

**Antimonato Polyoxovanadates extended by Transition Metal Complexes: Dimorphic
{Ni(dien)₂}₃[V₁₅Sb₆O₄₂(H₂O)] · 8 H₂O compounds and {Ni(dien)₂}₄[V₁₆Sb₄O₄₂(H₂O)]**

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Supplementary Information

Table S1: Sb-O, V-O and Ni-N bond lengths (Å) around the Ni²⁺ cations in compound 1.
Estimated standard deviations are given in parentheses.

Sb(1)-O(21) 1.934(7) Sb(1)-O(42) 1.937(7) Sb(1)-O(15) 1.966(7) Sb(2)-O(38) 1.920(7) Sb(2)-O(18) 1.953(7) Sb(2)-O(15) 1.967(8) Sb(3)-O(13) 1.936(8) Sb(3)-O(30) 1.956(7) Sb(3)-O(36) 1.959(8) Sb(4)-O(31) 1.935(7) Sb(4)-O(24) 1.946(7) Sb(4)-O(25) 1.956(7) Sb(5)-O(36) 1.938(8) Sb(5)-O(28) 1.940(7) Sb(5)-O(9) 1.982(7) Sb(6)-O(16) 1.931(7) Sb(6)-O(31) 1.939(7) Sb(6)-O(37) 1.945(7) V(1)-O(33) 1.606(7) V(1)-O(32) 1.913(7) V(1)-O(4) 1.934(7) V(1)-O(35) 1.967(7) V(1)-O(16) 2.029(7) V(1)-V(9) 2.884(3) V(2)-O(6) 1.615(7) V(2)-O(26) 1.919(8) V(2)-O(3) 1.944(7) V(2)-O(25) 1.953(7) V(2)-O(37) 1.979(7) V(2)-V(13) 2.847(3) V(3)-O(5) 1.637(7) V(3)-O(4) 1.905(7) V(3)-O(23) 1.926(7) V(3)-O(24) 1.971(7) V(3)-O(16) 1.984(7) V(4)-O(39) 1.605(8) V(4)-O(19) 1.913(7) V(4)-O(32) 1.944(7) V(4)-O(34) 1.960(7) V(4)-O(9) 2.017(7) V(5)-O(1) 1.620(8) V(5)-O(12) 1.907(7) V(5)-O(7) 1.948(7) V(5)-O(26) 1.948(7) V(5)-O(25) 1.985(7) V(6)-O(27) 1.616(8) V(6)-O(19) 1.919(7) V(6)-O(34) 1.936(7)	V(6)-O(42) 1.961(7) V(6)-O(18) 1.990(7) V(7)-O(17) 1.618(8) V(7)-O(14) 1.919(7) V(7)-O(34) 1.937(7) V(7)-O(28) 1.970(8) V(7)-O(18) 1.976(8) V(8)-O(29) 1.605(8) V(8)-O(4) 1.903(7) V(8)-O(19) 1.917(7) V(8)-O(23) 1.974(7) V(8)-O(42) 1.988(7) V(9)-O(40) 1.615(7) V(9)-O(32) 1.896(7) V(9)-O(35) 1.924(7) V(9)-O(30) 1.974(7) V(9)-O(9) 1.975(7) V(10)-O(2) 1.601(8) V(10)-O(7) 1.924(8) V(10)-O(23) 1.927(7) V(10)-O(21) 1.995(7) V(10)-O(24) 2.004(7) V(11)-O(11) 1.588(8) V(11)-O(10) 1.889(8) V(11)-O(14) 1.957(7) V(11)-O(28) 1.968(7) V(11)-O(13) 1.979(8) V(12)-O(41) 1.613(8) V(12)-O(12) 1.929(7) V(12)-O(10) 1.929(8) V(12)-O(14) 1.962(7) V(12)-O(38) 2.018(8) V(13)-O(8) 1.587(8) V(13)-O(26) 1.937(7) V(13)-O(10) 