

Electronic Supplementary Information

Role of Tetrel bonds in the Supramolecular Architecture of Tetranuclear Pb(II)[LL'Thiophene carboxylate] Complexes – An Experimental and Computational Study

Robert Swinton Darius^a, H Giftha Evangeline^a, Franc Perdih^b and, Swaminathan Angeline Vedha^{a*}

^a PG and Research Department of Chemistry, Bishop Heber College, Affiliated to Bharathidasan University. e-mail: angeline.ch@bhc.edu.in

^b Faculty of Chemistry and Chemical Technology, University of Ljubljana, Vecna pot, 113, PO Box 537, SI-1000 Ljubljana, Slovenia. E-mail: Franc.Perdih@fkkt.uni-lj.si

Tables

1. Table S1: Coordinates of complexes I -V
2. Table S2: RMSD of complex I
3. Table S3: Bite angles of complex I
4. Table S4: Jeffery's classification of Hydrogen Bonds
5. Table S5: Comparison of total energies of Complexes I, III, IV and V computed at BVP86/LanL2DZ basis set.
6. Table S6: Tetrel bond lengths (Å) in the structures of PbII complexes described in literature and in this work.
7. TablesS7: Electron density (ρ) of Pb tetrel bonds reported in literature and in present work

Figures

1. Figure S1: ORTEP view of complex I with displacement ellipsoids at a 50% probability level
2. Figure S2: Schematic representation of (i) Hemi-directional and (ii) Holo-directional
3. Figure S3: A view of three-dimensional supramolecular architecture in the complex (I) along c-axis and stacked along b-axis in close packed geometry.
4. Figure S4: A view of three-dimensional supramolecular architecture in the complex (I) along c-axis and stacked along b-axis in open packed geometry.
5. Figure S5: Molecular view of (i) AB and (ii) AC dimers in close packed structures
6. Figure S6: Molecular view of (i) AB and (ii) AC dimers in open packed structures
7. Figure S7: Molecular view of (i) AB and (ii) AC dimers of close packed complex IA where the Br atom involved in tetrel bond is replaced by H.
8. Figure S5: ESP map of asymmetric unit of complex II
9. Figure S9: ESP map of asymmetric unit of complex III
10. Figure S10: ESP map of asymmetric unit of complex V

CCDC No: 2364428

Table S1: Coordinates of complex I-V computed at BVP86/LanL2DZ basis set using Gaussian09w suite. QTAIM and NCI studies carried out at BVP86/LanL2DZ basis set using AIMALL professional and Multiwfn software.

Complex I

Pb4C80N8H48S4O12Br4

Pb	1.733280000000	0.995750000000	0.236407000000
Pb	-1.051353000000	1.818100000000	-3.124629000000
C	1.630659000000	3.408215000000	-2.870148000000
C	2.958381000000	4.066477000000	-2.807152000000
S	3.515702000000	5.036816000000	-4.254331000000
C	3.908295000000	4.075846000000	-1.789996000000
H	3.776063000000	3.555976000000	-0.835336000000
C	5.093797000000	4.833996000000	-2.102557000000
H	5.936680000000	4.942852000000	-1.417871000000
C	5.048136000000	5.407395000000	-3.365248000000
Br	6.423782000000	6.504574000000	-4.187595000000
C	4.322195000000	2.835222000000	3.466150000000
C	5.299837000000	3.822226000000	3.524474000000
H	5.648721000000	4.325506000000	2.620550000000
C	5.782669000000	4.106051000000	4.851903000000
H	6.547286000000	4.851371000000	5.078923000000
C	5.161030000000	3.325247000000	5.817084000000
S	3.931021000000	2.190483000000	5.125694000000
Br	5.493631000000	3.378497000000	7.730984000000
O	1.206473000000	2.713428000000	-1.836500000000
O	0.918601000000	3.540231000000	-3.960763000000
O	2.749944000000	1.325914000000	2.455596000000
O	3.859158000000	2.848433000000	1.111550000000
O	-0.042867000000	0.260492000000	1.518877000000
O	-2.221706000000	1.540550000000	-1.097643000000
N	0.525362000000	2.926093000000	1.208504000000
N	-1.854913000000	3.969652000000	-2.332606000000
N	-3.623140000000	1.751090000000	-3.977171000000
N	-1.695751000000	2.918476000000	-5.613494000000
C	3.611290000000	2.314630000000	2.268163000000
C	0.817825000000	4.227961000000	1.007725000000
H	1.560153000000	4.445624000000	0.236956000000
C	0.194594000000	5.264932000000	1.764860000000
H	0.468570000000	6.305429000000	1.570140000000
C	-0.746389000000	4.929759000000	2.743976000000
H	-1.232665000000	5.709132000000	3.341997000000
C	-1.088107000000	3.556771000000	2.972328000000

C	-2.048058000000	3.122096000000	3.942743000000
H	-2.556733000000	3.862946000000	4.569380000000
C	-2.325157000000	1.755451000000	4.071600000000
H	-3.060200000000	1.416417000000	4.810656000000
C	-1.673471000000	0.777073000000	3.260788000000
H	-1.917312000000	-0.284388000000	3.371096000000
C	-0.706674000000	1.162378000000	2.307210000000
C	-0.414892000000	2.572290000000	2.159216000000
C	-1.616249000000	5.150290000000	-2.944338000000
H	-0.927864000000	5.121512000000	-3.792345000000
C	-2.213692000000	6.363848000000	-2.490998000000
H	-1.989142000000	7.297205000000	-3.014694000000
C	-3.075505000000	6.333938000000	-1.389560000000
H	-3.553377000000	7.252902000000	-1.030216000000
C	-3.340646000000	5.098153000000	-0.712110000000
C	-4.205983000000	4.982768000000	0.421263000000
H	-4.710679000000	5.873079000000	0.811976000000
C	-4.390825000000	3.725493000000	1.014828000000
H	-5.048014000000	3.627830000000	1.886331000000
C	-3.738330000000	2.557824000000	0.525659000000
H	-3.887393000000	1.595720000000	1.025418000000
C	-2.870335000000	2.618066000000	-0.590335000000
C	-2.683576000000	3.914385000000	-1.224071000000
C	-4.562388000000	1.186678000000	-3.181124000000
H	-4.218364000000	0.881828000000	-2.190967000000
C	-5.907606000000	0.979679000000	-3.601449000000
H	-6.619516000000	0.520082000000	-2.911143000000
C	-6.280215000000	1.353850000000	-4.896660000000
H	-7.302862000000	1.196235000000	-5.256986000000
C	-5.309417000000	1.937929000000	-5.767863000000
C	-3.976236000000	2.128858000000	-5.257373000000
C	-5.625515000000	2.328561000000	-7.123785000000
H	-6.646149000000	2.167987000000	-7.489744000000
C	-4.662737000000	2.884258000000	-7.946420000000
H	-4.906077000000	3.172724000000	-8.975510000000
C	-3.314858000000	3.095759000000	-7.468259000000
C	-2.964669000000	2.726326000000	-6.119917000000
C	-2.291416000000	3.667509000000	-8.286433000000

H	-2.524766000000	3.956948000000	-9.317422000000
C	-1.006470000000	3.850436000000	-7.760728000000
H	-0.201926000000	4.285705000000	-8.360227000000
C	-0.746009000000	3.465753000000	-6.412581000000
H	0.233373000000	3.604494000000	-5.943922000000
Pb	-1.733280000000	-0.995750000000	-0.236407000000
Pb	1.051353000000	-1.818100000000	3.124629000000
C	-1.630659000000	-3.408215000000	2.870148000000
C	-2.958381000000	-4.066477000000	2.807152000000
S	-3.515702000000	-5.036816000000	4.254331000000
C	-3.908295000000	-4.075846000000	1.789996000000
H	-3.776063000000	-3.555976000000	0.835336000000
C	-5.093797000000	-4.833996000000	2.102557000000
H	-5.936680000000	-4.942852000000	1.417871000000
C	-5.048136000000	-5.407395000000	3.365248000000
Br	-6.423782000000	-6.504574000000	4.187595000000
C	-4.322195000000	-2.835222000000	-3.466150000000
C	-5.299837000000	-3.822226000000	-3.524474000000
H	-5.648721000000	-4.325506000000	-2.620550000000
C	-5.782669000000	-4.106051000000	-4.851903000000
H	-6.547286000000	-4.851371000000	-5.078923000000
C	-5.161030000000	-3.325247000000	-5.817084000000
S	-3.931021000000	-2.190483000000	-5.125694000000
Br	-5.493631000000	-3.378497000000	-7.730984000000
O	-1.206473000000	-2.713428000000	1.836500000000
O	-0.918601000000	-3.540231000000	3.960763000000
O	-2.749944000000	-1.325914000000	-2.455596000000
O	-3.859158000000	-2.848433000000	-1.111550000000
O	0.042867000000	-0.260492000000	-1.518877000000
O	2.221706000000	-1.540550000000	1.097643000000
N	-0.525362000000	-2.926093000000	-1.208504000000
N	1.854913000000	-3.969652000000	2.332606000000
N	3.623140000000	-1.751090000000	3.977171000000
N	1.695751000000	-2.918476000000	5.613494000000
C	-3.611290000000	-2.314630000000	-2.268163000000
C	-0.817825000000	-4.227961000000	-1.007725000000
H	-1.560153000000	-4.445624000000	-0.236956000000
C	-0.194594000000	-5.264932000000	-1.764860000000
H	-0.468570000000	-6.305429000000	-1.570140000000
C	0.746389000000	-4.929759000000	-2.743976000000
H	1.232665000000	-5.709132000000	-3.341997000000
C	1.088107000000	-3.556771000000	-2.972328000000
C	2.048058000000	-3.122096000000	-3.942743000000

