Supplementary materials:


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

| Metric* | $I$ | BOCROC | NUCLOO | QOCGIA |
| :--- | :--- | :--- | :--- | :--- |
| a | $1.720(2)$ | $1.711(4)$ | $1.7182(15)$ | $1.740(2)$ |
| b | $1.729(2)$ | $1.740(4)$ | $1.7373(15)$ | $1.735(3)$ |
| c | $1.419(2)$ | $1.417(5)$ | $1.3974(19)$ | $1.414(4)$ |
| d | $1.337(2)$ | $1.341(4)$ | $1.3314(19)$ | $1.373(4)$ |
| c | $1.341(3)$ | $1.329(5)$ | $1.328(2)$ | $1.309(3)$ |
| 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 | $121.16(15)$ | $123.0(3)$ | $124.94(11)$ | $126.51(19)$ |
| f | $125.43(18)$ | $123.8(3)$ | $122.85(13)$ | $122.3(2)$ |
| 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 $\mathbf{A}$ in Sobeme 2.