1.942(8) V(13)-O(3) 1.964(7) V(13)-O(13) 2.005(8) V(14)-O(20) 1.586(8) V(14)-O(12) 1.900(8) V(14)-O(7) 1.944(8) V(14)-O(21) 1.973(7) V(14)-O(38) 1.985(8) V(15)-O(22) 1.620(7) V(15)-O(35) 1.900(7) V(15)-O(3) 1.949(7) V(15)-O(30) 1.972(7) V(15)-O(37) 1.985(7)	Sb(11)-O(70) 1.922(7) Sb(11)-O(60) 1.956(8) Sb(11)-O(83) 1.980(7) Sb(12)-O(55) 1.940(7) Sb(12)-O(57) 1.947(7) Sb(12)-O(60) 1.968(7) Sb(13)-O(58) 1.932(7) Sb(13)-O(81) 1.939(7) Sb(13)-O(84) 1.970(7) Sb(14)-O(84) 1.925(7) Sb(14)-O(77) 1.938(7) Sb(14)-O(79) 1.962(7) Sb(15)-O(62) 1.925(6) Sb(15)-O(63) 1.941(7) Sb(15)-O(52) 1.954(7) Sb(16)-O(61) 1.930(7) Sb(16)-O(91) 1.947(7) Sb(16)-O(63) 1.961(7) V(51)-O(86) 1.612(7) V(51)-O(75) 1.893(7) V(51)-O(68) 1.949(7) V(51)-O(79) 1.974(7) V(51)-O(58) 1.993(7) V(52)-O(89) 1.618(8) V(52)-O(85) 1.918(7) V(52)-O(51) 1.933(7) V(52)-O(55) 1.980(7) V(52)-O(70) 1.989(7) V(53)-O(72) 1.598(7) V(53)-O(53) 1.902(7) V(53)-O(87) 1.933(7) V(53)-O(62) 1.980(7) V(53)-O(61) 1.990(7) V(54)-O(74) 1.594(8) V(54)-O(53) 1.907(7) V(54)-O(75) 1.943(7) V(54)-O(68) 1.945(6) V(54)-O(62) 2.040(7) V(55)-O(65) 1.627(8) V(55)-O(85) 1.916(7) V(55)-O(78) 1.931(7) V(55)-O(59) 1.941(7) V(55)-O(70) 1.994(7) V(56)-O(82) 1.592(7) V(56)-O(69) 1.926(7) V(65)-O(81) 1.988(7)	V(56)-O(75) 1.938(6) V(56)-O(73) 1.961(7) V(56)-O(58) 2.028(7) V(57)-O(92) 1.591(7) V(57)-O(85) 1.925(7) V(57)-O(66) 1.946(7) V(57)-O(51) 1.955(7) V(57)-O(91) 2.011(7) V(58)-O(67) 1.604(8) V(58)-O(51) 1.939(7) V(58)-O(87) 1.941(7) V(58)-O(55) 1.990(7) V(58)-O(61) 1.998(7) V(59)-O(90) 1.600(8) V(59)-O(69) 1.929(7) V(59)-O(53) 1.935(6) V(59)-O(87) 1.956(7) V(59)-O(57) 1.996(7) V(60)-O(88) 1.617(7) V(60)-O(69) 1.890(7) V(60)-O(73) 1.953(7) V(60)-O(83) 1.961(7) V(60)-O(57) 1.963(7) V(61)-O(76) 1.625(7) V(61)-O(68) 1.925(7) V(61)-O(80) 1.963(7) V(61)-O(79) 1.968(7) V(61)-O(52) 1.969(7) V(62)-O(56) 1.623(7) V(62)-O(66) 1.885(7) V(62)-O(91) 1.951(7) V(62)-O(80) 1.966(6) V(62)-O(52) 1.979(7) V(63)-O(54) 1.608(8) V(63)-O(73) 1.935(7) V(63)-O(59) 1.937(7) V(63)-O(83) 1.957(7) V(63)-O(81) 1.996(7) V(64)-O(64) 1.621(7) V(64)-O(66) 1.931(7) V(64)-O(78) 1.933(7) V(64)-O(80) 1.953(7) V(64)-O(77) 2.005(7) V(65)-O(71) 1.630(7) V(65)-O(78) 1.907(7) V(65)-O(59) 1.919(7) V(65)-O(77) 1.979(7)