H	2.556733000000	-3.862946000000	-4.569380000000
C	2.325157000000	-1.755451000000	-4.071600000000
H	3.060200000000	-1.416417000000	-4.810656000000
C	1.673471000000	-0.777073000000	-3.260788000000
H	1.917312000000	0.284388000000	-3.371096000000
C	0.706674000000	-1.162378000000	-2.307210000000
C	0.414892000000	-2.572290000000	-2.159216000000
C	1.616249000000	-5.150290000000	2.944338000000
H	0.927864000000	-5.121512000000	3.792345000000
C	2.213692000000	-6.363848000000	2.490998000000
H	1.989142000000	-7.297205000000	3.014694000000
C	3.075505000000	-6.333938000000	1.389560000000
H	3.553377000000	-7.252902000000	1.030216000000
C	3.340646000000	-5.098153000000	0.712110000000
C	4.205983000000	-4.982768000000	-0.421263000000
H	4.710679000000	-5.873079000000	-0.811976000000
C	4.390825000000	-3.725493000000	-1.014828000000
H	5.048014000000	-3.627830000000	-1.886331000000
C	3.738330000000	-2.557824000000	-0.525659000000
H	3.887393000000	-1.595720000000	-1.025418000000
C	2.870335000000	-2.618066000000	0.590335000000
C	2.683576000000	-3.914385000000	1.224071000000
C	4.562388000000	-1.186678000000	3.181124000000
H	4.218364000000	-0.881828000000	2.190967000000
C	5.907606000000	-0.979679000000	3.601449000000
H	6.619516000000	-0.520082000000	2.911143000000
C	6.280215000000	-1.353850000000	4.896660000000
H	7.302862000000	-1.196235000000	5.256986000000
C	5.309417000000	-1.937929000000	5.767863000000
C	3.976236000000	-2.128858000000	5.257373000000
C	5.625515000000	-2.328561000000	7.123785000000
H	6.646149000000	-2.167987000000	7.489744000000
C	4.662737000000	-2.884258000000	7.946420000000
H	4.906077000000	-3.172724000000	8.975510000000
C	3.314858000000	-3.095759000000	7.468259000000
C	2.964669000000	-2.726326000000	6.119917000000
C	2.291416000000	-3.667509000000	8.286433000000
H	2.524766000000	-3.956948000000	9.317422000000
C	1.006470000000	-3.850436000000	7.760728000000
H	-0.201926000000	4.285705000000	-8.360227000000
C	-0.746009000000	3.465753000000	-6.412581000000
H	0.233373000000	3.604494000000	-5.943922000000
Pb	-1.733280000000	-0.995750000000	-0.236407000000
Pb	1.051353000000	-1.818100000000	3.124629000000
C	-1.630659000000	-3.408215000000	2.870148000000
C	-2.958381000000	-4.066477000000	2.807152000000
S	-3.515702000000	-5.036816000000	4.254331000000
C	-3.908295000000	-4.075846000000	1.789996000000
H	-3.776063000000	-3.555976000000	0.835336000000
C	-5.093797000000	-4.833996000000	2.102557000000
H	-5.936680000000	-4.942852000000	1.417871000000
C	-5.048136000000	-5.407395000000	3.365248000000
Br	-6.423782000000	-6.504574000000	4.187595000000
C	-4.322195000000	-2.835222000000	-3.466150000000
C	-5.299837000000	-3.822226000000	-3.524474000000
H	-5.648721000000	-4.325506000000	-2.620550000000
C	-5.782669000000	-4.106051000000	-4.851903000000
H	-6.547286000000	-4.851371000000	-5.078923000000
C	-5.161030000000	-3.325247000000	-5.817084000000
S	-3.931021000000	-2.190483000000	-5.125694000000
Br	-5.493631000000	-3.378497000000	-7.730984000000
O	-1.206473000000	-2.713428000000	1.836500000000
O	-0.918601000000	-3.540231000000	3.960763000000
O	-2.749944000000	-1.325914000000	-2.455596000000
O	-3.859158000000	-2.848433000000	-1.111550000000
O	0.042867000000	-0.260492000000	-1.518877000000
O	2.221706000000	-1.540550000000	1.097643000000
N	-0.525362000000	-2.926093000000	-1.208504000000
N	1.854913000000	-3.969652000000	2.332606000000
N	3.623140000000	-1.751090000000	3.977171000000
N	1.695751000000	-2.918476000000	5.613494000000
C	-3.611290000000	-2.314630000000	-2.268163000000
C	-0.817825000000	-4.227961000000	-1.007725000000
H	-1.560153000000	-4.445624000000	-0.236956000000
C	-0.194594000000	-5.264932000000	-1.764860000000
H	-0.468570000000	-6.305429000000	-1.570140000000
C	0.746389000000	-4.929759000000	-2.743976000000
H	1.232665000000	-5.709132000000	-3.341997000000
C	1.088107000000	-3.556771000000	-2.972328000000
C	2.048058000000	-3.122096000000	-3.942743000000

Complex II

Pb4C76N8H48S4O12Cl4

Pb	-1.036716000000	-1.679718000000	0.418465000000
Pb	-3.404251000000	1.612876000000	-0.168488000000
N	-0.803453000000	-2.454996000000	-1.920558000000
C	-3.172589000000	2.125192000000	3.051755000000
C	-1.060858000000	-1.474864000000	-2.862482000000
N	-3.570510000000	2.832833000000	1.929139000000
C	-3.330465000000	2.668403000000	4.383914000000
C	-1.229892000000	-0.120445000000	-2.379230000000
C	-1.476780000000	0.898833000000	-3.324717000000
H	-1.583228000000	1.931537000000	-2.977544000000
C	-2.589314000000	0.809382000000	2.841422000000
C	-3.889922000000	3.984662000000	4.488000000000
H	-4.021643000000	4.431946000000	5.480244000000
C	-4.087116000000	4.074804000000	2.058493000000
H	-4.348870000000	4.587415000000	1.129758000000
C	-1.580813000000	0.592233000000	-4.715562000000
H	-1.784263000000	1.409532000000	-5.417093000000
C	-0.614003000000	-3.731292000000	-2.316518000000
H	-0.408773000000	-4.460330000000	-1.529939000000
C	-0.685690000000	-4.112053000000	-3.690008000000
H	-0.531497000000	-5.160030000000	-3.961076000000
C	-4.256686000000	4.687659000000	3.335554000000
H	-4.673066000000	5.697263000000	3.391104000000
C	-1.427159000000	-0.714280000000	-5.195370000000
H	-1.506133000000	-0.935915000000	-6.265373000000
C	-0.959581000000	-3.140990000000	-4.658609000000
H	-1.025063000000	-3.411962000000	-5.718741000000
C	-1.154612000000	-1.774838000000	-4.271791000000
C	-2.217572000000	0.070026000000	3.988944000000
H	-1.775137000000	-0.922074000000	3.856643000000
O	-2.443839000000	0.353017000000	1.572288000000
O	-1.136262000000	0.121849000000	-1.034636000000
O	-1.201415000000	3.239536000000	-0.385491000000
O	-3.195357000000	4.219361000000	-0.961555000000
C	-1.890085000000	4.256628000000	-0.856064000000
C	-1.181896000000	5.487142000000	-1.280780000000
S	-2.180878000000	6.883981000000	-1.916089000000
O	-3.356814000000	-2.020841000000	-0.367400000000
O	-2.631332000000	-4.123236000000	0.265987000000
C	-4.813403000000	-3.888258000000	-0.720770000000

C	-3.524654000000	-3.326608000000	-0.241373000000
C	-5.866922000000	-3.243842000000	-1.358195000000
H	-5.826079000000	-2.174626000000	-1.574836000000
S	-5.147309000000	-5.670171000000	-0.511756000000
C	-6.745500000000	-5.416843000000	-1.319029000000
C	-6.970613000000	-4.104223000000	-1.703106000000
H	-7.877470000000	-3.771294000000	-2.210932000000
Cl	-7.867855000000	-6.798130000000	-1.561285000000
N	-5.957668000000	2.705325000000	-0.557542000000
N	-5.598616000000	0.403623000000	0.902329000000
C	-7.086973000000	2.017228000000	-0.183829000000
C	-6.890964000000	0.827421000000	0.699697000000
C	-5.373884000000	-0.703744000000	1.667303000000
H	-4.327132000000	-0.999583000000	1.758117000000
C	-6.416493000000	-1.429922000000	2.284474000000
H	-6.183250000000	-2.313173000000	2.884429000000
C	-6.079450000000	3.797025000000	-1.371111000000
H	-5.137015000000	4.297645000000	-1.613251000000
C	-7.744786000000	-0.988009000000	2.101369000000
H	-8.580133000000	-1.517924000000	2.569949000000
C	-7.984833000000	0.148158000000	1.300126000000
H	-9.008681000000	0.502721000000	1.158391000000
C	0.176893000000	5.788484000000	-1.279081000000
H	0.949720000000	5.091679000000	-0.938238000000
C	-0.646372000000	7.812206000000	-2.143961000000
C	0.486245000000	7.108624000000	-1.768782000000
H	1.499314000000	7.508510000000	-1.834571000000
Cl	-0.690699000000	9.483411000000	-2.801246000000
C	-7.328274000000	4.252439000000	-1.851419000000
H	-7.376455000000	5.132555000000	-2.498836000000
C	-8.373031000000	2.417196000000	-0.639538000000
H	-9.266940000000	1.853529000000	-0.361353000000
C	-8.493425000000	3.544741000000	-1.478505000000
H	-9.478351000000	3.859990000000	-1.837878000000
C	-2.930014000000	1.883005000000	5.510704000000
H	-3.050022000000	2.284978000000	6.522637000000
C	-2.388510000000	0.607044000000	5.297060000000
H	-2.077522000000	-0.000879000000	6.154168000000
Pb	1.036719000000	1.679719000000	-0.418464000000
Pb	3.404251000000	-1.612880000000	0.168490000000
N	0.803457000000	2.454998000000	1.920559000000

