

SELECTIVITY, SYNTHESIS, CRYSTAL STRUCTURE AND BIOLOGICAL ACTIVITY OF THE ANION-COORDINATION PHENANTHROLINIUM TARTRATOGERMANATE

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Table S1

Selected geometric parameters (Å, °) for (HPhen)₄[(μ-O){Ge₂(OH)(μ-Tart)₂]₂·9H₂O.

Ge1A—O1A	1.766 (8)	Ge1B—O1B	1.767 (8)
Ge1A—O2A	1.928 (7)	Ge1B—O2B	1.923 (8)
Ge1A—O4A	1.779 (8)	Ge1B—O4B	1.778 (8)
Ge1A—O8A	1.893 (8)	Ge1B—O8B	1.897 (8)
Ge1A—O10A	1.788 (9)	Ge1B—O10B	1.786 (8)
Ge2A—O5A	1.769 (8)	Ge2B—O5B	1.769 (8)
Ge2A—O7A	1.899 (9)	Ge2B—O7B	1.926 (9)
Ge2A—O11A	1.783 (8)	Ge2B—O11B	1.805 (8)
Ge2A—O13A	1.938 (8)	Ge2B—O13B	1.922 (8)
Ge2A—O14A	1.766 (7)	Ge2B—O14B	1.752 (7)
Ge3A—O14A	1.739 (8)	Ge3B—O14B	1.755 (8)
Ge3A—O15A	1.929 (7)	Ge3B—O15B	1.909 (8)
Ge3A—O17A	1.770 (7)	Ge3B—O17B	1.792 (7)
Ge3A—O21A	1.916 (8)	Ge3B—O21B	1.919 (7)
Ge3A—O23A	1.801 (8)	Ge3B—O23B	1.793 (8)
Ge4A—O18A	1.769 (8)	Ge4B—O18B	1.768 (8)
Ge4A—O20A	1.947 (7)	Ge4B—O20B	1.926 (7)
Ge4A—O24A	1.793 (7)	Ge4B—O24B	1.787 (7)
Ge4A—O26A	1.919 (7)	Ge4B—O26B	1.904 (7)
Ge4A—O27A	1.756 (8)	Ge4B—O27B	1.762 (8)
O1A—Ge1A—O2A	93.3 (3)	O1B—Ge1B—O2B	92.4 (3)
O1A—Ge1A—O4A	122.8 (4)	O1B—Ge1B—O4B	117.3 (4)
O1A—Ge1A—O8A	89.7 (3)	O1B—Ge1B—O8B	91.4 (3)
O1A—Ge1A—O10A	115.3 (4)	O1B—Ge1B—O10B	118.9 (4)
O4A—Ge1A—O2A	86.5 (3)	O4B—Ge1B—O2B	87.4 (4)
O4A—Ge1A—O8A	91.3 (3)	O4B—Ge1B—O8B	92.5 (3)
O4A—Ge1A—O10A	121.9 (4)	O4B—Ge1B—O10B	123.7 (4)
O10A—Ge1A—O2A	91.5 (3)	O10B—Ge1B—O2B	88.3 (4)
O10A—Ge1A—O8A	87.8 (3)	O10B—Ge1B—O8B	88.2 (4)
O5A—Ge2A—O7A	89.2 (4)	O5B—Ge2B—O7B	88.0 (4)
O5A—Ge2A—O11A	120.1 (3)	O5B—Ge2B—O11B	123.4 (4)
O5A—Ge2A—O13A	93.1 (4)	O5B—Ge2B—O13B	91.0 (4)
O11A—Ge2A—O7A	89.0 (4)	O11B—Ge2B—O7B	90.2 (3)
O11A—Ge2A—O13A	86.9 (3)	O11B—Ge2B—O13B	87.1 (4)
O14A—Ge2A—O5A	110.1 (4)	O14B—Ge2B—O5B	114.5 (4)

