



STRUCTURAL
CHEMISTRY

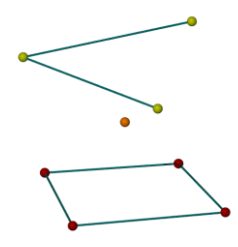
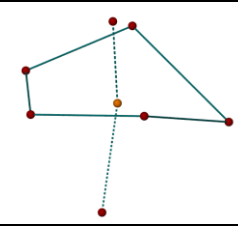
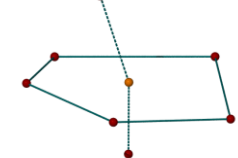
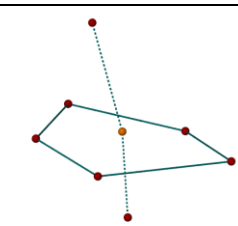
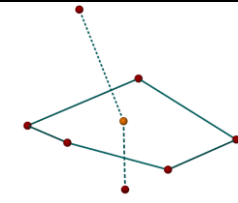
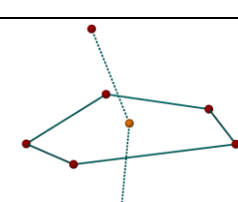
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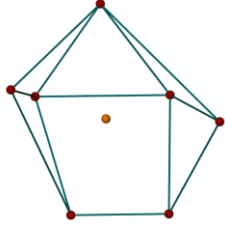
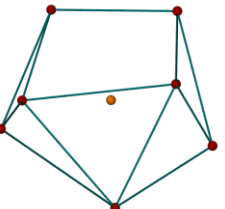
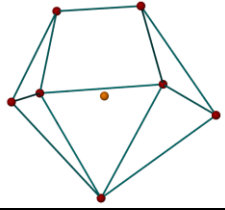
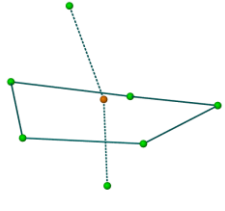
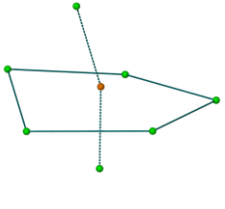
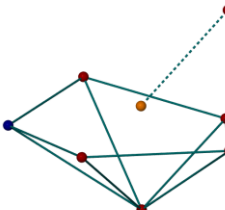
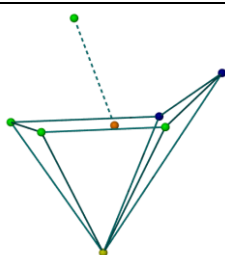
Supporting information for article:

Ψ -Polyhedral symbols for bismuth(III) with an active electron lone-pair

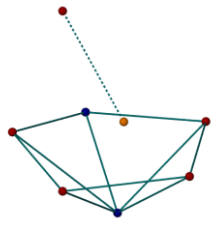
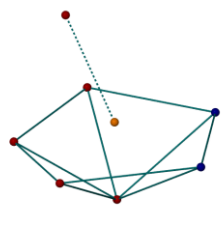
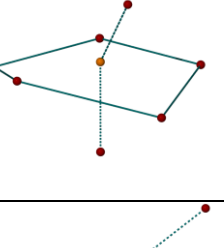
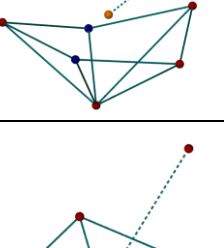
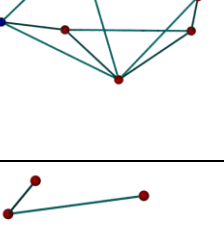
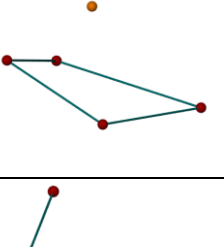
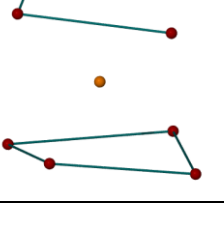
Seik Weng Ng

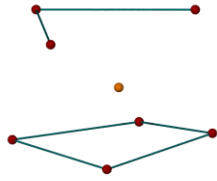
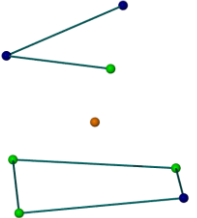
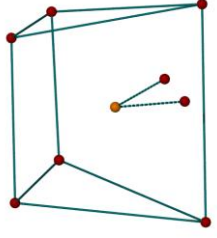
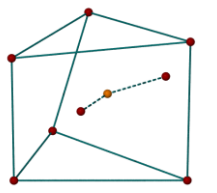
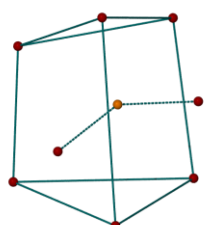
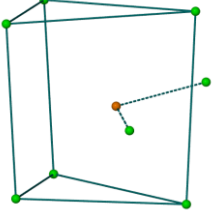
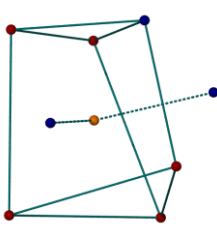
Table S1 Bi(III) in high coordination (C.N. ≥ 8) showing stereochemical activity*

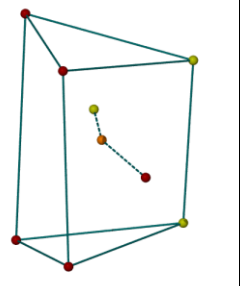
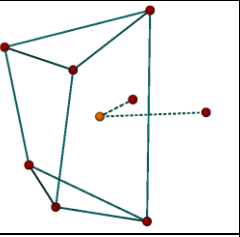
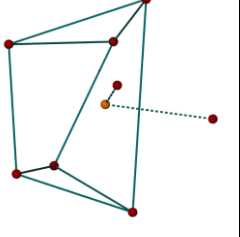
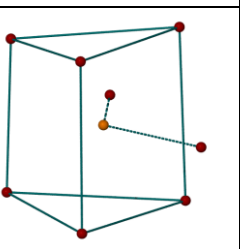
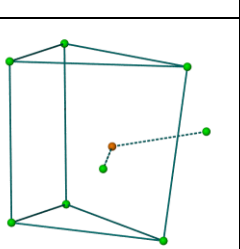
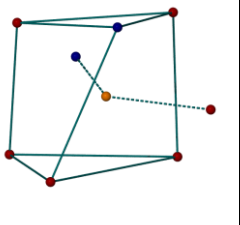
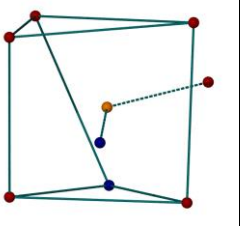
Formula	C.N.		Polyhedral symbol	Reference
$\text{Bi}_2\text{Cl}_6(\text{H}_2\text{O})(\text{C}_{12}\text{H}_{24}\text{O}_6)_2$ Bi at (0, 0.1473, 0)	8		$\Psi\text{-CU-8}$	Drew <i>et al.</i> , 1990
$[\text{Bi}_4\text{O}_2(\text{H}_2\text{O})_2(\text{C}_8\text{H}_4\text{O}_7\text{S})_3]\cdot\text{H}_2\text{O}$ Bi at (-0.0506, 0.2383, -0.0884)	8		$\Psi\text{-DD-8}$	Albat <i>et al.</i> , 2017
$\text{Bi}_4\text{O}_3(\text{H}_2\text{O})_2(\text{C}_8\text{H}_4\text{O}_7\text{S})_2$ Bi at (0.5048, 0.0253, 0.2737)	8		$\Psi\text{-DD-8}$	Albat <i>et al.</i> , 2017
$\text{Bi}_4\text{O}_3(\text{H}_2\text{O})_2(\text{C}_8\text{H}_4\text{O}_7\text{S})_2$ Bi at (0.7432, 0.7241, 0.2225)	8		$\Psi\text{-DD-8}$	Albat <i>et al.</i> , 2017
$\text{Bi}_2(\text{OH})_2(\text{C}_{12}\text{H}_2\text{O}_8\text{S})$ Bi at (0.0213, 0.9424, 0.7961)	8		$\Psi\text{-DD-8}$	Albat & Stock, 2018
$\text{Bi}_2(\text{OH})_2(\text{C}_{12}\text{H}_2\text{O}_8\text{S})$ Bi at (0.9210, 0.6342, 0.2793)	8		$\Psi\text{-DD-8}$	Albat & Stock, 2018