C	3.172591000000	-2.125192000000	-3.051754000000
C	1.060862000000	1.474865000000	2.862483000000
N	3.570510000000	-2.832836000000	-1.929138000000
C	3.330467000000	-2.668402000000	-4.383914000000
C	1.229896000000	0.120446000000	2.379232000000
C	1.476785000000	-0.898832000000	3.324719000000
H	1.583232000000	-1.931536000000	2.977546000000
C	2.589317000000	-0.809381000000	-2.841419000000
C	3.889922000000	-3.984662000000	-4.488001000000
H	4.021643000000	-4.431944000000	-5.480245000000
C	4.087114000000	-4.074807000000	-2.058494000000
H	4.348868000000	-4.587419000000	-1.129760000000
C	1.580818000000	-0.592231000000	4.715564000000
H	1.784268000000	-1.409530000000	5.417095000000
C	0.614007000000	3.731293000000	2.316520000000
H	0.408777000000	4.460331000000	1.529940000000
C	0.685693000000	4.112055000000	3.690009000000
H	0.531500000000	5.160031000000	3.961077000000
C	4.256684000000	-4.687661000000	-3.335556000000
H	4.673063000000	-5.697264000000	-3.391107000000
C	1.427163000000	0.714282000000	5.195372000000
H	1.506138000000	0.935917000000	6.265374000000
C	0.959585000000	3.140991000000	4.658610000000
H	1.025067000000	3.411964000000	5.718742000000
C	1.154616000000	1.774839000000	4.271792000000
C	2.217577000000	-0.070024000000	-3.988941000000
H	1.775143000000	0.922077000000	-3.856638000000
O	2.443843000000	-0.353018000000	-1.572285000000
O	1.136266000000	-0.121848000000	1.034638000000
O	1.201417000000	-3.239537000000	0.385493000000
O	3.195356000000	-4.219369000000	0.961554000000
C	1.890083000000	-4.256632000000	0.856064000000
C	1.181891000000	-5.487145000000	1.280778000000
S	2.180869000000	-6.883989000000	1.916080000000
O	3.356818000000	2.020848000000	0.367397000000
O	2.631327000000	4.123242000000	-0.265985000000
C	4.813404000000	3.888268000000	0.720763000000
C	3.524654000000	3.326616000000	0.241371000000

C	5.866927000000	3.243855000000	1.358182000000
H	5.826087000000	2.174638000000	1.574821000000
S	5.147310000000	5.670180000000	0.511737000000
C	6.745494000000	5.416859000000	1.319026000000
C	6.970616000000	4.104239000000	1.703093000000
H	7.877473000000	3.771312000000	2.210919000000
Cl	7.867840000000	6.798152000000	1.561293000000
N	5.957668000000	-2.705333000000	0.557543000000
N	5.598619000000	-0.403628000000	-0.902324000000
C	7.086974000000	-2.017237000000	0.183831000000
C	6.890966000000	-0.827429000000	-0.699693000000
C	5.373888000000	0.703741000000	-1.667296000000
H	4.327136000000	0.999582000000	-1.758109000000
C	6.416498000000	1.429917000000	-2.284468000000
H	6.183256000000	2.313169000000	-2.884421000000
C	6.079448000000	-3.797034000000	1.371111000000
H	5.137013000000	-4.297654000000	1.613250000000
C	7.744790000000	0.988001000000	-2.101365000000
H	8.580138000000	1.517916000000	-2.569945000000
C	7.984836000000	-0.148167000000	-1.300123000000
H	9.008684000000	-0.502732000000	-1.158389000000
C	-0.176899000000	-5.788483000000	1.279078000000
H	-0.949724000000	-5.091675000000	0.938236000000
C	0.646360000000	-7.812207000000	2.143959000000
C	-0.486255000000	-7.108622000000	1.768778000000
H	-1.499325000000	-7.508505000000	1.834568000000
Cl	0.690681000000	-9.483412000000	2.801244000000
C	7.328272000000	-4.252450000000	1.851419000000
H	7.376452000000	-5.132567000000	2.498835000000
C	8.373031000000	-2.417207000000	0.639540000000
H	9.266941000000	-1.853540000000	0.361356000000
C	8.493424000000	-3.544753000000	1.478506000000
H	9.478349000000	-3.860030000000	1.837879000000
C	2.930017000000	-1.883001000000	-5.510703000000
H	3.050025000000	-2.284974000000	-6.522636000000
C	2.388514000000	-0.607040000000	-5.297057000000
H	2.077528000000	0.000884000000	-6.154165000000

Complex III

Pb4C80N8H48S4O12Cl4

Pb	0.937768000000	1.730640000000	-0.428382000000
----	----------------	----------------	-----------------

Pb	3.455712000000	-1.437227000000	0.188151000000
Cl	1.094970000000	-9.412176000000	2.883588000000

Cl	7.546900000000	7.102208000000	1.654413000000
S	4.892104000000	5.873382000000	0.550767000000
C	6.477943000000	5.681412000000	1.398551000000
C	6.737271000000	4.380836000000	1.801489000000
H	7.641486000000	4.083140000000	2.335300000000
C	5.672005000000	3.480498000000	1.438148000000
H	5.661735000000	2.412950000000	1.666512000000
S	2.484125000000	-6.758546000000	1.994439000000
O	1.114283000000	-0.053617000000	1.037658000000
O	2.445091000000	-0.241201000000	-1.566300000000
O	3.398284000000	-4.063799000000	1.025887000000
O	1.370829000000	-3.171154000000	0.422333000000
O	3.232654000000	2.163208000000	0.394672000000
O	2.446852000000	4.235353000000	-0.267710000000
N	0.641492000000	2.505948000000	1.904799000000
N	3.689189000000	-2.670238000000	-1.895260000000
N	6.057074000000	-2.417394000000	0.584093000000
N	5.564013000000	-0.115993000000	-0.904101000000
C	0.955852000000	1.549455000000	2.853621000000
C	1.200283000000	0.203252000000	2.380446000000
C	1.509540000000	-0.792940000000	3.331852000000
H	1.677373000000	-1.820015000000	2.992043000000
C	1.599433000000	-0.470307000000	4.720111000000
H	1.852157000000	-1.269034000000	5.426940000000
C	1.371371000000	0.828666000000	5.190650000000
H	1.440003000000	1.062582000000	6.258754000000
C	1.036273000000	1.865074000000	4.260107000000
C	0.765329000000	3.221003000000	4.637392000000
H	0.818817000000	3.503637000000	5.695150000000
C	0.432736000000	4.167049000000	3.662329000000
H	0.218644000000	5.206399000000	3.925781000000
C	0.379430000000	3.771982000000	2.291983000000
H	0.129201000000	4.481889000000	1.500815000000
C	3.274748000000	-1.985787000000	-3.026272000000
C	2.629111000000	-0.696989000000	-2.830293000000
C	2.236994000000	0.018073000000	-3.986639000000
H	1.745516000000	0.988194000000	-3.864659000000
C	2.450027000000	-0.516178000000	-5.289592000000
H	2.121676000000	0.072325000000	-6.153778000000
C	3.053355000000	-1.766422000000	-5.489653000000
H	3.205005000000	-2.167169000000	-6.497827000000
C	3.474345000000	-2.527447000000	-4.353646000000
C	4.091738000000	-3.818641000000	-4.443700000000
H	4.256380000000	-4.263959000000	-5.431900000000

C	4.472799000000	-4.500219000000	-3.283123000000
H	4.933576000000	-5.490893000000	-3.328366000000
C	4.260369000000	-3.889373000000	-2.011544000000
H	4.532612000000	-4.385296000000	-1.076675000000
C	7.130893000000	-1.658898000000	0.164337000000
C	6.290269000000	-3.526008000000	1.330397000000
H	5.397196000000	-4.088423000000	1.619656000000
C	7.603686000000	-3.941060000000	1.699917000000
H	7.731569000000	-4.843593000000	2.304232000000
C	8.703022000000	-3.185166000000	1.274891000000
H	9.725201000000	-3.479736000000	1.538421000000
C	8.490737000000	-2.011956000000	0.486062000000
C	9.580584000000	-1.187752000000	0.013397000000
H	10.606771000000	-1.477444000000	0.267497000000
C	9.334920000000	-0.056554000000	-0.743640000000
H	10.163412000000	0.565905000000	-1.100955000000
C	7.983412000000	0.335990000000	-1.076792000000
C	7.695644000000	1.507120000000	-1.844467000000
H	8.520021000000	2.133347000000	-2.203348000000
C	6.365752000000	1.843602000000	-2.117492000000
H	6.107841000000	2.737641000000	-2.690640000000
C	5.323935000000	1.007012000000	-1.622803000000
H	4.270614000000	1.242234000000	-1.787325000000
C	6.871661000000	-0.460914000000	-0.624608000000
C	2.098181000000	-4.155796000000	0.909011000000
C	1.434311000000	-5.410240000000	1.336312000000
C	0.987876000000	-7.749424000000	2.212384000000
C	-0.169129000000	-7.097501000000	1.818921000000
H	-1.165046000000	-7.539512000000	1.876304000000
C	0.089477000000	-5.769174000000	1.321951000000
H	-0.709774000000	-5.110394000000	0.966839000000
C	3.355959000000	3.473445000000	0.264087000000
C	4.613582000000	4.082785000000	0.768472000000
Pb	-0.937767000000	-1.730640000000	0.428401000000
Pb	-3.455709000000	1.437218000000	-0.188136000000
Cl	-1.094972000000	9.412154000000	-2.883606000000
Cl	-7.546906000000	-7.102136000000	-1.654570000000
S	-4.892120000000	-5.873348000000	-0.550857000000
C	-6.477949000000	-5.681350000000	-1.398655000000
C	-6.737272000000	-4.380759000000	-1.801547000000
H	-7.641487000000	-4.083044000000	-2.335353000000
C	-5.672006000000	-3.480436000000	-1.438180000000
H	-5.661731000000	-2.412882000000	-1.666514000000
S	-2.484136000000	6.758552000000	-1.994385000000

