sub>6</sub> units (a central CN<sub>3</sub> triangle, two H bonded to each N; perpendicular to [001]) and O<sub>3</sub>S-SO<sub>3</sub> units (parallel to [001]) in an approximate Ni<sub>2</sub>In-type (ht-Co<sub>2</sub>Ge) arrangement.

Russell V.A. et al. (1997) [1]

C<sub>2</sub>H<sub>12</sub>N<sub>6</sub>O<sub>6</sub>S<sub>2</sub>

*a* = 0.7504, *c* = 1.2129 nm, *c/a* = 1.616, *V* = 0.5915 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	6 <i>c</i>	. <i>m</i> .	0.2258	0.7742	0.2578		single atom S
O2	6 <i>c</i>	. <i>m</i> .	0.4406	0.5594	0.0242		single atom S
N3	6 <i>c</i>	. <i>m</i> .	0.7686	0.2314	0.254		single atom C
N4	6 <i>c</i>	. <i>m</i> .	0.8979	0.1021	0.0013		single atom C
S5	2 <i>b</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.053		tetrahedron O <sub>3</sub> S
S6	2 <i>b</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.228		tetrahedron O <sub>3</sub> S
C7	2 <i>b</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.755		non-coplanar triangle N <sub>3</sub>
C8	2 <i>a</i>	3 <i>m</i> .	0	0	0.0		non-coplanar triangle N <sub>3</sub>
H9	12 <i>d</i>	1	0.2773	0.029	0.003		
H10	12 <i>d</i>	1	0.3894	0.085	0.2537		

Transformation from published data: -*x*, -*y*, -*z*; origin shift 0 0 0.609

Experimental: single crystal, diffractometer, X-rays, *R* = 0.066, *T* = 293 K

Remarks: Bis(guanidinium) dithionate. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Russell V.A., Evans C.C., Li W., Ward M.D. (1997), *Science* (Washington D.C.) 276, 575-579.