Sb(21)-O(114) 1.930(7) Sb(21)-O(130) 1.954(7) Sb(21)-O(142) 1.956(7) Sb(22)-O(128) 1.956(7) Sb(22)-O(114) 1.966(7) Sb(22)-O(136) 1.978(7) Sb(23)-O(124) 1.929(7) Sb(23)-O(115) 1.940(7) Sb(23)-O(109) 1.947(7) Sb(24)-O(125) 1.941(7) Sb(24)-O(132) 1.958(6) Sb(24)-O(115) 1.968(7)	V(106)-O(124) 1.968(7) V(106)-O(125) 1.989(7) V(107)-O(102) 1.617(7) V(107)-O(138) 1.900(7) V(107)-O(132) 1.956(7) V(107)-O(126) 1.963(7) V(107)-O(109) 1.982(7) V(108)-O(140) 1.607(8) V(108)-O(135) 1.956(7) V(108)-O(127) 1.967(7) V(108)-O(136) 1.973(7) V(108)-O(119) 1.983(7)	Sb(31)-O(159) 1.961(7) Sb(31)-O(153) 1.963(6) Sb(31)-O(154) 1.988(7) Sb(32)-O(154) 1.927(7) Sb(32)-O(180) 1.930(7) Sb(32)-O(169) 1.932(7) Sb(33)-O(173) 1.921(8) Sb(33)-O(185) 1.936(8) Sb(33)-O(183) 1.953(7) Sb(34)-O(182) 1.914(7) Sb(34)-O(173) 1.944(8) Sb(34)-O(171) 1.976(7)	V(156)-O(167) 1.973(7) V(156)-O(172) 1.980(7) V(157)-O(189) 1.616(7) V(157)-O(156) 1.911(7) V(157)-O(188) 1.934(7) V(157)-O(159) 2.002(7) V(157)-O(165) 2.014(7) V(158)-O(157) 1.595(7) V(158)-O(156) 1.921(7) V(158)-O(177) 1.941(7) V(158)-O(175) 1.960(7) V(158)-O(176) 2.032(7)

Sb(25)-O(116) 1.918(7) Sb(25)-O(118) 1.928(7) Sb(25)-O(139) 1.969(7) Sb(26)-O(106) 1.931(7) Sb(26)-O(116) 1.950(7) Sb(26)-O(121) 1.955(7) V(101)-O(108) 1.636(7) V(101)-O(101) 1.892(7) V(101)-O(137) 1.921(7) V(101)-O(139) 1.959(8) V(101)-O(121) 1.984(7) V(102)-O(113) 1.633(7) V(102)-O(127) 1.896(7) V(102)-O(134) 1.952(7) V(102)-O(133) 1.972(8) V(102)-O(118) 2.004(7) V(103)-O(123) 1.609(7) V(103)-O(138) 1.932(7) V(103)-O(111) 1.940(7) V(103)-O(141) 1.954(7) V(103)-O(132) 1.974(7) V(104)-O(122) 1.613(7) V(104)-O(138) 1.922(7) V(104)-O(101) 1.929(7) V(104)-O(126) 1.975(7) V(104)-O(121) 2.023(8) V(105)-O(105) 1.603(8) V(105)-O(119) 1.915(7) V(105)-O(141) 1.948(7) V(105)-O(125) 1.978(7) V(105)-O(128) 1.986(7) V(106)-O(120) 1.610(8) V(106)-O(135) 1.908(7) V(106)-O(119) 1.919(6)	V(109)-O(104) 