O	-1.114274000000	0.053615000000	-1.037639000000
O	-2.445085000000	0.241197000000	1.566318000000
O	-3.398286000000	4.063781000000	-1.025874000000
O	-1.370827000000	3.171148000000	-0.422316000000
O	-3.232656000000	-2.163186000000	-0.394653000000
O	-2.446866000000	-4.235352000000	0.267675000000
N	-0.641498000000	-2.505953000000	-1.904782000000
N	-3.689189000000	2.670233000000	1.895273000000
N	-6.057073000000	2.417380000000	-0.584082000000
N	-5.564012000000	0.115981000000	0.904117000000
C	-0.955853000000	-1.549458000000	-2.853604000000
C	-1.200277000000	-0.203253000000	-2.380428000000
C	-1.509532000000	0.792941000000	-3.331832000000
H	-1.677361000000	1.820015000000	-2.992022000000
C	-1.599428000000	0.470309000000	-4.720091000000
H	-1.852151000000	1.269037000000	-5.426919000000
C	-1.371372000000	-0.828664000000	-5.190631000000
H	-1.440007000000	-1.062580000000	-6.258735000000
C	-1.036278000000	-1.865075000000	-4.260089000000
C	-0.765339000000	-3.221005000000	-4.637377000000
H	-0.818829000000	-3.503637000000	-5.695135000000
C	-0.432748000000	-4.167053000000	-3.662315000000
H	-0.218659000000	-5.206403000000	-3.925768000000
C	-0.379439000000	-3.771988000000	-2.291968000000
H	-0.129210000000	-4.481898000000	-1.500802000000
C	-3.274742000000	1.985787000000	3.026285000000
C	-2.629101000000	0.696991000000	2.830309000000
C	-2.236975000000	-0.018064000000	3.986657000000
H	-1.745493000000	-0.988184000000	3.864679000000
C	-2.450005000000	0.516191000000	5.289609000000
H	-2.121648000000	-0.072306000000	6.153796000000
C	-3.053338000000	1.766433000000	5.489666000000
H	-3.204987000000	2.167184000000	6.497840000000
C	-3.474337000000	2.527452000000	4.353658000000
C	-4.091735000000	3.818643000000	4.443710000000

Complex IV

Pb4C80N8H48S4O12Cl4

Pb	1.731955000000	0.996854000000	0.235446000000
Pb	-1.054095000000	1.817512000000	-3.123226000000
C	1.628303000000	3.408735000000	-2.869505000000
C	2.956627000000	4.065268000000	-2.804513000000
S	3.514053000000	5.035498000000	-4.253359000000

H	-4.256374000000	4.263964000000	5.431909000000
C	-4.472802000000	4.500216000000	3.283131000000
H	-4.933581000000	5.490888000000	3.328372000000
C	-4.260372000000	3.889366000000	2.011554000000
H	-4.532618000000	4.385288000000	1.076684000000
C	-7.130891000000	1.658882000000	-0.164330000000
C	-6.290267000000	3.525990000000	-1.330391000000
H	-5.397194000000	4.088407000000	-1.619649000000
C	-7.603684000000	3.941038000000	-1.699920000000
H	-7.731567000000	4.843569000000	-2.304237000000
C	-8.703020000000	3.185141000000	-1.274897000000
H	-9.725198000000	3.479706000000	-1.538434000000
C	-8.490734000000	2.011933000000	-0.486063000000
C	-9.580581000000	1.187726000000	-0.013404000000
H	-10.606768000000	1.477414000000	-0.267512000000
C	-9.334918000000	0.056529000000	0.743634000000
H	-10.163409000000	-0.565934000000	1.100943000000
C	-7.983410000000	-0.336010000000	1.076793000000
C	-7.695643000000	-1.507142000000	1.844466000000
H	-8.520020000000	-2.133373000000	2.203340000000
C	-6.365752000000	-1.843621000000	2.117496000000
H	-6.107841000000	-2.737663000000	2.690642000000
C	-5.323935000000	-1.007028000000	1.622813000000
H	-4.270614000000	-1.242250000000	1.787337000000
C	-6.871660000000	0.460898000000	0.624617000000
C	-2.098183000000	4.155784000000	-0.908999000000
C	-1.434316000000	5.410229000000	-1.336303000000
C	-0.987879000000	7.749407000000	-2.212388000000
C	0.169128000000	7.097476000000	-1.818948000000
H	1.165048000000	7.539474000000	-1.876362000000
C	-0.089479000000	5.769153000000	-1.321966000000
H	0.709775000000	5.110361000000	-0.966883000000
C	-3.355966000000	-3.473426000000	-0.264108000000
C	-4.613589000000	-4.082747000000	-0.768517000000

C	3.905592000000	4.073301000000	-1.786530000000
H	3.771514000000	3.553075000000	-0.832284000000
C	5.092744000000	4.830466000000	-2.097181000000
H	5.937608000000	4.941437000000	-1.415657000000
C	5.041762000000	5.400128000000	-3.358795000000
C	4.322996000000	2.825835000000	3.471107000000
C	5.306308000000	3.806657000000	3.535218000000
H	5.658987000000	4.311872000000	2.633861000000
C	5.790388000000	4.081211000000	4.864740000000

H	6.559176000000	4.818820000000	5.101444000000
C	5.159871000000	3.297256000000	5.818157000000
S	3.923785000000	2.173035000000	5.127161000000
O	1.202747000000	2.714134000000	-1.836233000000
O	0.917909000000	3.542025000000	-3.960848000000
O	2.747001000000	1.325603000000	2.454904000000
O	3.861365000000	2.850092000000	1.116539000000
O	-0.043517000000	0.260992000000	1.517438000000
O	-2.222205000000	1.539696000000	-1.095388000000
N	0.524070000000	2.926896000000	1.208849000000
N	-1.858535000000	3.968552000000	-2.332014000000
N	-3.625447000000	1.748616000000	-3.974489000000
N	-1.697933000000	2.912550000000	-5.613105000000
C	3.611047000000	2.312657000000	2.270730000000
C	0.815920000000	4.229016000000	1.008895000000
H	1.556908000000	4.447667000000	0.237110000000
C	0.193710000000	5.265195000000	1.767989000000
H	0.467182000000	6.305922000000	1.573814000000
C	-0.745684000000	4.928985000000	2.748283000000
H	-1.231131000000	5.707707000000	3.347809000000
C	-1.086830000000	3.555721000000	2.975851000000
C	-2.045192000000	3.119941000000	3.947354000000
H	-2.552995000000	3.860058000000	4.575548000000
C	-2.321818000000	1.753133000000	4.075379000000
H	-3.055567000000	1.413283000000	4.815341000000
C	-1.671227000000	0.775655000000	3.262588000000
H	-1.914562000000	-0.285998000000	3.372282000000
C	-0.706146000000	1.162111000000	2.307788000000
C	-0.414722000000	2.572133000000	2.160700000000
C	-1.621752000000	5.148992000000	-2.944848000000
H	-0.934991000000	5.120221000000	-3.794157000000
C	-2.219197000000	6.362419000000	-2.491171000000
H	-1.996285000000	7.295611000000	-3.015849000000
C	-3.079066000000	6.332569000000	-1.388211000000
H	-3.556954000000	7.251414000000	-1.028611000000
C	-3.342307000000	5.096971000000	-0.709681000000
C	-4.205916000000	4.981632000000	0.425016000000
H	-4.710586000000	5.871826000000	0.816009000000
C	-4.389338000000	3.724529000000	1.019343000000
H	-5.045364000000	3.626877000000	1.891712000000
C	-3.736912000000	2.556986000000	0.529719000000
H	-3.885008000000	1.594948000000	1.029897000000
C	-2.870497000000	2.617243000000	-0.587461000000
C	-2.685331000000	3.913342000000	-1.222057000000

C	-4.565089000000	1.187110000000	-3.176840000000
H	-4.221694000000	0.886465000000	-2.185161000000
C	-5.909990000000	0.978225000000	-3.597214000000
H	-6.622482000000	0.521852000000	-2.905362000000
C	-6.281598000000	1.346483000000	-4.894458000000
H	-7.303936000000	1.187154000000	-5.254919000000
C	-5.310214000000	1.926860000000	-5.767481000000
C	-3.977690000000	2.121049000000	-5.256519000000
C	-5.625106000000	2.310728000000	-7.125621000000
H	-6.645004000000	2.146980000000	-7.492202000000
C	-4.661963000000	2.863782000000	-7.949606000000
H	-4.904338000000	3.146974000000	-8.980370000000
C	-3.315022000000	3.079477000000	-7.470643000000
C	-2.965940000000	2.716301000000	-6.120338000000
C	-2.291480000000	3.649474000000	-8.289915000000
H	-2.523942000000	3.934149000000	-9.322414000000
C	-1.007539000000	3.836831000000	-7.763306000000
H	-0.203007000000	4.270977000000	-8.363623000000
C	-0.748096000000	3.458119000000	-6.413284000000
H	0.230587000000	3.600218000000	-5.944163000000
Pb	-1.731955000000	-0.996854000000	-0.235446000000
Pb	1.054095000000	-1.817512000000	3.123226000000
C	-1.628303000000	-3.408735000000	2.869505000000
C	-2.956627000000	-4.065268000000	2.804513000000
S	-3.514053000000	-5.035498000000	4.253359000000
C	-3.905592000000	-4.073301000000	1.786530000000
H	-3.771514000000	-3.553075000000	0.832284000000
C	-5.092744000000	-4.830466000000	2.097181000000
H	-5.937608000000	-4.941437000000	1.415657000000
C	-5.041762000000	-5.400128000000	3.358795000000
C	-4.322996000000	-2.825835000000	-3.471107000000
C	-5.306308000000	-3.806657000000	-3.535218000000
H	-5.658987000000	-4.311872000000	-2.633861000000
C	-5.790388000000	-4.081211000000	-4.864740000000
H	-6.559176000000	-4.818820000000	-5.101444000000
C	-5.159871000000	-3.297256000000	-5.818157000000
S	-3.923785000000	-2.173035000000	-5.127161000000
O	-1.202747000000	-2.714134000000	1.836233000000
O	-0.917909000000	-3.542025000000	3.960848000000
O	-2.747001000000	-1.325603000000	-2.454904000000
O	-3.861365000000	-2.850092000000	-1.116539000000
O	0.043517000000	-0.260992000000	-1.517438000000
O	2.222205000000	-1.539696000000	1.095388000000
N	-0.524070000000	-2.926896000000	-1.208849000000

