Supplementary materials:

B = BOCROC, C = NUCLOO

Comparison of pertinent bond lengths and angles $(\mathring{A}, {}^{\circ})$.

Metric*	1	BOCROC	NUCLOO	QOCGIA
a	1.720(2)	1.711(4)	1.7182 (15)	1.740(2)
ь	1.729(2)	1.740(4)	1.7373 (15)	1.735 (3)
c	1.419(2)	1.417 (5)	1.3974 (19)	1.414(4)
d	1.337(2)	1.341(4)	1.3314 (19)	1.373 (4)
e	1.341(3)	1.329 (5)	1.328(2)	1.309(3)
f	1.396(2)	1.395 (4)	1.3806 (17)	1.381(3)
g	1.283(3)	1.275 (5)	1.280(2)	1.293 (4)
h	121.16 (15)	123.0(3)	124.94 (11)	126.51 (19)
i	125.43 (18)	123.8 (3)	122.85 (13)	122.3 (2)
j	111.65 (17)	114.9(3)	117.49 (12)	109.4(2)
k	118.09 (17)	115.5 (3)	114.40 (13)	116.0(2)

^{*}Key is A in Scheme 2.