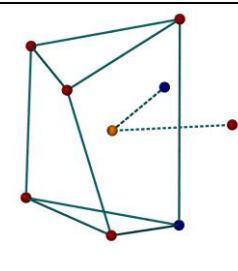
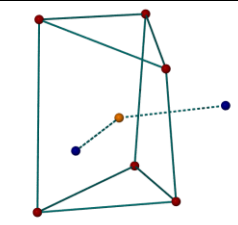
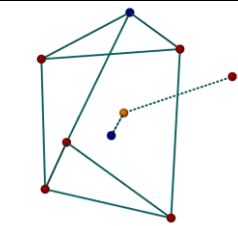
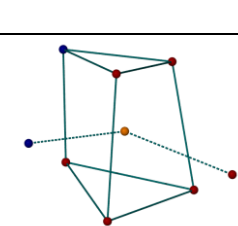
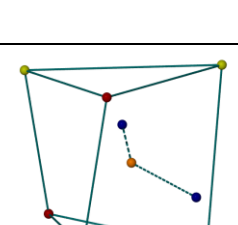
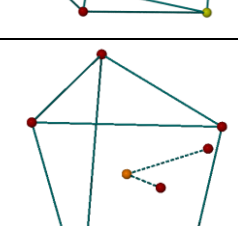
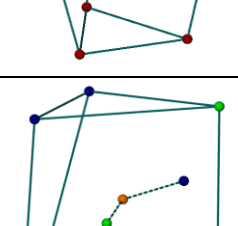
$\text{Bi}_2(\text{OH})_2(\text{C}_{12}\text{H}_2\text{O}_8\text{S})$ Bi at (0.9909, 0.8220, 0.4303)	8		Ψ-DD-8	Albat & Stock, 2018
$\text{Bi}_8\text{O}_7(\text{OH})_2(\text{H}_2\text{O})_2(\text{C}_{12}\text{H}_2\text{O}_8\text{S}_2)_2$	8		Ψ-DD-8	Albat & Stock, 2018
$[\text{Bi}_7\text{O}_5(\text{OH})_3(\text{H}_2\text{O})_4(\text{C}_{12}\text{H}_2\text{O}_8\text{S}_2)_2] \cdot 4\text{H}_2\text{O}$	8		Ψ-DD-8	Albat & Stock, 2018
$\text{Bi}_2(\text{C}_{13}\text{H}_{11}\text{N}_2\text{O}_3\text{S}_2)_6$	8		Ψ-DD-8	Anamika <i>et al.</i> , 2019
$\text{Bi}_2(\text{C}_{16}\text{H}_{16}\text{NOS}_2)_6$	8		Ψ-DD-8	Anamika <i>et al.</i> , 2019
$\text{Bi}_4\text{O}_4(\text{C}_7\text{H}_3\text{NO}_4)_2$ Bi at (0.3581, 0.1965, 0.7551)	8		Ψ-DD-8	Feng, Chen <i>et al.</i> , 2018
$\text{Bi}(\text{C}_{12}\text{H}_8\text{N}_2)(\text{C}_4\text{H}_8\text{NOS}_2)_2$	8		Ψ-DD-8	Li <i>et al.</i> , 2014

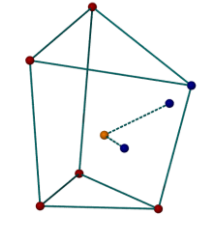
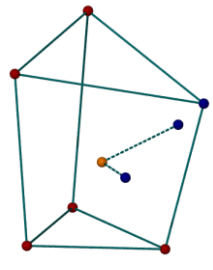
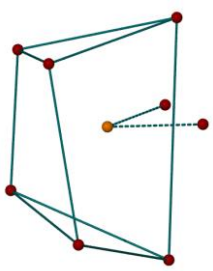
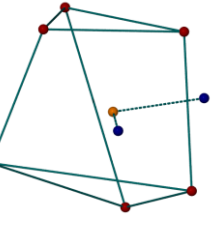
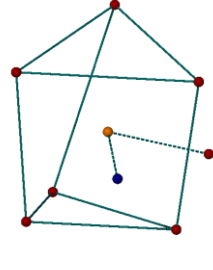
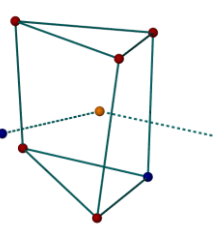
$\text{Bi}_2\text{Br}_5(\text{NO}_3)(\text{C}_{12}\text{H}_8\text{N}_2)_2$	8		Ψ -DD-8	Morsali & Mahjoub, 2006
$[\text{Bi}_2(\text{C}_6\text{H}_6\text{NO}_3)_6] \cdot 0.5\text{C}_3\text{H}_6\text{O}$ Bi at (0.4646, 0.8740, 0.4529)	8		Ψ -DD-8	Pathak <i>et al.</i> , 2015
$[\text{Bi}_2(\text{C}_6\text{H}_6\text{NO}_3)_6] \cdot 0.5\text{C}_3\text{H}_6\text{O}$ Bi at (0.5618, 0.6262, 0.9256)	8		Ψ -DD-8	Pathak <i>et al.</i> , 2015
$[\text{Bi}_2(\text{C}_{13}\text{H}_{10}\text{NO}_2)_6] \cdot \text{C}_2\text{H}_6\text{O}$	8		Ψ -DD-8	Pathak <i>et al.</i> , 2015
$[\text{Bi}_2(\text{C}_7\text{H}_5\text{NO}_3)_3(\text{C}_7\text{H}_7\text{NO}_3)_3][\text{Bi}_2(\text{C}_7\text{H}_5\text{NO}_3)(\text{C}_7\text{H}_5\text{NO}_3)_3(\text{C}_2\text{H}_6\text{O}_5)_4] \cdot 4\text{C}_2\text{H}_6\text{OS}$ Bi at (0.7394, 0.5312, 0.0126)	8		Ψ -DD-8	Pathak <i>et al.</i> , 2105
$2\text{C}_2\text{H}_8\text{N} \cdot [\text{Bi}(\text{C}_3\text{H}_7\text{NO})(\text{C}_8\text{H}_2\text{NO}_6)(\text{C}_8\text{H}_3\text{NO}_6)] \cdot 0.5\text{C}_2\text{H}_7\text{N}$ Bi at (0.5994, 0.5091, 0.6637)	8		Ψ -DD-8	Senior & Linden, 2020
$\text{Bi}(\text{C}_8\text{H}_7\text{O}_2)_3$	8		Ψ -DD-8	Sharutin <i>et al.</i> , 2004

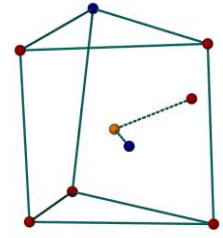
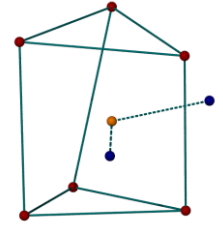
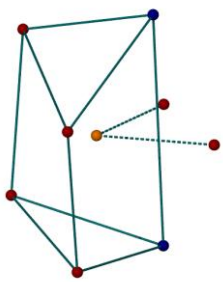
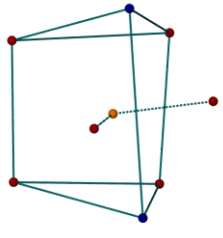
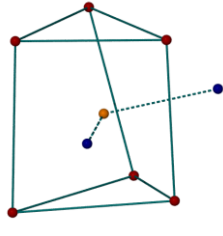
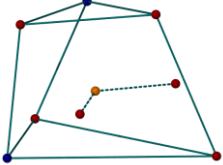
$[\text{Bi}_2(\text{C}_{10}\text{H}_8\text{N}_2)_2(\text{C}_7\text{H}_5\text{O}_3)_6] \cdot 2\text{C}_7\text{H}_8$	8		Ψ -DD-8	Thurston <i>et al.</i> , 2002
$[\text{Bi}_2(\text{C}_{12}\text{H}_8\text{N}_2)_2(\text{C}_7\text{H}_5\text{O}_3)_2(\text{C}_7\text{H}_6\text{O}_3)_2] \cdot 2\text{C}_7\text{H}_8$	8		Ψ -DD-8	Thurston <i>et al.</i> , 2002
$\text{Bi}_2\text{O}_2(\text{C}_7\text{H}_3\text{NO}_4)$ Bi at (0.3499, 0.2106, 0.1329)	8		Ψ -DD-8	Wibowo <i>et al.</i> , 2012
$\text{Bi}(\text{H}_2\text{O})(\text{C}_7\text{H}_3\text{NO}_4)(\text{C}_7\text{H}_4\text{NO}_4)$	8		Ψ -DD-8	Wibowo <i>et al.</i> , 2011b
$[\text{Bi}_3\text{O}_2(\text{H}_2\text{O})(\text{C}_7\text{H}_3\text{NO}_4)_2(\text{C}_7\text{H}_4\text{NO}_4)] \cdot \text{H}_2\text{O}$ Bi at (0.5121, 0.6039, 0.2702)	8		Ψ -DD-8	Wibowo <i>et al.</i> , 2010
$\text{Bi}_2(\text{OH})_2(\text{C}_{12}\text{H}_2\text{O}_8\text{S}_2)$ Bi at (1.2587, 0.8645, 0.2466)	8		Ψ -SAPR-8	Albat & Stock, 2018
$\text{Bi}_2(\text{OH})_2(\text{H}_2\text{O})_2(\text{C}_{12}\text{H}_2\text{O}_8\text{S}_2)(\text{C}_{12}\text{H}_4\text{O}_8\text{S}_2)$ Bi at (0.4355, 0.0951, 0.5401)	8		Ψ -SAPR-8	Albat & Stock, 2018