1.606(7) V(109)-O(135) 1.905(7) V(109)-O(134) 1.929(7) V(109)-O(131) 1.949(7) V(109)-O(124) 2.018(7) V(110)-O(103) 1.616(7) V(110)-O(111) 1.900(7) V(110)-O(141) 1.925(7) V(110)-O(142) 1.962(7) V(110)-O(128) 1.986(7) V(111)-O(117) 1.602(7) V(111)-O(111) 1.916(7) V(111)-O(101) 1.937(7) V(111)-O(137) 1.955(7) V(111)-O(142) 2.017(7) V(112)-O(107) 1.604(7) V(112)-O(127) 1.903(7) V(112)-O(136) 1.954(7) V(112)-O(133) 1.958(7) V(112)-O(130) 1.970(7) V(113)-O(110) 1.614(7) V(113)-O(131) 1.924(7) V(113)-O(126) 1.924(7) V(113)-O(106) 1.958(7) V(113)-O(109) 1.967(7) V(114)-O(112) 1.611(7) V(114)-O(133) 1.909(8) V(114)-O(137) 1.935(7) V(114)-O(130) 1.968(7) V(114)-O(139) 1.978(8) V(115)-O(129) 1.596(8) V(115)-O(134) 1.899(7) V(115)-O(131) 1.961(7) V(115)-O(106) 1.984(7) V(115)-O(118) 1.987(7)	Sb(35)-O(187) 1.912(7) Sb(35)-O(176) 1.928(7) Sb(35)-O(172) 1.954(7) Sb(36)-O(187) 1.959(7) Sb(36)-O(174) 1.960(7) Sb(36)-O(167) 1.962(7) V(151)-O(178) 1.594(7) V(151)-O(156) 1.908(7) V(151)-O(165) 1.920(7) V(151)-O(174) 1.946(7) V(151)-O(176) 1.988(7) V(152)-O(190) 1.620(7) V(152)-O(181) 1.908(7) V(152)-O(175) 1.942(7) V(152)-O(171) 1.945(7) V(152)-O(172) 1.992(7) V(153)-O(155) 1.610(7) V(153)-O(170) 1.929(7) V(153)-O(152) 1.932(7) V(153)-O(168) 1.957(7) V(153)-O(180) 2.012(7) V(154)-O(160) 1.606(7) V(154)-O(165) 1.906(7) V(154)-O(163) 1.931(7) V(154)-O(153) 1.971(7) V(154)-O(174) 2.013(7) V(155)-O(184) 1.589(7) V(155)-O(151) 1.930(7) V(155)-O(168) 1.931(7) V(155)-O(183) 1.956(7) V(155)-O(169) 1.979(7) V(156)-O(179) 1.600(7) V(156)-O(161) 1.909(7) V(156)-O(181) 1.946(7)	V(159)-O(162) 1.614(7) V(159)-O(177) 1.867(7) V(159)-O(175) 1.925(7) V(159)-O(171) 1.976(7) V(159)-O(185) 1.986(7) V(160)-O(164) 1.642(8) V(160)-O(152) 1.927(7) V(160)-O(161) 1.930(7) V(160)-O(163) 1.962(7) V(160)-O(167) 1.986(7) V(161)-O(191) 1.606(7) V(161)-O(152) 1.911(7) V(161)-O(163) 1.937(6) V(161)-O(153) 1.960(7) V(161)-O(180) 1.976(7) V(162)-O(158) 1.626(7) V(162)-O(188) 1.890(7) V(162)-O(151) 1.942(7) V(162)-O(159) 1.951(7) V(162)-O(169) 1.990(6) V(163)-O(186) 