N	1.858535000000	-3.968552000000	2.332014000000
N	3.625447000000	-1.748616000000	3.974489000000
N	1.697933000000	-2.912550000000	5.613105000000
C	-3.611047000000	-2.312657000000	-2.270730000000
C	-0.815920000000	-4.229016000000	-1.008895000000
H	-1.556908000000	-4.447667000000	-0.237110000000
C	-0.193710000000	-5.265195000000	-1.767989000000
H	-0.467182000000	-6.305922000000	-1.573814000000
C	0.745684000000	-4.928985000000	-2.748283000000
H	1.231131000000	-5.707707000000	-3.347809000000
C	1.086830000000	-3.555721000000	-2.975851000000
C	2.045192000000	-3.119941000000	-3.947354000000
H	2.552995000000	-3.860058000000	-4.575548000000
C	2.321818000000	-1.753133000000	-4.075379000000
H	3.055567000000	-1.413283000000	-4.815341000000
C	1.671227000000	-0.775655000000	-3.262588000000
H	1.914562000000	0.285998000000	-3.372282000000
C	0.706146000000	-1.162111000000	-2.307788000000
C	0.414722000000	-2.572133000000	-2.160700000000
C	1.621752000000	-5.148992000000	2.944848000000
H	0.934991000000	-5.120221000000	3.794157000000
C	2.219197000000	-6.362419000000	2.491171000000
H	1.996285000000	-7.295611000000	3.015849000000
C	3.079066000000	-6.332569000000	1.388211000000
H	3.556954000000	-7.251414000000	1.028611000000
C	3.342307000000	-5.096971000000	0.709681000000
C	4.205916000000	-4.981632000000	-0.425016000000
H	4.710586000000	-5.871826000000	-0.816009000000
C	4.389338000000	-3.724529000000	-1.019343000000

H	5.045364000000	-3.626877000000	-1.891712000000
C	3.736912000000	-2.556986000000	-0.529719000000
H	3.885008000000	-1.594948000000	-1.029897000000
C	2.870497000000	-2.617243000000	0.587461000000
C	2.685331000000	-3.913342000000	1.222057000000
C	4.565089000000	-1.187110000000	3.176840000000
H	4.221694000000	-0.886465000000	2.185161000000
C	5.909990000000	-0.978225000000	3.597214000000
H	6.622482000000	-0.521852000000	2.905362000000
C	6.281598000000	-1.346483000000	4.894458000000
H	7.303936000000	-1.187154000000	5.254919000000
C	5.310214000000	-1.926860000000	5.767481000000
C	3.977690000000	-2.121049000000	5.256519000000
C	5.625106000000	-2.310728000000	7.125621000000
H	6.645004000000	-2.146980000000	7.492202000000
C	4.661963000000	-2.863782000000	7.949606000000
H	4.904338000000	-3.146974000000	8.980370000000
C	3.315022000000	-3.079477000000	7.470643000000
C	2.965940000000	-2.716301000000	6.120338000000
C	2.291480000000	-3.649474000000	8.289915000000
H	2.523942000000	-3.934149000000	9.322414000000
C	1.007539000000	-3.836831000000	7.763306000000
H	0.203007000000	-4.270977000000	8.363623000000
C	0.748096000000	-3.458119000000	6.413284000000
H	-0.230587000000	-3.600218000000	5.944163000000
Cl	6.315491000000	6.414292000000	-4.119275000000
Cl	5.467614000000	3.331879000000	7.589092000000
Cl	-6.315491000000	-6.414292000000	4.119275000000
Cl	-5.467614000000	-3.331879000000	-7.589092000000

Complex V

Pb4C80N8H48S4O12Br4

Pb	1.690474000000	-1.026621000000	0.380382000000
Pb	2.229363000000	3.026150000000	0.030740000000
S	7.179072000000	-2.529874000000	-0.666002000000
C	8.477417000000	-1.519828000000	-1.423181000000
C	8.054622000000	-0.234205000000	-1.733010000000
H	8.695049000000	0.514793000000	-2.202708000000
C	6.678629000000	-0.007769000000	-1.370261000000
H	6.143028000000	0.929334000000	-1.534272000000
S	-1.318068000000	7.171499000000	-1.612624000000
O	0.943298000000	0.693695000000	-0.985092000000

O	1.980916000000	1.370339000000	1.683535000000
O	0.829565000000	5.276993000000	-0.673219000000
O	-0.475765000000	3.451157000000	-0.186074000000
O	3.886999000000	-0.156779000000	-0.378082000000
O	4.235612000000	-2.382203000000	0.138837000000
N	1.834880000000	-1.694454000000	-1.996352000000
N	1.795980000000	4.066386000000	2.182686000000
N	3.954629000000	5.226758000000	-0.235581000000
N	4.717486000000	2.916123000000	1.114579000000
C	1.628081000000	-0.653914000000	-2.884131000000
C	1.158572000000	0.600492000000	-2.334301000000

C	0.933977000000	1.674799000000	-3.222534000000
H	0.565842000000	2.626649000000	-2.826602000000
C	1.179309000000	1.526109000000	-4.621630000000
H	1.001403000000	2.386190000000	-5.277453000000
C	1.633801000000	0.318671000000	-5.165938000000
H	1.813708000000	0.216206000000	-6.241789000000
C	1.860613000000	-0.800877000000	-4.301409000000
C	2.307884000000	-2.084370000000	-4.755951000000
H	2.498271000000	-2.237270000000	-5.824547000000
C	2.492751000000	-3.126778000000	-3.841935000000
H	2.829597000000	-4.115504000000	-4.165077000000
C	2.244821000000	-2.895387000000	-2.455701000000
H	2.380978000000	-3.680623000000	-1.709289000000
C	1.782214000000	3.196454000000	3.260674000000
C	1.888829000000	1.773962000000	2.974316000000
C	1.900861000000	0.886591000000	4.076634000000
H	1.970328000000	-0.188719000000	3.885336000000
C	1.799920000000	1.371029000000	5.412078000000
H	1.808754000000	0.643700000000	6.231781000000
C	1.681567000000	2.739061000000	5.698930000000
H	1.599886000000	3.096106000000	6.731331000000
C	1.665077000000	3.678760000000	4.620312000000
C	1.535687000000	5.095681000000	4.798967000000
H	1.443282000000	5.499645000000	5.813984000000
C	1.522426000000	5.948044000000	3.689733000000
H	1.412985000000	7.030182000000	3.803025000000
C	1.659303000000	5.395952000000	2.381536000000
H	1.643868000000	6.017988000000	1.483095000000
C	5.262518000000	5.111213000000	0.188576000000
C	3.582551000000	6.339107000000	-0.917001000000
H	2.529072000000	6.373806000000	-1.212200000000
C	4.491471000000	7.397340000000	-1.213909000000
H	4.136274000000	8.270565000000	-1.768355000000
C	5.819800000000	7.297362000000	-0.782308000000
H	6.541288000000	8.095690000000	-0.990284000000
C	6.242560000000	6.137973000000	-0.060284000000
C	7.597417000000	5.971081000000	0.416404000000
H	8.325512000000	6.766356000000	0.218967000000
C	7.969315000000	4.831524000000	1.106715000000
H	8.997364000000	4.708493000000	1.466647000000
C	7.016915000000	3.774030000000	1.364061000000
C	7.373090000000	2.576836000000	2.059768000000
H	8.399688000000	2.447003000000	2.420015000000
C	6.409592000000	1.582803000000	2.260473000000

H	6.648983000000	0.649796000000	2.776717000000
C	5.089025000000	1.788003000000	1.766097000000
H	4.308423000000	1.032648000000	1.876293000000
C	5.657461000000	3.905660000000	0.906432000000
C	-0.339380000000	4.690436000000	-0.609382000000
C	-1.540483000000	5.452807000000	-1.026381000000
C	-3.108043000000	7.275606000000	-1.861616000000
C	-3.771102000000	6.105012000000	-1.522474000000
H	-4.851626000000	5.974450000000	-1.602193000000
C	-2.880065000000	5.075303000000	-1.050039000000
H	-3.235349000000	4.087558000000	-0.738767000000
C	4.649639000000	-1.234754000000	-0.312403000000
C	6.049978000000	-1.103292000000	-0.790194000000
Pb	-1.690471000000	1.026611000000	-0.380421000000
Pb	-2.229365000000	-3.026156000000	-0.030780000000
S	-7.179083000000	2.529830000000	0.665937000000
C	-8.477388000000	1.519815000000	1.423225000000
C	-8.054602000000	0.234177000000	1.733007000000
H	-8.695017000000	-0.514815000000	2.202730000000
C	-6.678623000000	0.007732000000	1.370212000000
H	-6.143021000000	-0.929373000000	1.534210000000
S	1.318064000000	-7.171534000000	1.612522000000
O	-0.943293000000	-0.693703000000	0.985054000000
O	-1.980913000000	-1.370348000000	-1.683576000000
O	-0.829570000000	-5.276996000000	0.673185000000
O	0.475765000000	-3.451164000000	0.186041000000
O	-3.886990000000	0.156760000000	0.378044000000
O	-4.235616000000	2.382182000000	-0.138877000000
N	-1.834877000000	1.694446000000	1.996313000000
N	-1.795595000000	-4.066395000000	-2.182723000000
N	-3.954632000000	-5.226762000000	0.235540000000
N	-4.717484000000	-2.916130000000	-1.114627000000
C	-1.628079000000	0.653905000000	2.884092000000
C	-1.158569000000	-0.600500000000	2.334263000000
C	-0.933976000000	-1.674807000000	3.222496000000
H	-0.565843000000	-2.626658000000	2.826656000000
C	-1.179310000000	-1.526117000000	4.621592000000
H	-1.001406000000	-2.386198000000	5.277416000000
C	-1.633802000000	-0.318679000000	5.165899000000
H	-1.813710000000	-0.216214000000	6.241750000000
C	-1.860612000000	0.800869000000	4.301371000000
C	-2.307884000000	2.084362000000	4.755911000000
H	-2.498272000000	2.237262000000	5.824507000000
C	-2.492750000000	3.126770000000	3.841895000000

H	-2.829597000000	4.115495000000	4.165037000000
C	-2.244819000000	2.895378000000	2.455661000000
H	-2.380975000000	3.680614000000	1.709249000000
C	-1.782207000000	-3.196466000000	-3.260712000000
C	-1.888822000000	-1.773973000000	-2.974356000000
C	-1.900851000000	-0.886604000000	-4.076676000000
H	-1.970317000000	0.188707000000	-3.885380000000
C	-1.799906000000	-1.371044000000	-5.412119000000
H	-1.808737000000	-0.643716000000	-6.231824000000
C	-1.681553000000	-2.739077000000	-5.698969000000
H	-1.599869000000	-3.096123000000	-6.731369000000
C	-1.665066000000	-3.678774000000	-4.620349000000
C	-1.535676000000	-5.095695000000	-4.799001000000
H	-1.443268000000	-5.499660000000	-5.814018000000
C	-1.522418000000	-5.948057000000	-3.689766000000
H	-1.412977000000	-7.030195000000	-3.803056000000
C	-1.659299000000	-5.395963000000	-2.381570000000
H	-1.643867000000	-6.017997000000	-1.483128000000
C	-5.262520000000	-5.111217000000	-0.188621000000
C	-3.582557000000	-6.339110000000	0.916962000000
H	-2.529078000000	-6.373810000000	1.212164000000
C	-4.491478000000	-7.397342000000	1.213871000000
H	-4.136283000000	-8.270567000000	1.768318000000
C	-5.819806000000	-7.297364000000	0.782267000000
H	-6.541295000000	-8.095691000000	0.990242000000