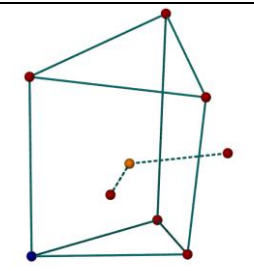
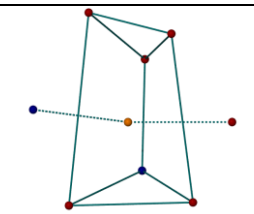
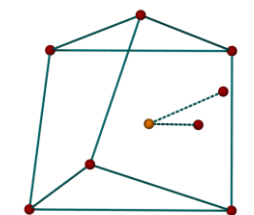
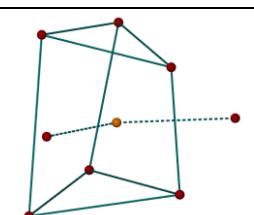
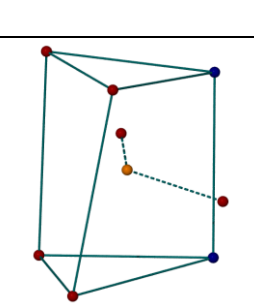
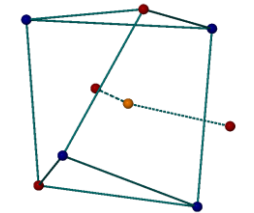
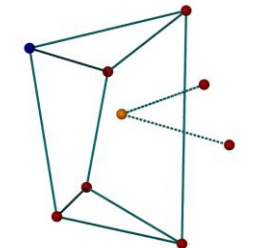
$[\text{Bi}_6\text{O}_4(\text{OH})_4(\text{H}_2\text{O})_{12}(\text{C}_{12}\text{H}_4\text{O}_8\text{S}_2)_3] \cdot x\text{H}_2\text{O}$ Bi at (0.1576, 1.0325, 1.0921)	8		Ψ-SAPR-8	Albat & Stock, 2018
$\text{Bi}(\text{SCN})_3 \cdot 0.5\text{H}_2\text{O}$ Bi at (0.3016, 0.2691, 0.0783)	8		Ψ-SAPR-8	Koch & Ruck, 2010
$[\text{Bi}_4\text{O}_2(\text{H}_2\text{O})_2(\text{C}_8\text{H}_4\text{O}_7\text{S})_3] \cdot \text{H}_2\text{O}$ Bi at (0.0455, 0.2839, 0.0887)	9		Ψ-TPRS-9	Albat <i>et al.</i> , 2017
$\text{Bi}_4\text{O}_3(\text{H}_2\text{O})_2(\text{C}_8\text{H}_4\text{O}_7\text{S})_2$ Bi at (0.6928, 0.2837, 0.2841)	9		Ψ-TPRS-9	Albat <i>et al.</i> , 2017
$\text{Bi}_4\text{O}_3(\text{H}_2\text{O})_2(\text{C}_8\text{H}_4\text{O}_7\text{S})_2$ Bi at (1.2291, 0.7989, 0.2857)	9		Ψ-TPRS-9	Albat <i>et al.</i> , 2017
$\text{Bi}_2(\text{C}_{10}\text{H}_{12}\text{N}_3\text{S}_2)_6$	9		Ψ-TPRS-9	Anamika <i>et al.</i> , 2019
$[\text{Co}(\text{CH}_4\text{N}_2\text{S})_3][\text{Bi}(\text{C}_{14}\text{H}_{18}\text{N}_3\text{O}_{10})] \cdot 0.5(\text{SO}_4) \cdot 3\text{H}_2\text{O}$	9		Ψ-TPRS-9	Bulimestru <i>et al.</i> , 2005

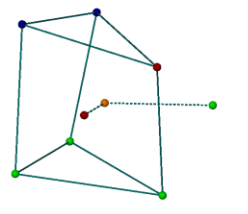
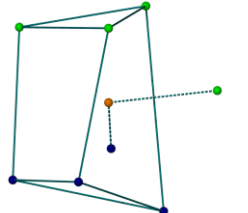
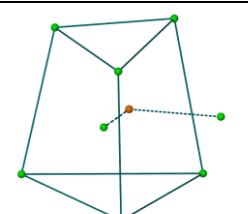
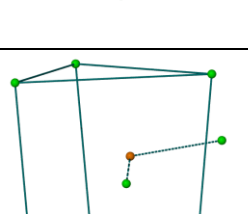
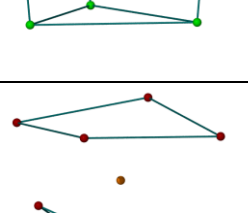
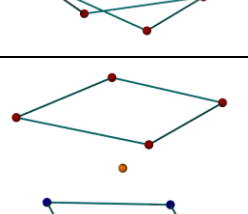
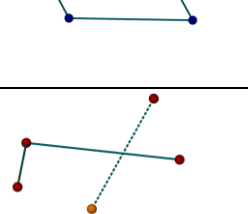
$\text{Bi}_2\text{Cl}_6(\text{H}_2\text{O})(\text{C}_{12}\text{H}_{24}\text{O}_6)_2$ Bi at (0.5474, 0.3256, 0.3687)	9		Ψ -TPRS-9	Drew <i>et al.</i> , 1990
$\text{Bi}(\text{C}_8\text{H}_2\text{O}_8)(\text{C}_8\text{H}_3\text{O}_8)] \cdot 2.5\text{C}_3\text{H}_7\text{NO}$	9		Ψ -TPRS-9	Gao & Zhang, 2012
$\text{Bi}_2(\text{H}_2\text{O})_4(\text{C}_2\text{H}_4\text{O}_6\text{S}_2)_3$	9		Ψ -TPRS-9	Gschwind & Jansen, 2012
$[\text{Bi}(\text{C}_2\text{H}_6\text{OS})_3][\text{Fe}(\text{NCS})_6]$	9		Ψ -TPRS-9	Gumbris <i>et al.</i> , 2012
$\text{Bi}_2(\text{C}_{10}\text{H}_{12}\text{NS}_2)_6$	9		Ψ -TPRS-9	Guo <i>et al.</i> , 2015
$\text{C}_6\text{H}_{16}\text{N}_3[\text{Bi}_2(\text{H}_2\text{O})_2(\text{C}_7\text{H}_3\text{NO}_4)_3(\text{C}_7\text{H}_4\text{NO}_4)] \cdot 5\text{H}_2\text{O}$ Bi at (0.0721, 0.3569, 0.4871)	9		Ψ -TPRS-9	Hakimi <i>et al.</i> , 2015
$\text{C}_6\text{H}_{16}\text{N}_3[\text{Bi}_2(\text{H}_2\text{O})_2(\text{C}_7\text{H}_3\text{NO}_4)_3(\text{C}_7\text{H}_4\text{NO}_4)] \cdot 5\text{H}_2\text{O}$ Bi at (0.5801, 0.1413, 0.5179)	9		Ψ -TPRS-9	Hakimi <i>et al.</i> , 2015

