$BaFe_4O_7$	*hP*24	(176) $P6_3/m$ – ifeda

$BaFe_4O_7$ [1]
Structural features: Two close-packed O_3 and deficient triangle-mesh Ba□O (hexagon-mesh BaO) layers in c_2h stacking; Fe in octahedral (O_6) and tetrahedral (O_4) voids. Infinite layers of edge-linked FeO_6 octahedra with 6-rings are interconnected via common vertices with units of two vertex-linked FeO_4 tetrahedra to form a 3D-framework.

Okamoto S. et al. (1973) [1]
$BaFe_4O_7$
$a = 0.516$, $c = 1.3811$ nm, $c/a = 2.677$, $V = 0.3185$ nm^3, $Z = 2$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
O1	12*i*	1	0.3435	0.0058	0.079		non-coplanar triangle Fe_3
Fe2	4*f*	3..	$^1/_3$	$^2/_3$	0.0089		octahedron O_6
Fe3	4*e*	3..	0	0	0.1149		tetrahedron O_4
Ba4	2*d*	-6..	$^2/_3$	$^1/_3$	$^1/_4$		tricapped trigonal prism O_9
O5	2*a*	-6..	0	0	$^1/_4$		colinear Fe_2

Transformation from published data: *y*,*x*,-*z*
Experimental: single crystal, Weissenberg photographs, X-rays, R = 0.080

References: [1] Okamoto S., Okamoto S.I., Ito T. (1973), Acta Crystallogr. B 29, 832-838.