C	-6.242563000000	-6.137976000000	0.060240000000
C	-7.597419000000	-5.971084000000	-0.416452000000
H	-8.325515000000	-6.766358000000	-0.219015000000
C	-7.969315000000	-4.831528000000	-1.106767000000
H	-8.997363000000	-4.708497000000	-1.466702000000
C	-7.016914000000	-3.774036000000	-1.364113000000
C	-7.373085000000	-2.576842000000	-2.059824000000
H	-8.399683000000	-2.447010000000	-2.420073000000
C	-6.409585000000	-1.582811000000	-2.260529000000
H	-6.648975000000	-0.649805000000	-2.776776000000
C	-5.089021000000	-1.788011000000	-1.766149000000
H	-4.308417000000	-1.032658000000	-1.876345000000
C	-5.657460000000	-3.905665000000	-0.906480000000
C	0.339376000000	-4.690442000000	0.609352000000
C	1.540476000000	-5.452815000000	1.026356000000
C	3.108006000000	-7.275547000000	1.861791000000
C	3.771080000000	-6.104988000000	1.522556000000
H	4.851595000000	-5.974404000000	1.602349000000
C	2.880059000000	-5.075318000000	1.050007000000
H	3.235346000000	-4.087575000000	0.738729000000
C	-4.649636000000	1.234730000000	0.312364000000
C	-6.049974000000	1.103261000000	0.790155000000
Br	10.245516000000	-2.259689000000	-1.735495000000
Br	3.914956000000	-8.906931000000	2.538762000000
Br	-3.915027000000	8.907074000000	-2.538343000000

Table S2: RMSD of complex I

Atom Labels	Bond Length (Å) Expt	Bond Length (Å) Opt	RMSD
Pb1 - O20	2.811	2.743	0.034
Pb1 - O22	2.472	2.463	0.004
Pb1 - O24	2.334	2.311	0.011
Pb1 - O104	2.642	2.742	0.05
Pb1 - O105	2.602	2.723	0.060
Pb2 - O21	2.671	2.747	0.038
Pb2 - O25	2.349	2.357	0.004
Pb81 - O24	2.642	2.742	0.050
Pb81 - O25	2.602	2.723	0.061
Pb81 - O100	2.811	2.743	0.034
Pb81 - O102	2.472	2.463	0.005
Pb81 - O104	2.334	2.311	0.012

Pb82 - O101	2.671	2.747	0.038
Pb82 - O105	2.349	2.357	0.004
Pb1 - N26	2.485	2.476	0.005
Pb2 - N27	2.454	2.429	0.013
Pb2 - N28	2.734	2.710	0.012
Pb81 - N106	2.485	2.476	0.005
Pb82 - N107	2.454	2.429	0.013
Pb82 - N108	2.734	2.710	0.012

Table S3: Bite angles around the lead centres in complex I

6-coordinated Pb centre	
Atom Label	Bite angle
O3-Pb-N	69.83
7-coordinated Pb centre	
Atom Label	Bite angle
N1-Pb-N2	60.73
N3-Pb-O4	70.1
O1-Pb-O3	49.42

Table S4: Jeffery's classification of Hydrogen Bonds

Type	Strong	moderate	weak
Interaction type	Strongly covalent	Mostly electrostatic	electrostatic / dispersion
Bond length [Å]	1.2 - 1.5	1.5 - 2.2	2.2 - 3.2
Bond angle [°]	175 - 180	130 - 180	90 - 150

Table S5: Comparison of total energies of Complexes I, III, IV and V computed at BVP86/LanL2DZ basis set.

Complex	Arrangement	Types of Bonds	Total Energy (Hartree)	Difference (open-close) (Kcal/mol)
V	open Br (Theoretical)	H-bond	-9048.464910	27.010
I	close Br (Experimental)	Tetrel	-9048.507954	
III	open Cl (Experimental)	H-Bond	-9062.655624	64.460
IV	close Cl (Theoretical)	Tetrel	-9062.758350	

Table S6: Tetrel bond lengths (Å) in the structures of PbII complexes described in literature and in this work.

Complex	Bond	Ligand	Length Å	Reference
[Pb(L2)(Br)].H2O	Pb...Br	L	3.375	50
Complex I	Pb...Br	BTC	3.819	Present work
[Pb(HLV)Cl2] _n	Pb...Cl	Cl-	3.382	48
[Pb3(LVI)2Cl4] _n ·nMeOH	Pb...Cl	Cl-	3.440	48
[Pb3(LVI)2Cl4] _n ·nMeOH	Pb...Cl	Cl-	3.467	48
[Pb3(LVI)2Cl4] _n ·nMeOH	Pb...Cl	Cl-	3.490	48
[(H2O)(DMSO)NiLPbCl](SCN)	Pb...Cl	Cl-	3.339	7
Complex IV	Pb...Cl	BTC	3.863	Present work
[Pb(HL1)(I)2]2	Pb...I	I-	3.575	51
[Pb(L)(SCN)] _n	Pb...N	NCS-	3.542	51
[(H2O)Ni(SCN)L1 Pb(OAc)].DMSO	Pb...N	NCS-	3.379	45
[Pb(L)(I)]	Pb...N	L	3.247	47
[Pb(L)(μ-NO2)]CH3OH	Pb...N	L	3.408	47
[Pb(L)(NCS)]2	Pb...N	L	3.195	47
[Pb(HLII)Cl2] _n ·nMeOH	Pb...N	L	3.391	48
[Pb3(LVI)2Cl4] _n ·nMeOH	Pb...N	L	3.093	48
[Pb3(LVI)2Cl4] _n ·nMeOH	Pb...N	L	2.989	48
[Pb(MeOH)2(H2L3)(NCS)][NCS]	Pb...N	NCS-	3.329	50
Pb2(MeOH)2(L1)2(μ1,1-N3)2	Pb...N	L	3.200	50
[Pb(L1)(CH3COO)]	Pb...N	L	2.940	51
[Pb2(L2)(CH3COO)(SCN)2]2	Pb...N	L	2.978	51
[Pb(HL2)2(SCN)2](C2H5OH)	Pb...N	L	3.419	51
[PbL(NO2)] _n	Pb...N	L	3.235	38
[PbL(NO2)] _n	Pb...N	L	3.039	38
[Pb2(H2L ^{II})(NO3)4]	Pb...O	NO3	3.061	46
[Pb2(HL ^{II})(CH3COO)3] _n	Pb...O	CH3COO-	3.518	46
[Pb(HL ^I)(NO3)2] _n	Pb...O	NO3	3.117	46
[Pb(HL)(SCN)2]·CH3OH	Pb...S	NCS-	3.041	49
[Pb(HL)(SCN)2]·CH3OH	Pb...S	NCS-	3.404	49
[Pb(HL)(SCN)2]	Pb...S	NCS-	3.473	49
[(H2O)Ni(SCN)L1 Pb(OAc)].DMSO	Pb...S	NCS-	3.064	45
Pb(L4)(NCS)2	Pb...S	NCS-	3.051	50
Pb(L5)(NCS)2	Pb...S	NCS-	3.409	50
Pb(L5)(NCS)2	Pb...S	L	3.229	50
[Pb(HL2)2(SCN)2](C2H5OH)	Pb...S	NCS-	3.275	51
[Pb2(L2)(CH3COO)(SCN)2]2	Pb...S	NCS-	3.022	51

Tables7: Electron density (ρ) of Pb tetrel bonds reported in literature and in present work

Complex	Bond	ρ x 10 ² a.u	Reference
[Pb(L1)(CH3COO)]	Pb...N	1.88	51
[Pb2(L2)(CH3COO)(SCN)2]2	Pb...N	1.79	51
[Pb2(L2)(CH3COO)(SCN)2]2	Pb...N	1.75	51
[Pb2(L2)(CH3COO)(SCN)2]2	Pb...S	1.82	51
[Pb(HL2)2(SCN)2](C2H5OH)	Pb...S	1.93	51
[Pb(HL1)(I)2]2	Pb...I	1.34	51
[PbL(NO2)] _n	Pb...N	1.20	39
[PbL(NO2)] _n	Pb...N	1.76	39
Complex I	Pb...Br	0.73	present work
Complex IV	Pb...Cl	0.55	Present work

Figure S1: ORTEP view of complex I showing the atom numbering scheme with displacement ellipsoids drawn at a 50% probability level. Disordered bromine atoms are omitted for clarity. H atoms not involved in hydrogen bonding have been omitted for clarity.