$\text{Bi}_2(\text{C}_{10}\text{H}_8\text{N}_2)_2(\text{C}_7\text{H}_5\text{O}_2)_6$ Bi at (0.2610, 0.2679, 0.6642)	9		Ψ -TPRS-9	He <i>et al.</i> , 2020
$[\text{Bi}_2(\text{C}_7\text{H}_3\text{NO}_4)_2(\text{C}_7\text{H}_4\text{NO}_4)_2] \cdot \text{H}_2\text{O}$ Bi at (-0.2107, 0.7218, 0.0879)	9		Ψ -TPRS-9	Huang <i>et al.</i> , 2016
$[\text{Bi}_2(\text{C}_7\text{H}_3\text{NO}_4)_2(\text{C}_7\text{H}_4\text{NO}_4)_2] \cdot \text{H}_2\text{O}$ Bi at (0.0230, 0.5656, 0.2490)	9		Ψ -TPRS-9	Huang <i>et al.</i> , 2016
$[\text{BaBi}_2(\text{H}_2\text{O})(\text{C}_{10}\text{H}_{12}\text{N}_2\text{O}_8)_2] \cdot 3\text{H}_2\text{O}$ Bi at (0.3558, 0.1678, -0.1234)	9		Ψ -TPRS-9	Ilyukhin & Poznyak, 2000
$[\text{BiCl}_3(\text{C}_{10}\text{H}_{10}\text{N}_6\text{O}_4)] \cdot 2\text{C}_5\text{H}_5\text{N}_3\text{O}_2 \cdot \text{H}_2\text{O}$	9		Ψ -TPRS-9	Luo <i>et al.</i> , 2021
$[\text{Bi}(\text{NO}_3)(\text{C}_5\text{H}_4\text{NO}_3)_2] \cdot 1.5\text{H}_2\text{O}$	9		Ψ -TPRS-9	Marandi <i>et al.</i> , 2013
$\text{Bi}_2(\text{NO}_3)_2(\text{C}_{19}\text{H}_{25}\text{N}_7\text{O}_2\text{S}_2)_2$	9		Ψ -TPRS-9	Nomiya <i>et al.</i> , 2004

$[\text{Bi}(\text{H}_2\text{O})(\text{NO}_3)(\text{C}_{13}\text{H}_{15}\text{N}_7\text{O}_3)]\cdot\text{NO}_3$	9		Ψ-TPRS-9	Nomiya <i>et al.</i> , 2004
$[\text{Bi}(\text{H}_2\text{O})(\text{C}_{11}\text{H}_{14}\text{N}_7\text{O}_2)]\cdot 2\text{NO}_3\cdot\text{H}_2\text{O}$	9		Ψ-TPRS-9	Nomiya <i>et al.</i> , 2004
$[\text{Bi}_2(\text{C}_7\text{H}_5\text{NO}_3)_3(\text{C}_7\text{H}_7\text{NO}_3)_3][\text{Bi}_2(\text{C}_7\text{H}_5\text{NO}_3)(\text{C}_7\text{H}_5\text{NO}_3)_3(\text{C}_2\text{H}_6\text{O}_5)_4]\cdot 4\text{C}_2\text{H}_6\text{OS}$ Bi at (0.7586, 0.9563, 0.49487)	9		Ψ-TPRS-9	Pathak <i>et al.</i> , 2105
$\text{H}_3\text{O}[\text{Bi}_2(\text{H}_2\text{O})_2(\text{C}_8\text{H}_2\text{NO}_6)(\text{C}_8\text{H}_3\text{NO}_6)_2]$ Bi at (0.9442, 0.1636, 0.0700)	9		Ψ-TPRS-9	Rhauderwiek <i>et al.</i> , 2018
$\text{H}_3\text{O}[\text{Bi}_2(\text{H}_2\text{O})_2(\text{C}_8\text{H}_2\text{NO}_6)(\text{C}_8\text{H}_3\text{NO}_6)_2]$ Bi at (0.8437, 0.1733, 0.4681)	9		Ψ-TPRS-9	Rhauderwiek <i>et al.</i> , 2018
$3\text{C}_2\text{H}_8\text{N}[\text{Bi}(\text{C}_8\text{H}_2\text{NO}_6)_2]$	9		Ψ-TPRS-9	Senior & Linden, 2020

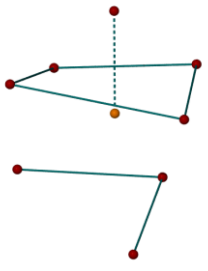
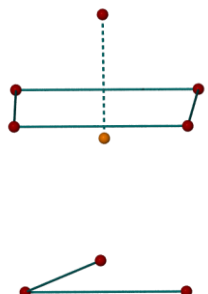
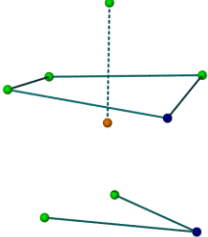
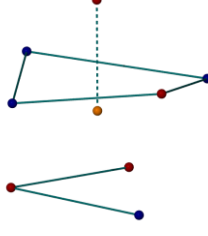
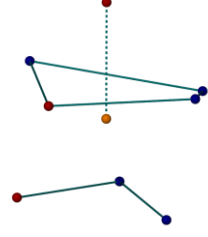
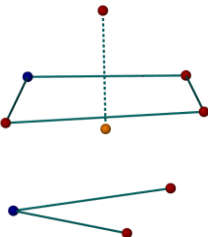
$2\text{C}_2\text{H}_8\text{N}[\text{Bi}(\text{C}_3\text{H}_7\text{NO})(\text{C}_8\text{H}_2\text{NO}_6)(\text{C}_8\text{H}_3\text{NO}_6)] \cdot 0.5\text{C}_2\text{H}_7\text{N}$ Bi at (0.5394, 0.3886, 0.912)	9		Ψ-TPRS-9	Senior & Linden, 2020
$\text{C}_2\text{H}_8\text{N}[\text{Bi}(\text{C}_3\text{H}_7\text{NO})(\text{C}_7\text{H}_4\text{N}_2\text{O}_4)_2]$	9		Ψ-TPRS-9	Senior & Linden, 2020
$2\text{C}_2\text{H}_8\text{N}[\text{Bi}_2(\text{C}_3\text{H}_7\text{NO})_2(\text{C}_7\text{H}_3\text{NO}_5)_4]$	9		Ψ-TPRS-9	Senior & Linden, 2020
$\text{C}_2\text{H}_8\text{N}[\text{Bi}(\text{C}_3\text{H}_7\text{NO})(\text{C}_9\text{H}_8\text{N}_2\text{O}_4)_2]$	9		Ψ-TPRS-9	Senior & Linden, 2020
$\text{C}_6\text{H}_7\text{N}_2\text{O}[\text{Bi}(\text{H}_2\text{O})_2(\text{C}_7\text{H}_3\text{NO}_4)_2] \cdot \text{H}_2\text{O}$	9		Ψ-TPRS-9	Soleimannejad & Gholizadeh, 2012
$\text{C}_4\text{H}_{10}\text{N}_2[\text{Bi}(\text{C}_7\text{H}_3\text{NO}_4)(\text{C}_7\text{H}_4\text{NO}_4)] \cdot \text{H}_2\text{O}$	9		Ψ-TPRS-9	Sushrutha & Natarajan, 2013