O14A—Ge2A—O7A	92.0 (4)	O14B—Ge2B—O7B	89.4 (4)
O14A—Ge2A—O11A	129.8 (4)	O14B—Ge2B—O11B	122.0 (4)
O14A—Ge2A—O13A	90.6 (4)	O14B—Ge2B—O13B	94.5 (4)
O14A—Ge3A—O15A	89.9 (3)	O14B—Ge3B—O15B	90.6 (4)
O14A—Ge3A—O17A	113.9 (4)	O14B—Ge3B—O17B	109.2 (4)
O14A—Ge3A—O21A	93.5 (3)	O14B—Ge3B—O21B	92.3 (4)
O14A—Ge3A—O23A	122.5 (4)	O14B—Ge3B—O23B	128.9 (4)
O17A—Ge3A—O15A	87.5 (3)	O17B—Ge3B—O15B	88.3 (3)
O17A—Ge3A—O21A	91.2 (3)	O17B—Ge3B—O21B	93.3 (3)
O17A—Ge3A—O23A	123.6 (4)	O17B—Ge3B—O23B	121.8 (4)
O23A—Ge3A—O15A	91.4 (3)	O23B—Ge3B—O15B	88.3 (4)
O23A—Ge3A—O21A	86.7 (4)	O23B—Ge3B—O21B	87.8 (4)
O18A—Ge4A—O20A	88.1 (4)	O18B—Ge4B—O20B	87.2 (3)
O18A—Ge4A—O24A	123.0 (4)	O18B—Ge4B—O24B	123.0 (4)
O18A—Ge4A—O26A	90.9 (4)	O18B—Ge4B—O26B	89.5 (3)
O24A—Ge4A—O20A	89.4 (3)	O24B—Ge4B—O20B	91.5 (3)
O24A—Ge4A—O26A	87.3 (3)	O24B—Ge4B—O26B	88.3 (3)
O27A—Ge4A—O18A	118.1 (4)	O27B—Ge4B—O18B	121.6 (4)
O27A—Ge4A—O20A	94.1 (4)	O27B—Ge4B—O20B	93.7 (4)
O27A—Ge4A—O24A	118.9 (4)	O27B—Ge4B—O24B	115.4 (4)
O27A—Ge4A—O26A	90.4 (4)	O27B—Ge4B—O26B	89.9 (3)

Table S2

Hydrogen-bond geometry (Å, °) for (HPhen)₄[(μ-O){Ge₂(OH)(μ-Tart)₂]₂·9H₂O.

<i>D—H···A</i>	<i>H···A</i>	<i>D···A</i>	<i>D—H···A</i>
O1A—H1A···O20A ⁱ	1.96	2.759 (11)	159
O27A—H27A···O2A ⁱⁱ	2.12	2.809 (11)	139
O1B—H1B···O37 ⁱⁱⁱ	2.08	2.788 (11)	141
O27B—H27B···O2B ⁱⁱ	2.18	2.873 (11)	139
O28—H28A···O3A	2.15	2.979 (13)	165
O28—H28B···O9B ^{iv}	2.04	2.840 (12)	155
O29—H29A···O19A	2.00	2.802 (12)	157
O29—H29B···O25B	2.06	2.840 (12)	153
O30—H30A···O25B	1.96	2.753 (11)	155
O30—H30B···O31	1.92	2.710 (13)	150
O31—H31A···O6A	2.05	2.792 (11)	146
O31—H31B···O12B	1.99	2.749 (13)	148
O32—H32A···O29 ⁱ	2.04	2.885 (12)	165
O32—H32B···O27B ⁱ	2.12	2.938 (13)	156
O33—H33A···O16A	2.27	2.932 (12)	139
O33—H33B···O22B ^{iv}	1.91	2.759 (11)	170
O34—H34A···O35	1.94	2.754 (12)	160
O34—H34B···O9B ^{iv}	2.06	2.824 (13)	150
O35—H35A···O14A	2.05	2.895 (11)	162
O35—H35B···O33	1.92	2.735 (12)	155
O36—H36A···O16A	2.39	2.966 (14)	125
O37—H37B···O36	1.90	2.722 (13)	156
O38—H38A···O26A	2.00	2.872 (12)	161
O38—H38B···O39	1.92	2.730 (14)	157
O39—H39A···O41 ^v	2.02	2.828 (14)	157
O39—H39B···O19B ^{vi}	2.10	2.792 (13)	137
O40—H40A···O1A ⁱⁱ	2.17	2.888 (12)	143
O40—H40B···O41 ⁱⁱ	2.22	2.977 (16)	148
O41—H41A···O9A	2.03	2.789 (11)	146
O41—H41B···O3B ^{vii}	1.92	2.766 (13)	166
O42—H42A···O6B ^{vi}	2.07	2.900 (11)	167
O42—H42B···O12A	2.08	2.813 (11)	144
O43—H43A···O42	2.24	3.095 (13)	167
O43—H43B···O14B ^{vi}	2.06	2.887 (12)	158
O44—H44A···O43	1.97	2.832 (12)	169
O44—H44B···O25A	1.84	2.699 (12)	168
O45—H45A···O16B ^{vii}	2.26	3.071 (12)	161
O45—H45B···O22A	2.40	3.044 (12)	133
N2—H2···O37 ^{viii}	1.78	2.593 (10)	153
C27—H27···O19B ^{ix}	2.27	3.074 (9)	142
N3—H3···O44	1.95	2.655 (10)	136
N5—H5···O42 ^x	1.91	2.713 (9)	151
N7—H7···O30	1.92	2.660 (11)	141
C52—H52···O17A	2.17	3.069 (9)	158
N10—H10···O38	1.79	2.631 (11)	160
N12—H12···O34	1.88	2.638 (11)	143
N14—H14···O45	1.88	2.706 (10)	155
N15—H15···O28 ^{vii}	1.88	2.725 (11)	161