1.598(7) V(163)-O(188) 1.910(7) V(163)-O(177) 1.942(7) V(163)-O(151) 1.971(7) V(163)-O(185) 2.030(7) V(164)-O(166) 1.609(7) V(164)-O(170) 1.923(7) V(164)-O(161) 1.928(7) V(164)-O(181) 1.979(7) V(164)-O(182) 2.017(7) V(165)-O(192) 1.602(7) V(165)-O(170) 1.911(7) V(165)-O(168) 1.945(8) V(165)-O(183) 1.980(7) V(165)-O(182) 1.992(7)
Ni(5)-N(46) 2.090(12) Ni(5)-N(41) 2.097(9) Ni(5)-N(45) 2.132(9) Ni(6)-N(56) 2.082(10) Ni(6)-N(55) 2.106(10) Ni(6)-N(53) 2.125(10)	Ni(5)-N(43) 2.135(10) Ni(5)-N(42) 2.140(10) Ni(5)-N(44) 2.164(10) Ni(6)-N(54) 2.137(10) Ni(6)-N(51) 2.137(11) Ni(6)-N(52) 2.152(10)	Ni(7)-N(62) 2.046(13) Ni(7)-N(66) 2.072(16) Ni(7)-N(65) 2.098(12) Ni(8)-N(76) 2.058(13) Ni(8)-N(73) 2.109(11) Ni(8)-N(74) 2.126(11)	Ni(7)-N(61) 2.116(11) Ni(7)-N(63) 2.137(11) Ni(7)-N(64) 2.150(11) Ni(8)-N(72) 2.137(10) Ni(8)-N(75) 2.162(10) Ni(8)-N(71) 2.172(10)
Ni(1)-N(2) 2.063(12) Ni(1)-N(5) 2.091(13) Ni(1)-N(1) 2.103(11) Ni(2)-N(16) 2.086(11) Ni(2)-N(15) 2.097(12) Ni(2)-N(11) 2.102(11)	Ni(1)-N(3) 2.104(11) Ni(1)-N(4) 2.136(15) Ni(1)-N(6) 2.167(13) Ni(2)-N(12) 2.118(11) Ni(2)-N(14) 2.121(13) Ni(2)-N(13) 2.143(10)	Ni(3)-N(21) 2.084(10) Ni(3)-N(24) 2.106(9) Ni(3)-N(26) 2.110(9) Ni(4)-N(36) 2.094(9) Ni(4)-N(33) 2.094(10) Ni(4)-N(34) 2.111(8)	Ni(3)-N(23) 2.113(9) Ni(3)-N(25) 2.153(9) Ni(3)-N(22) 2.177(10) Ni(4)-N(35) 2.142(9) Ni(4)-N(32) 2.145(10) Ni(4)-N(31) 2.156(9)
Ni(9)-N(86) 2.043(9) Ni(9)-N(84) 2.089(10) Ni(9)-N(83) 2.103(10) Ni(10)-N(92) 2.084(10) Ni(10)-N(94) 2.085(13) Ni(10)-N(93) 2.087(11)	Ni(9)-N(81) 2.127(9) Ni(9)-N(85) 2.140(9) Ni(9)-N(82) 2.156(10) Ni(10)-N(96) 2.096(11) Ni(10)-N(91) 2.130(11) Ni(10)-N(95) 2.144(14)	Ni(11)-N(105) 2.025(19) Ni(11)-N(102) 2.042(16) Ni(11)-N(106) 2.066(15) Ni(12)-N(115) 2.13(3) Ni(12)-N(112) 2.17(3) Ni(12)-N(116) 2.17(3)	Ni(11)-N(101) 2.144(15) Ni(11)-N(104) 2.19(2) Ni(11)-N(103) 2.207(16) Ni(12)-N(111) 2.22(3) Ni(12)-N(114) 2.27(3) Ni(12)-N(113) 2.33(3)

Table S2: Bond lengths (Å) around the Ni²⁺ cations and also Sb-O and V-O bond lengths in compound 2. Estimated standard deviations are given in parentheses.