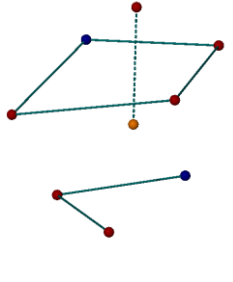
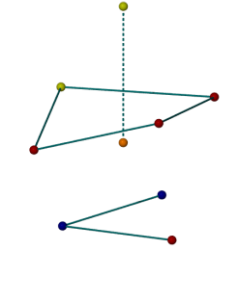
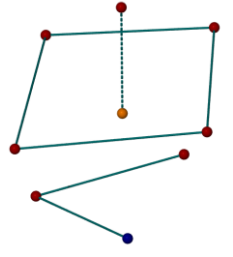
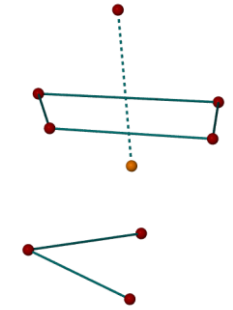
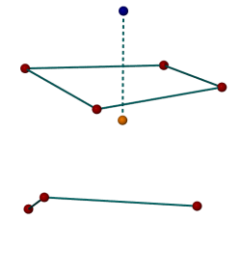
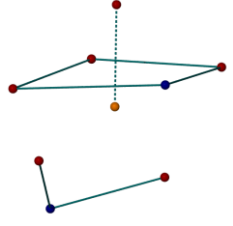
$\text{Bi}(\text{OH})(\text{C}_7\text{H}_2\text{NO}_4)$	9		Ψ -TPRS-9	Sushrutha & Natarajan, 2013
$\text{C}_6\text{H}_9\text{N}_2[\text{Bi}(\text{NO}_3)(\text{C}_7\text{H}_3\text{NO}_4)(\text{C}_7\text{H}_4\text{NO}_4)] \cdot 2\text{H}_2\text{O}$	9		Ψ -TPRS-9	Tabatabaee <i>et al.</i> , 2014
$\text{C}_2\text{H}_8\text{N}[\text{Bi}(\text{C}_3\text{H}_7\text{NO})(\text{C}_8\text{H}_4\text{O}_4)_2] \cdot 2\text{C}_3\text{H}_7\text{NO}$	9		Ψ -TPRS-9	Thirumurugan & Cheetham, 2010
$\text{Bi}_4(\text{OH})_2(\text{H}_2\text{O})_4(\text{C}_{16}\text{H}_6\text{N}_2\text{O}_8)_2(\text{C}_{16}\text{H}_7\text{N}_2\text{O}_8) \cdot 7\text{H}_2\text{O}$ Bi at (0.3590, 0.9058, 0.0794)	9		Ψ -TPRS-9	Vilela <i>et al.</i> , 2019
$[\text{Bi}(\text{H}_3\text{O})(\text{C}_7\text{H}_3\text{NO}_4)_2] \cdot 0.83\text{H}_2\text{O}$	9		Ψ -TPRS-9	Wibowo <i>et al.</i> , 2011a
$3\text{C}_2\text{H}_8\text{N}[\text{Bi}(\text{C}_7\text{H}_3\text{NO}_4)_2(\text{C}_7\text{H}_4\text{NO}_4)_2]$	9		Ψ -TPRS-9	Wibowo <i>et al.</i> , 2011b
$\text{Bi}(\text{C}_7\text{H}_6\text{NO}_2)_3 \cdot 0.5\text{C}_2\text{H}_3\text{N}$	9		Ψ -TPRS-9	Wrobel <i>et al.</i> , 2017

[Bi(NO ₃)(C ₁₂ H ₈ N ₂)(C ₆ H ₁₀ NS ₂) ₂].0.5H ₂ O	9		Ψ-TPRS-9	Yin <i>et al.</i> , 2004a
[Bi(NO ₃)(C ₁₂ H ₈ N ₂) ₂ (C ₅ H ₁₀ NO ₂ S ₂) ₂].3H ₂ O	9		Ψ-TPRS-9	Yin <i>et al.</i> , 2004b
Bi ₂ (C ₅ H ₁₀ NO ₂ S) ₆ Bi at (0.3926, 0.5604, 0.9597)	9		Ψ-TPRS-9	Yin <i>et al.</i> , 2004b
Bi ₂ (C ₅ H ₁₀ NO ₂ S) ₆ Bi at (-0.8933, 0.4659, 0.5688)	9		Ψ-TPRS-9	Yin <i>et al.</i> , 2004b
Bi ₂ (OH) ₂ (H ₂ O) ₂ (C ₁₂ H ₂ O ₈ S ₂)(C ₁₂ H ₄ O ₈ S ₂) Bi at (0.3252, -0.0739, 0.3587)	9		Ψ-SAPRS-9	Albat & Stock, 2018
Bi(ClO ₄) ₃ (C ₈ H ₂₂ N ₄ O)	9		Ψ-SAPRS-9	Luckay <i>et al.</i> , 1997
Bi ₄ O ₃ (H ₂ O) ₂ (C ₈ H ₄ O ₇ S) ₂ Bi at (0.0161, -0.0461, 0.2140)	9		Ψ-SAPRS-9	Albat <i>et al.</i> , 2017

Bi ₄ O ₃ (H ₂ O) ₂ (C ₈ H ₄ O ₇ S) ₂ Bi at (0.2584, 0.2346, 0.2270)	9		Ψ-SAPRS-9	Albat <i>et al.</i> , 2017
Bi ₄ O ₃ (H ₂ O) ₂ (C ₈ H ₄ O ₇ S) ₂ Bi at (0.9868, 0.5191, 0.2761)	9		Ψ-SAPRS-9	Albat <i>et al.</i> , 2017
2C ₃ H ₅ N ₂ [Bi ₂ (C ₆ H ₃ N ₃ O ₃) ₄]·2H ₂ O Bi at (0.1450, 0.2652, 0.7637)	9		Ψ-SAPRS-9	Al-Nubi <i>et al.</i> , 2021
KBi(C ₆ H ₄ O ₇)·3.5H ₂ O Bi at (0.2498, 0.7065, 0.6459)	9		Ψ-SAPRS-9	Antsyshkina <i>et al.</i> , 2006
[Bi ₂ (H ₂ O) ₄ (C ₄ O ₄) ₃]·4H ₂ O	9		Ψ-SAPRS-9	Busch <i>et al.</i> , 2012
C ₂ H ₈ N·[Bi(C ₆ H ₂ O ₄ S) ₂]·1.5C ₃ H ₇ NO	9		Ψ-SAPRS-9	Kan <i>et al.</i> , 2017
3NH ₄ ·3K[Bi ₆ (H ₂ O) ₄ (C ₆ H ₅ O ₇) ₆]·14H ₂ O Bi at (0.2464, 0.4517, 0.0023)	9		Ψ-SAPRS-9	Li <i>et al.</i> , 2003

$\text{Bi}(\text{H}_2\text{O})_2(\text{C}_8\text{H}_2\text{NO}_6)$	9		Ψ -SAPRS-9	Rhauderwiek <i>et al.</i> , 2018
$\text{Bi}_4\text{Na}_4(\text{C}_{10}\text{H}_{14}\text{O}_4)_8(\text{C}_2\text{H}_6\text{O})_{3.1}(\text{H}_2\text{O})_{3.4}$ Bi at (0.1707, 0.3991, 0.4337)	9		Ψ -SAPRS-9	Wibowo <i>et al.</i> , 2012
$\text{Bi}_4\text{Na}_4(\text{C}_{10}\text{H}_{14}\text{O}_4)_8(\text{C}_2\text{H}_6\text{O})_{3.1}(\text{H}_2\text{O})_{3.4}$ Bi at (0.1657, 0.8894, 0.0680)	9		Ψ -SAPRS-9	Wibowo <i>et al.</i> , 2012
$2\text{C}_3\text{H}_{12}\text{N}_2[\text{Bi}_2(\text{C}_2\text{O}_4)_5]\cdot 2\text{H}_2\text{O}$	9		Ψ -SAPRS-9	Yu <i>et al.</i> , 2007
$\text{Bi}(\text{OH})(\text{C}_7\text{H}_5\text{O}_5\text{S})$	9		Ψ -SAPRS-9	Albat <i>et al.</i> , 2017
$[\text{Bi}_4\text{O}_2(\text{H}_2\text{O})_2(\text{C}_8\text{H}_4\text{O}_7\text{S})_3]\cdot \text{H}_2\text{O}$ Bi (0.3942, 0.2060, 0.0147)	9		Ψ -SAPRS-9	Albat <i>et al.</i> , 2017
$[\text{Bi}_4\text{O}_2(\text{H}_2\text{O})_2(\text{C}_8\text{H}_4\text{O}_7\text{S})_3]\cdot \text{H}_2\text{O}$ Bi at (0.4757, 0.2483, 0.1951)	9		Ψ -SAPRS-9	Albat <i>et al.</i> , 2017