Symmetry codes: (i) *x*, *y*-1, *z*; (ii) *x*, *y*+1, *z*; (iii) *x*+1, *y*-1, *z*; (iv) *x*-1, *y*, *z*; (v) *x*-1, *y*+1, *z*; (vi) *x*-1, *y*, *z*+1; (vii) *x*, *y*, *z*+1; (viii) *x*, *y*-1, *z*+1; (ix) *x*-1, *y*-1, *z*+1; (x) *x*+1, *y*, *z*.

Table S3

The geometry of stacking interactions.

Plane A	Plane B	Symmetry	Angle, °	Centroid- centroid distance, Å	Shift distance, Å
C49 C45 C44 C46 C47 C48	C81 C85 C84 C83 C82 C80	(1+X,+Y,+Z)	3.126	3.646	0.854
C49 C45 C44 C46 C47 C49	N11 C81 C80 C79 C78 C77	(1+X,+Y,+Z)	2.197	3.878	1.578
N5 C41 C42 C43 C44 C45	N12 C85 C84 C86 C87 C88	(1+X,+Y,+Z)	4.168	3.827	1.290
N1 C17 C18 C19 C20 C21	C104 C106 C107 C108 C109 C105	(+X,+Y,+Z)	5.343	3.888	1.975
N1 C17 C18 C19 C20 C22	N16 C112 C111 C110 C108 C109	(+X,+Y,+Z)	5.349	3.570	1.097
N1 C17 C18 C19 C20 C23	N4 C40 C39 C38 C36 C37	(+X,-1+Y,+Z)	1.473	3.687	1.662
N15 C101 C102 C103 C104 C105	N14 C100 C99 C98 C96 C97	(+X,+Y,+Z)	2.879	3.701	1.354
N16 C112 C111 C110 C108 C109	C93 C97 C96 C95 C94 C92	(+X,+Y,+Z)	2.923	3.675	1.480
N16 C112 C111 C110 C108 C110	N13 C93 C92 C91 C90 C89	(+X,+Y,+Z)	3.009	3.530	1.344
N11 C81 C80 C79 C78 C77	C68 C70 C71 C72 C73 C69	(+X,-1+Y,+Z)	7.071	3.785	1.236
N11 C81 C80 C79 C78 C78	N10 C73 C72 C74 C75 C76	(+X,-1+Y,+Z)	6.162	3.875	1.660
C33 C37 C36 C35 C34 C32	C93 C97 C96 C95 C94 C92	(+X,+Y,+Z)	2.353	3.944	1.976
C33 C37 C36 C35 C34 C33	N14 C100 C99 C98 C96 C97	(+X,+Y,+Z)	2.606	3.779	1.763
N3 C33 C32 C31 C30 C29	C93 C97 C96 C95 C94 C92	(+X,+Y,+Z)	4.112	3.738	1.459
N3 C33 C32 C31 C30 C30	N13 C93 C92 C91 C90 C89	(+X,+Y,+Z)	3.862	3.564	1.156
C58 C59 C60 C61 C57 C56	N10 C73 C72 C74 C75 C76	(1+X,+Y,+Z)	4.863	3.693	1.271
N8 C64 C63 C62 C60 C61	C68 C70 C71 C72 C73 C69	(1+X,+Y,+Z)	0.221	3.777	1.458
N8 C64 C63 C62 C60 C62	N10 C73 C72 C74 C75 C76	(1+X,+Y,+Z)	1.564	3.582	0.972