Sb(1)-O(13)	1.937(5)	V(3)-O(8)	2.032(6)
Sb(1)-O(3)	1.941(6)	V(4)-O(4)	1.605(5)
Sb(1)-O(12)	1.944(5)	V(4)-O(2)	1.909(5)
Sb(2)-O(8)	1.935(5)	V(4)-O(10)	1.931(5)
Sb(2)-O(9)	1.945(5)	V(4)-O(9)	1.972(5)
V(1)-O(5)	1.610(5)	V(4)-O(13)	1.985(6)
V(1)-O(11)	1.910(5)	V(5)-O(14)	1.599(6)
V(1)-O(10)	1.937(5)	V(5)-O(6)	1.897(6)
V(1)-O(12)	2.014(5)	V(5)-O(2)	1.947(5)
V(1)-V(2)	2.8303(15)	V(5)-O(13)	1.996(5)
V(2)-O(7)	1.610(5)	Ni(1)-N(2)	2.059(9)
V(2)-O(11)	1.905(5)	Ni(1)-N(5)	2.089(10)
V(2)-O(10)	1.938(5)	Ni(1)-N(6)	2.121(7)
V(2)-O(9)	1.982(5)	Ni(1)-N(3)	2.130(6)
V(3)-O(6)	1.916(5)	Ni(1)-N(1)	2.131(8)
V(3)-O(2)	1.961(5)	Ni(1)-N(4)	2.169(6)

Table S3: Sb-O, V-O and Ni-N bond lengths (Å) in compound 3. Estimated standard deviations are given in parentheses.

Sb(1)-O(10)	1.949(3)	V(2)-O(3)	1.967(3)
Sb(2)-O(20)	1.934(3)	V(3)-O(4)	1.614(3)
Sb(2)-O(18)	1.934(3)	V(3)-O(2)	1.926(3)
Sb(2)-O(15)	1.955(3)	V(3)-O(1)	1.959(3)
Ni(1)-N(2)	2.123(5)	V(3)-O(15)	2.000(3)
Ni(1)-N(3)	2.129(5)	V(4)-O(11)	1.627(3)
Ni(1)-N(1)	2.135(4)	V(4)-O(12)	1.917(3)
Ni(2)-N(7)	2.100(5)	V(4)-O(9)	1.925(3)
Ni(2)-N(6)	2.107(5)	V(4)-O(1)	1.949(3)
Ni(2)-N(5)	2.113(4)	V(4)-O(18)	2.000(3)
Ni(2)-N(9)	2.119(4)	V(5)-O(19)	1.639(3)
Ni(2)-N(8)	2.143(4)	V(5)-O(2)	1.908(3)
Ni(2)-N(4)	2.152(5)	V(5)-O(9)	1.934(3)
Ni(3)-N(10)	2.107(4)	V(5)-O(8)	1.958(3)
Ni(3)-N(11)	2.130(5)	V(5)-O(1)	1.961(3)
Ni(3)-N(12)	2.134(5)	V(6)-O(21)	1.607(4)
V(1)-O(5)	1.629(3)	V(6)-O(12)	1.926(3)
V(1)-O(6)	1.912(3)	V(6)-O(13)	1.938(3)
V(1)-O(9)	1.920(3)	V(6)-O(17)	1.966(3)
V(1)-O(8)	1.957(3)	V(6)-O(18)	1.987(3)
V(1)-O(10)	1.983(3)	V(7)-O(7)	1.624(3)
V(1)-V(5)	2.9594(10)	V(7)-O(2)	1.927(3)
V(1)-V(8)	3.0086(10)	V(7)-O(8)	1.952(3)
V(2)-O(16)	1.618(3)	V(8)-O(14)	1.622(3)
V(2)-O(12)	1.946(3)	V(8)-O(6)	1.919(3)
V(2)-O(6)	1.951(3)	V(8)-O(3)	1.941(3)
V(2)-O(13)	1.953(3)	V(8)-O(10)	1.983(3)