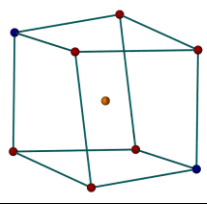
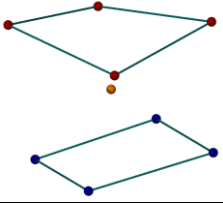
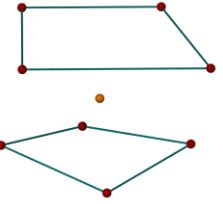
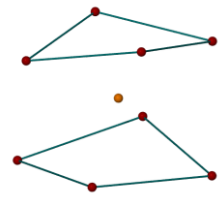
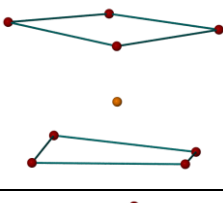
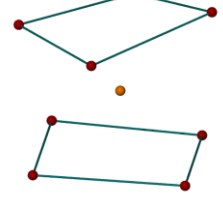
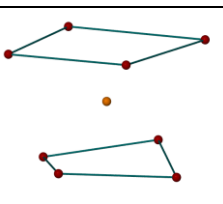
$\text{Bi}_4\text{O}_3(\text{H}_2\text{O})_2(\text{C}_8\text{H}_4\text{O}_7\text{S})_2$ Bi at (0.5549, 0.4665, 0.2149)			Ψ-SAPRS-9	Albat <i>et al.</i> , 2017
$\text{Bi}_6\text{O}_6(\text{OH})_2(\text{H}_2\text{O})_4(\text{C}_{12}\text{H}_2\text{O}_8\text{S}_2)$ Bi at (0.7337, 0.7500, 0.8673)	9		Ψ-SAPRS-9	Albat & Stock, 2018
$\text{Bi}_2(\text{C}_{14}\text{H}_{12}\text{N}_2\text{S}_2\text{Br})_6$	9		Ψ-SAPRS-9	Anamika <i>et al.</i> , 2019
$\text{C}_5\text{H}_6\text{N}[\text{Bi}(\text{C}_6\text{H}_4\text{NO}_3)_4]\text{C}_5\text{H}_5\text{N}$	9		Ψ-SAPRS-9	Anjaneyulu <i>et al.</i> , 2012
$[\text{Bi}_2(\text{H}_2\text{O})_2(\text{N}_3)_2(\text{C}_{12}\text{H}_8\text{N}_2)_2(\text{C}_7\text{H}_3\text{NO}_4)_2] \cdot 2\text{H}_2\text{O}$	9		Ψ-SAPRS-9	Feng, Zhong <i>et al.</i> , 2018
$\text{Bi}_2(\text{C}_{10}\text{H}_8\text{N}_2)_2(\text{C}_7\text{H}_5\text{O}_2)_6$ Bi at (0.2573, 0.2910, 0.4970)	9		Ψ-SAPRS-9	He <i>et al.</i> , 2020

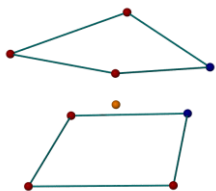
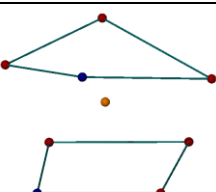
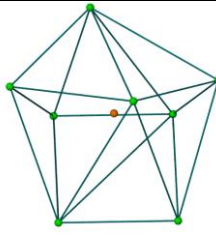
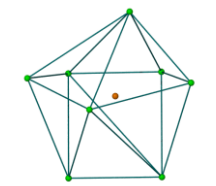
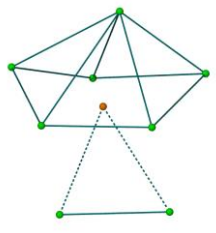
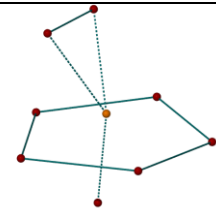
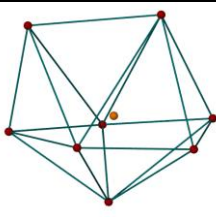
$\text{Bi}_2(\text{H}_2\text{O})(\text{C}_7\text{H}_3\text{NO}_4)_2(\text{C}_7\text{H}_4\text{NO}_4)_2$ Bi at (0.1759, 0.3809, 0.33368)	9		Ψ-SAPRS-9	Kowalik <i>et al.</i> , 2020
$\text{BiCl}(\text{H}_2\text{O})(\text{C}_{12}\text{H}_6\text{N}_2\text{O}_4)$	9		Ψ-SAPRS-9	Luo <i>et al.</i> , 2021
$\text{Bi}(\text{C}_8\text{H}_2\text{NO}_6)$	9		Ψ-SAPRS-9	Rhauderwiek <i>et al.</i> , 2018
$\text{Bi}_4(\text{OH})_2(\text{H}_2\text{O})_4(\text{C}_{16}\text{H}_6\text{N}_2\text{O}_8)_2(\text{C}_{16}\text{H}_7\text{N}_2\text{O}_8) \cdot 7\text{H}_2\text{O}$ Bi at (-0.0167, 1.1003, -0.1562)	9		Ψ-SAPRS-9	Vilela <i>et al.</i> , 2019
$\text{Bi}_2(\text{H}_2\text{O})_2(\text{C}_{10}\text{H}_4\text{O}_8)(\text{C}_7\text{H}_3\text{NO}_4)_2$	9		Ψ-SAPRS-9	Wang, Huang <i>et al.</i> , 2017
$\text{Bi}_3\text{O}_2(\text{H}_2\text{O})_2(\text{C}_7\text{H}_3\text{NO}_4)_2(\text{C}_7\text{H}_4\text{NO}_4)$ Bi at (0.8565, 0.7531, 0.2917)	9		Ψ-SAPRS-9	Wibowo <i>et al.</i> , 2010

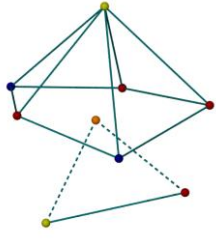
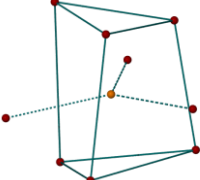
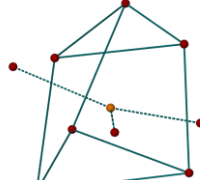
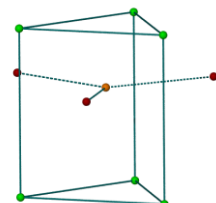
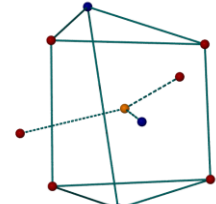
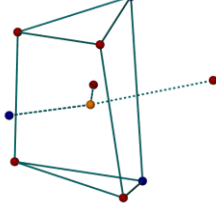
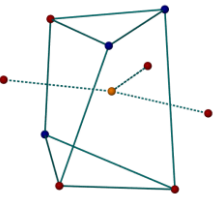
$C_2H_8N[Bi(C_7H_3NO_4)(C_8H_4O_4)] \cdot 2C_3H_7NO$	10		Ψ -SAPRS-10	Kan <i>et al.</i> , 2017
$[Bi_2(C_3H_4N_2)(C_8H_4O_4)_{3.5}] \cdot 3C_3H_7NO$ Bi at (0.1424, 0.6552, 0.2418)	10		Ψ -SAPRS-10	Thirumurugan & Cheetham, 2010
$Bi_4Na_4(C_{10}H_{14}O_4)_8(C_2H_6O)_{3.1}(H_2O)_{3.4}$ Bi at (0.3185, 0.2978, 0.5770)	10		Ψ -SAPRS-10	Wibowo <i>et al.</i> , 2012
Cation $[Bi(H_2O)(C_{14}H_8O_4)_2]$ Guest	10		Ψ -CUS-10	Kan <i>et al.</i> , 2017

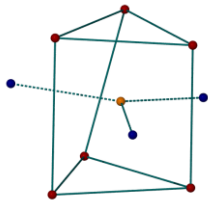
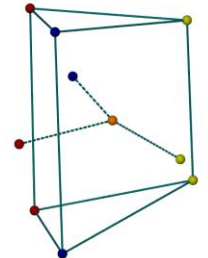
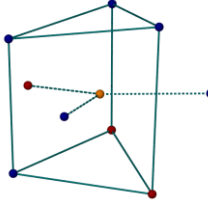
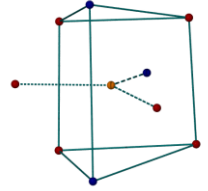
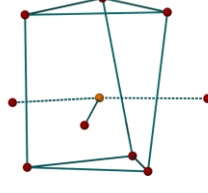
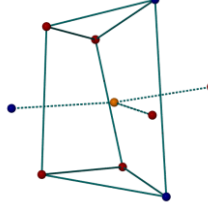
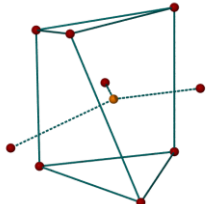
*Color codes of atoms: orange Bi, purple Br, yellow Cl, green S, red O, blue N.