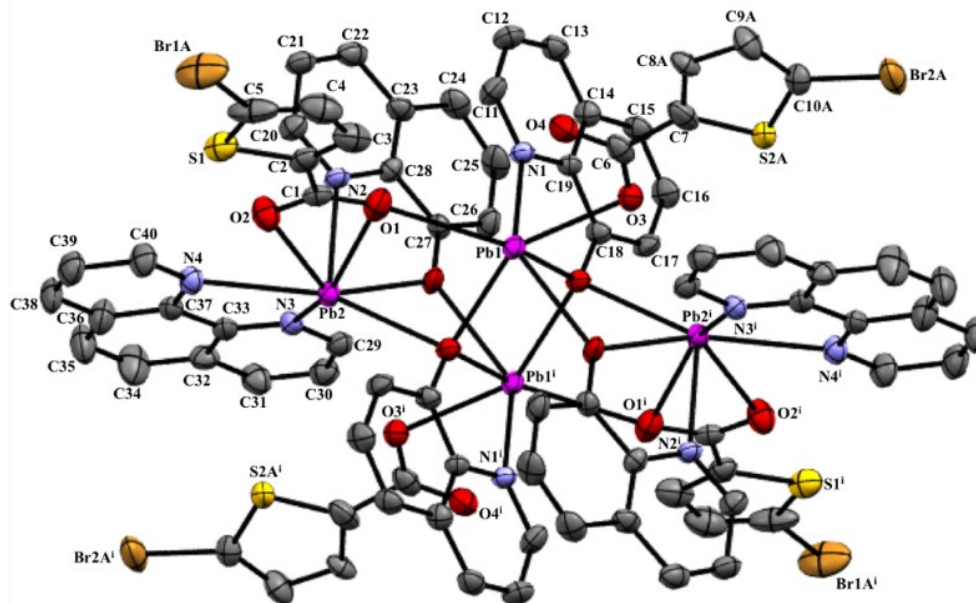


Figure S2: Schematic representation of (i) Hemi-directional and (ii) Holo-directional

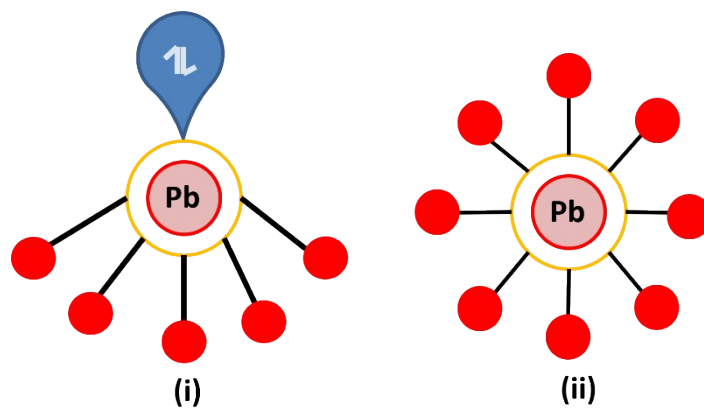


Figure S3: A view of three-dimensional supramolecular architecture in the complex (I) along c-axis and stacked along b-axis in close packed arrangement

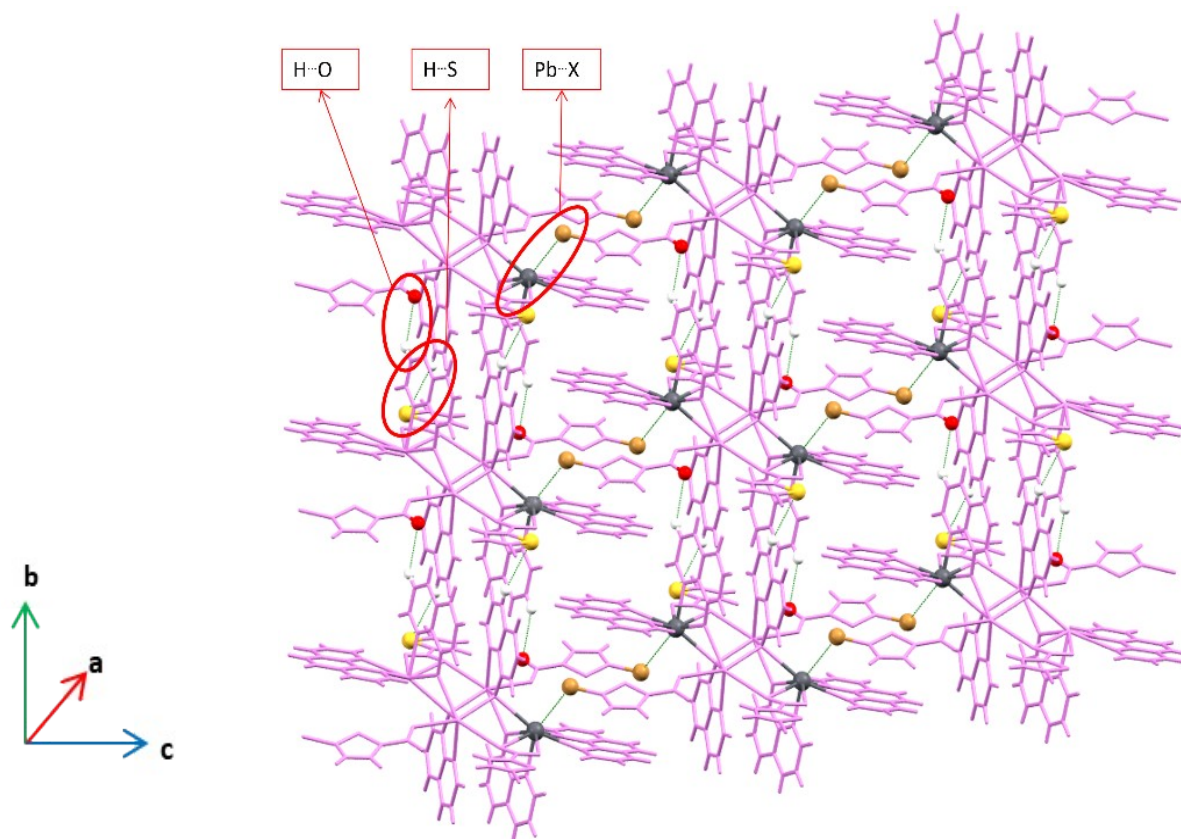


Figure S4: A view of three-dimensional supramolecular architecture in the complex (I) along c-axis and stacked along b-axis in open packed arrangement

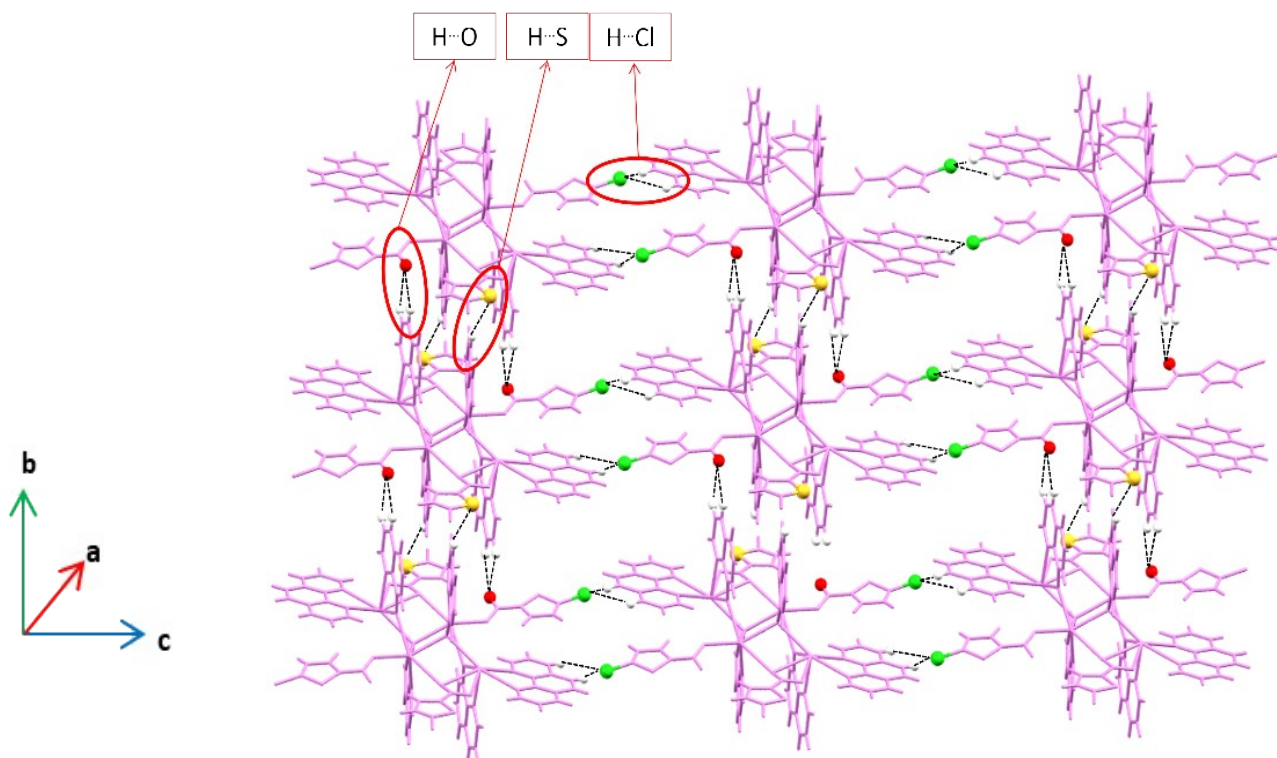


Figure S5: Molecular view of (i) AB and (ii) AC dimers in close packed structures

