Table 27A-2-001. HBr, DBr. Unit cell parameters.

Compound	Phase	T [K]	a, b, c [Å]	Ref.
HBr	I	130	a = 5.815(2)	71Sim
	II	115	a = 5.785(2)	
	III	100	a = 5.555(3) b = 5.648(2) c = 6.086(2)	
	IV	85	a = 5.462(3) b = 5.643(3) c = 6.111(3)	
DBr	III	107	a = 5.559(5) b = 5.649(5) c = 6.095(5)	68San
	IV	84	a = 5.44(2) b = 5.614(5) c = 6.120(5)	

Table 27A-2-002. DBr. Fractional coordinates and temperature parameters [68San]. B is defined by Eq. (e) in Introduction.

Atom	x	y	z	B [Å^2]	x	y	z	B [Å^2]
	T = 84 K (phase IV)				T = 107 K (phase III)			
D	0.075(2)	0.179(3)	0	5.0(5)	–0.172(6)	0.177(4)	0	8.4(8)
Br	0.25	0	0	2.1(4)	0	0	0	4.4(8)

Table 27A-2-003. HBr. Linear thermal expansion coefficients [71Sim].

Phase	T [K]	α_{ij} [$\cdot 10^{-6}$ K^{-1}]
I	130	α_{11} = 225(15)
II	115	α_{11} = 225(40)
III	100	α_{11} = 430(20) α_{22} = 370(20) α_{33} = –60(30)

Table 27A-2-004. HBr, DBr. Transition heats and transition entropies.

Compound	Transition	ΔQ_m [J mol^{-1}]	ΔS_m [J K^{-1} mol^{-1}]	Ref.
HBr	I–II–III	691	5.98	24Euc
	III–IV	472	5.27	
DBr	I–III	1267	10.5	47Clu
	III–IV	709	7.6	