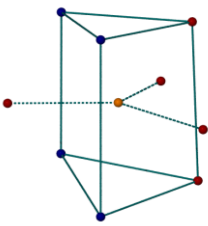
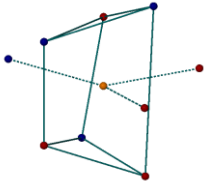
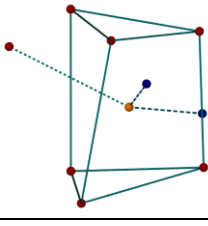
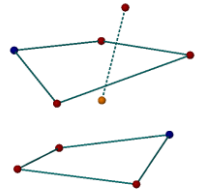
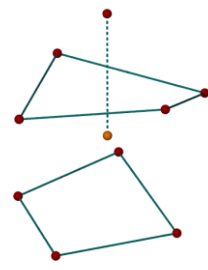
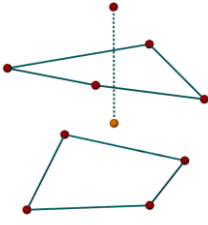
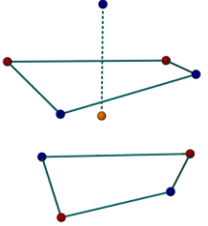
Table S2 Bi(III) in high coordination (C.N. ≥ 8) showing no stereochemical activity*

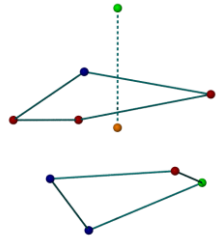
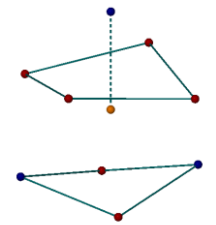
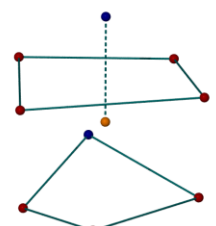
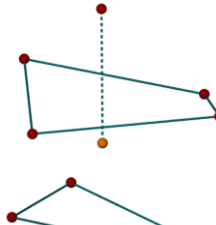
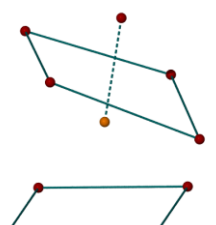
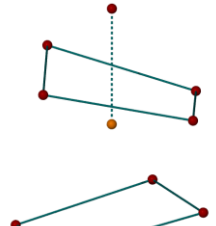
Formula	C.N.		Polyhedral Symbol	Reference
$3K[Bi(C_6H_6NO_6)] \cdot 2H_2O$	8		CU-8	Davidovich <i>et al.</i> , 1998
$[Bi(C_{14}H_{23}N_4O_6)] \cdot 3.5H_2O$	8		SAPR-8	Adcock <i>et al.</i> , 2018
$Bi_6O_6(OH)_2(H_2O)_4(C_{12}H_2O_8S_2)$ Bi at (1.1421, 0.7500, 1.3077)	8		SAPR-8	Albat & Stock, 2018
$Bi_6O_6(OH)_2(H_2O)_4(C_{12}H_2O_8S_2)$ Bi at (1.0404, 0.6549, 0.9989)	8		SAPR-8	Albat & Stock, 2018
$[Bi_6O_4(OH)_4(H_2O)_{12}(C_{12}H_4O_8S_2)_3] \cdot xH_2O$ Bi at (0.2082, 0.8271, 0.9189)	8		SAPR-8	Albat & Stock, 2018
$Bi_2(C_3H_7NO)_4(C_2O_4)_2(C_{10}H_6O_8)$	8		SAPR-8	Gao & Zhang, 2012
$Bi_2(C_3H_7NO)_4(C_2O_4)(C_{10}H_6O_8)_2$	8		SAPR-8	Gao & Zhang, 2012

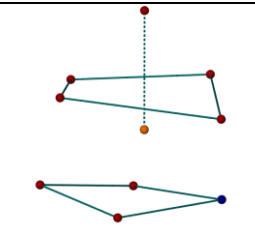
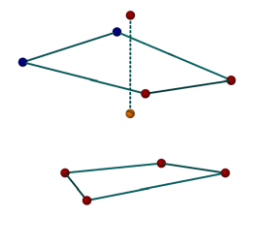
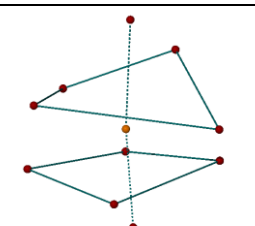
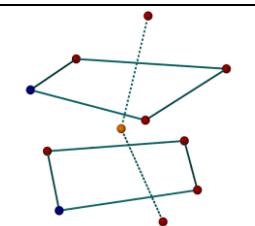
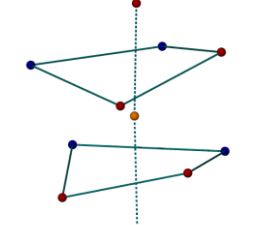
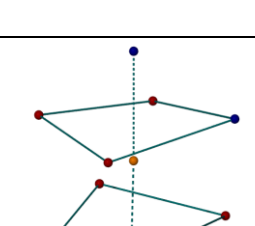
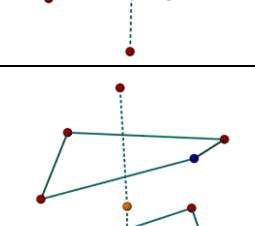
$[\text{BaBi}_2(\text{H}_2\text{O})(\text{C}_{10}\text{H}_{12}\text{N}_2\text{O}_8)_2] \cdot 3\text{H}_2\text{O}$ Bi at (0.2045, 0.2988, 0.1734)	8		SAPR-8	Ilyukhin & Poznyak, 2000
$\text{Bi}_2(\text{H}_2\text{O})(\text{C}_7\text{H}_3\text{NO}_4)_2(\text{C}_7\text{H}_4\text{NO}_4)_2$ Bi at (0.4144, 0.3469, 0.5637)	8		SAPR-8	Kowalik <i>et al.</i> , 2020
$\text{Bi}_2(\text{C}_{14}\text{H}_{12}\text{N}_2\text{S}_2\text{Cl})_6$	8		DD-8	Anamika <i>et al.</i> , 2019
$\text{Bi}_2(\text{C}_{10}\text{H}_{12}\text{NS}_2)_6$ Bi at (0.1800, 0.0383, 0.2902)	8		DD-8	Guo <i>et al.</i> , 2015
$\text{Bi}(\text{C}_{10}\text{H}_{12}\text{N}_3\text{S}_2)_3$ Bi at (0.3076, 0.1075, 0.1985)	8		DD-8	Guo <i>et al.</i> , 2015
$3\text{NH}_4 \cdot 3\text{K}[\text{Bi}_6(\text{H}_2\text{O})_4(\text{C}_6\text{H}_5\text{O}_7)_6] \cdot 14\text{H}_2\text{O}$ Bi at (0.2464, 0.4517, 0.0023)	8		DD-8	Li <i>et al.</i> , 2003
$3\text{NH}_4 \cdot 3\text{K}[\text{Bi}_6(\text{H}_2\text{O})_4(\text{C}_6\text{H}_5\text{O}_7)_6] \cdot 14\text{H}_2\text{O}$ Bi at (0.0111, 0.5909, 0.14420)	8		DD-8	Li <i>et al.</i> , 2003

$2\text{C}_6\text{H}_{16}\text{N}[\text{BiCl}_2(\text{C}_7\text{H}_3\text{NO}_4)(\text{C}_7\text{H}_4\text{NO}_4)]$	8		DD-8	Kowalik <i>et al.</i> , 2020
$\text{C}_5\text{H}_6\text{N}[\text{Bi}(\text{C}_6\text{H}_2\text{O}_4\text{S})(\text{C}_6\text{H}_3\text{O}_4\text{S})]\cdot 1.5\text{H}_2\text{O}$			TPRS-9	Adcock <i>et al.</i> , 2018
$3\text{C}_5\text{H}_6\text{N}[\text{Bi}_2(\text{H}_2\text{O})(\text{C}_6\text{H}_2\text{O}_4\text{S})_4(\text{C}_6\text{H}_3\text{O}_4\text{S})]\cdot \text{H}_2\text{O}$ Bi at (0.5792, 1.1237, 0.5853)	9		TPRS-9	Adcock <i>et al.</i> , 2018
$\text{Bi}(\text{C}_7\text{H}_5\text{OS})_3$	9		TPRS-9	Andrews <i>et al.</i> , 2012
$2\text{C}_5\text{H}_7\text{N}_2[\text{Bi}(\text{C}_7\text{H}_3\text{NO}_4)_2(\text{C}_7\text{H}_4\text{NO}_4)]\cdot 2\text{H}_2\text{O}$	9		TPRS-9	Hakimi <i>et al.</i> , 2015
$\text{C}_5\text{H}_7\text{N}_2[\text{Bi}(\text{C}_7\text{H}_3\text{NO}_4)(\text{C}_7\text{H}_4\text{NO}_4)_2]\cdot 4\text{H}_2\text{O}$	9		TPRS-9	Hakimi <i>et al.</i> , 2015
$[\text{Bi}(\text{NO}_3)_2(\text{C}_{12}\text{H}_{10}\text{N}_4\text{O})]\cdot \text{CH}_4\text{O}$	9		TPRS-9	Hanifehpour <i>et al.</i> , 2015

$C_7H_{11}N_2[Bi(C_7H_3NO_4)(C_7H_4NO_4)_5] \cdot 5H_2O$ Bi at (0.5492, 1.5207, 0.2634)	9		TPRS-9	Lu <i>et al.</i> , 2021
$BiCl_3(C_{11}H_{11}N_3O_2S)_3$	9		TPRS-9	Marzano <i>et al.</i> , 2013
$Bi(NO_3)(SCN)_2(C_{12}H_8N_2)(CH_4O)$	9		TPRS-9	Morsali, 2005
$C_{10}H_{10}N_2[Bi(C_7H_3NO_4)_2(C_7H_4NO_4)] \cdot 5H_2O$	9		SAPRS-9	Qi <i>et al.</i> , 2020
$[Bi_2(C_3H_4N_2)(C_8H_4O_4)_{3.5}] \cdot 3C_3H_7NO$ Bi at (-0.3068, 1.1902, 0.6755)	9		TPRS-9	Thirumurugan & Cheetham, 2010
$3C_2H_8N[Bi(C_7H_3NO_4)_3]$	9		TPRS-9	Thirumurugan <i>et al.</i> , 2012
$[Bi(C_3H_7NO)(C_9H_3O_6)] \cdot C_3H_7NO \cdot 2CH_4O$	9		TPRS-9	Wang <i>et al.</i> , 2015

$4\text{K}[\text{Bi}(\text{C}_7\text{H}_3\text{NO}_4)_3(\text{C}_7\text{H}_4\text{NO}_4)] \cdot 0.33\text{H}_2\text{O}$	9		TPRS-9	Wibowo <i>et al.</i> , 2011b
$2\text{CH}_6\text{N}_3[\text{Bi}(\text{C}_{18}\text{H}_{25}\text{N}_4\text{O}_{12})] \cdot 4\text{H}_2\text{O}$	9		TPRS-9	Wullens <i>et al.</i> , 1998
$[\text{BiCu}(\text{H}_2\text{O})(\text{NO}_3)(\text{C}_7\text{H}_3\text{NO}_4)_2(\text{C}_{12}\text{H}_8\text{N}_2)] \cdot 2\text{H}_2\text{O}$	9		TPRS-9	Yue <i>et al.</i> , 2015
$2\text{C}_3\text{H}_5\text{N}_2[\text{Bi}_2(\text{C}_6\text{H}_3\text{N}_3\text{O}_3)_4] \cdot 2\text{H}_2\text{O}$ Bi at (0.6415, 0.2433, 0.5086)	9		SAPRS-9	Al-Nubi <i>et al.</i> , 2021
$\text{KBi}(\text{C}_6\text{H}_4\text{O}_7) \cdot 3.5\text{H}_2\text{O}$ Bi at (0.2310, 0.8829, 0.9046)	9		SAPRS-9	Antsyshkina <i>et al.</i> , 2006
$[\text{Bi}_2(\text{H}_2\text{O})_6(\text{C}_4\text{O}_4)_3] \cdot 2\text{H}_2\text{O}$	9		SAPRS-9	Busch <i>et al.</i> , 2012
$\text{Bi}(\text{NO}_3)(\text{C}_{19}\text{H}_{13}\text{N}_7\text{O}_2)$	9		SAPRS-9	Gungor & Kose, 2018

$[\text{Bi}(\text{NO}_3)_2(\text{C}_{13}\text{H}_{19}\text{N}_7\text{S}_2)]\text{NO}_3$	9		SAPRS-9	Li <i>et al.</i> , 2012
$\text{C}_7\text{H}_{11}\text{N}_2[\text{Bi}(\text{C}_7\text{H}_3\text{NO}_4)(\text{C}_7\text{H}_4\text{NO}_4)_5]5\text{H}_2\text{O}$ Bi at (0.5720, 1.0077, -0.2365)	9		SAPRS-9	Lu <i>et al.</i> , 2021
$\text{Bi}(\text{C}_5\text{H}_2\text{N}_2\text{O}_4)(\text{C}_5\text{H}_3\text{N}_2\text{O}_4)$	9		SAPRS-9	Sushrutha & Natarajan, 2013
$\text{C}_2\text{H}_8\text{N}[\text{Bi}(\text{C}_8\text{H}_4\text{O}_4)_2]$ Bi at (0.6667, 0.3333, 0.1835)	9		SAPRS-9	Thirumurugan & Cheetham, 2010
$\text{Bi}(\text{C}_{10}\text{H}_{14}\text{O}_4)(\text{C}_{10}\text{H}_{15}\text{O}_4)$ Bi at (0.3626, -0.1432, 0.7563)	9		SAPRS-9	Vilela <i>et al.</i> , 2018
$\text{Bi}(\text{C}_{10}\text{H}_{14}\text{O}_4)(\text{C}_{10}\text{H}_{15}\text{O}_4)$ Bi at (0.8641, 0.1558, 0.2525)	9		SAPRS-9	Vilela <i>et al.</i> , 2018

$\text{Bi}(\text{H}_2\text{O})_2(\text{C}_9\text{H}_5\text{O}_6)(\text{C}_7\text{H}_3\text{NO}_4)$	9		SAPRS-9	Wang, Huang <i>et al.</i> , 2017
$\text{Bi}_2(\text{C}_{12}\text{H}_8\text{N}_2)_2(\text{C}_8\text{H}_7\text{O}_2)_6$	9		SAPRS-9	Yang <i>et al.</i> , 2012
$\text{C}_{10}\text{H}_{10}\text{N}_2[\text{Bi}(\text{C}_8\text{H}_7\text{O}_3)_5(\text{C}_8\text{H}_8\text{O}_3)] \cdot 4\text{H}_2\text{O}$	10		SAPRS-10	Chen <i>et al.</i> , 2013
$\text{C}_{10}\text{H}_9\text{N}_2[\text{Bi}(\text{NO}_3)_4(\text{C}_{10}\text{H}_8\text{N}_2)]$	10		SAPRS-10	Meng & Zhang, 2011
$[\text{Bi}(\text{NO}_3)_3(\text{C}_6\text{H}_4\text{N}_2\text{S}_2)_2] \cdot 0.5\text{H}_2\text{O}$	10		SAPRS-10	Morsali <i>et al.</i> , 2001
$\text{Bi}(\text{NO}_3)_3(\text{C}_{12}\text{H}_{10}\text{N}_4\text{O})(\text{CH}_4\text{O})$	10		SAPRS-10	Roodsari <i>et al.</i> , 2015
$\text{C}_2\text{H}_8\text{N}[\text{Bi}(\text{C}_8\text{H}_4\text{O}_4)_2] \cdot \text{C}_3\text{H}_7\text{NO}$	10		SAPRS-10	Thirumurugan & Cheetham, 2010

$\text{Bi}(\text{C}_7\text{H}_6\text{NO}_2)_3 \cdot 0.5\text{H}_2\text{O} \cdot 0.5\text{CH}_3\text{NO}_2$	10		SAPRS-10	Wrobel <i>et al.</i> , 2017
$3\text{C}_5\text{H}_6\text{N}[\text{Bi}_2(\text{H}_2\text{O})(\text{C}_6\text{H}_2\text{O}_4)_4(\text{C}_6\text{H}_3\text{O}_4\text{S})] \cdot \text{H}_2\text{O}$ Bi at (0.0649, 0.6008, 0.8368)	10		CUS-10	Adcock <i>et al.</i> , 2018
$2\text{C}_5\text{H}_6\text{N}[\text{Bi}(\text{C}_6\text{H}_2\text{O}_4)_2(\text{C}_6\text{H}_3\text{O}_4\text{S})] \cdot x\text{H}_2\text{O}$	10		CUS-10	Adcock <i>et al.</i> , 2018
$\text{C}_2\text{H}_8\text{N}[\text{Bi}(\text{C}_8\text{H}_4\text{O}_4)_2]$ Bi at (0, 0, 0)	12		PPRP-12	Thirumurugan & Cheetham, 2010

*Color codes of atoms: orange Bi, green S, red O, blue N.