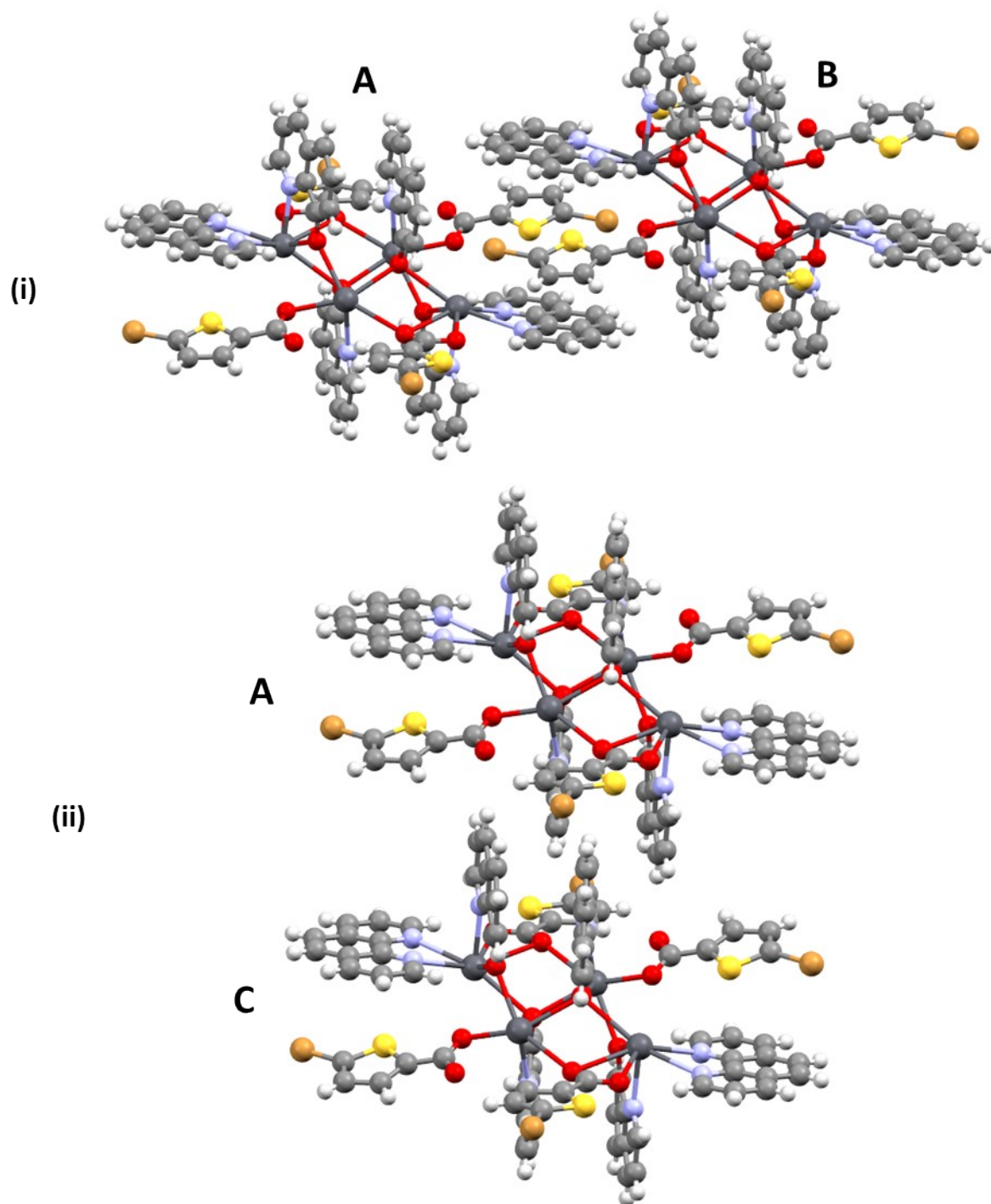


Figure S6: Molecular view of (i) AB and (ii) AC dimers in open packed structures

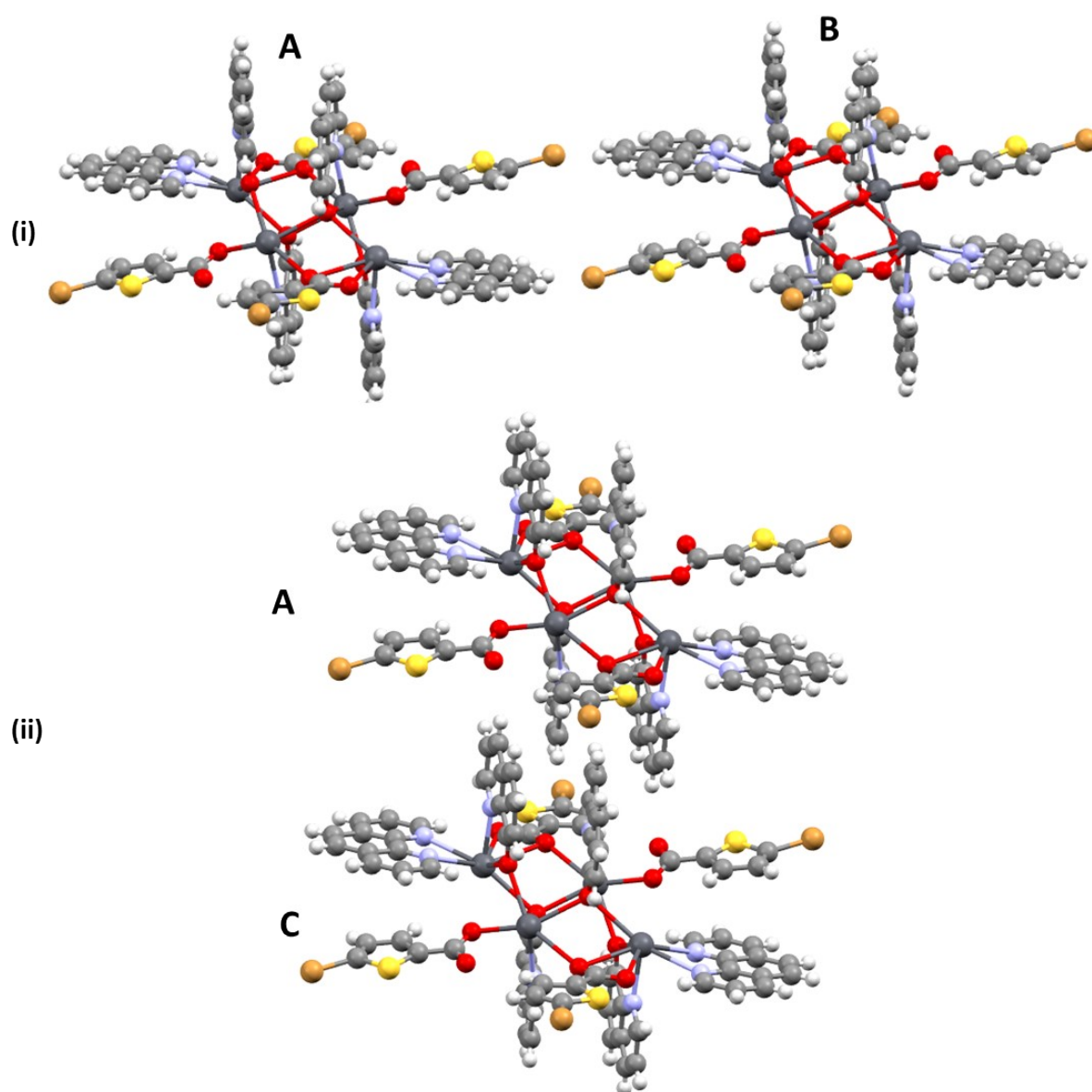


Figure S7: Molecular view of (i) AB and (ii) AC dimers of close packed complex IA where the Br atom involved in tetrel bond is replaced by H.

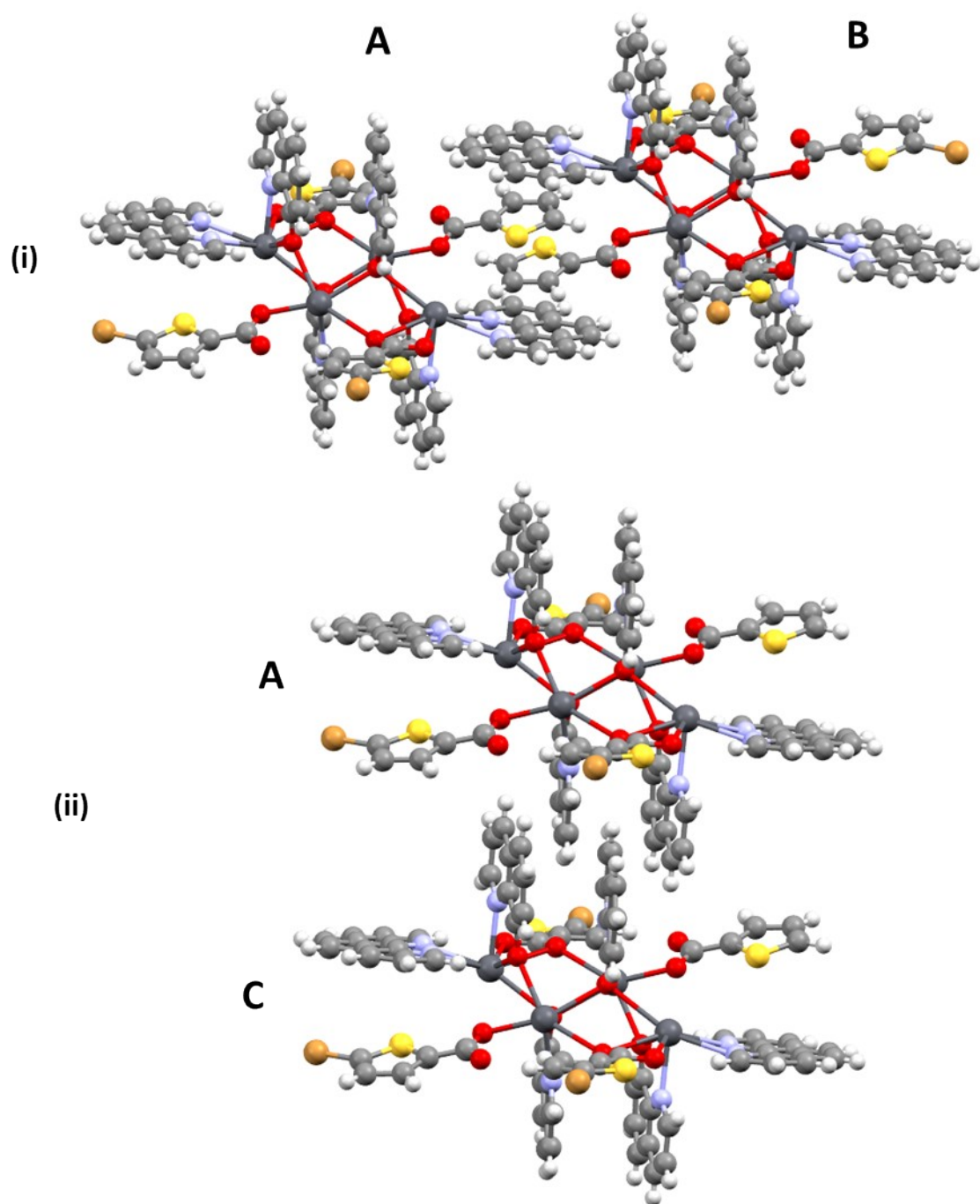


Figure S8: ESP map of asymmetric unit of complex II (computed at BVP86/LanL2DZ basis set using Gaussian 09w suite with isovalue 0.002 a.u.). Other atoms not taking part in intermolecular interactions are removed for clarity. H...Cl hydrogen bonding interactions are denoted by green dotted lines

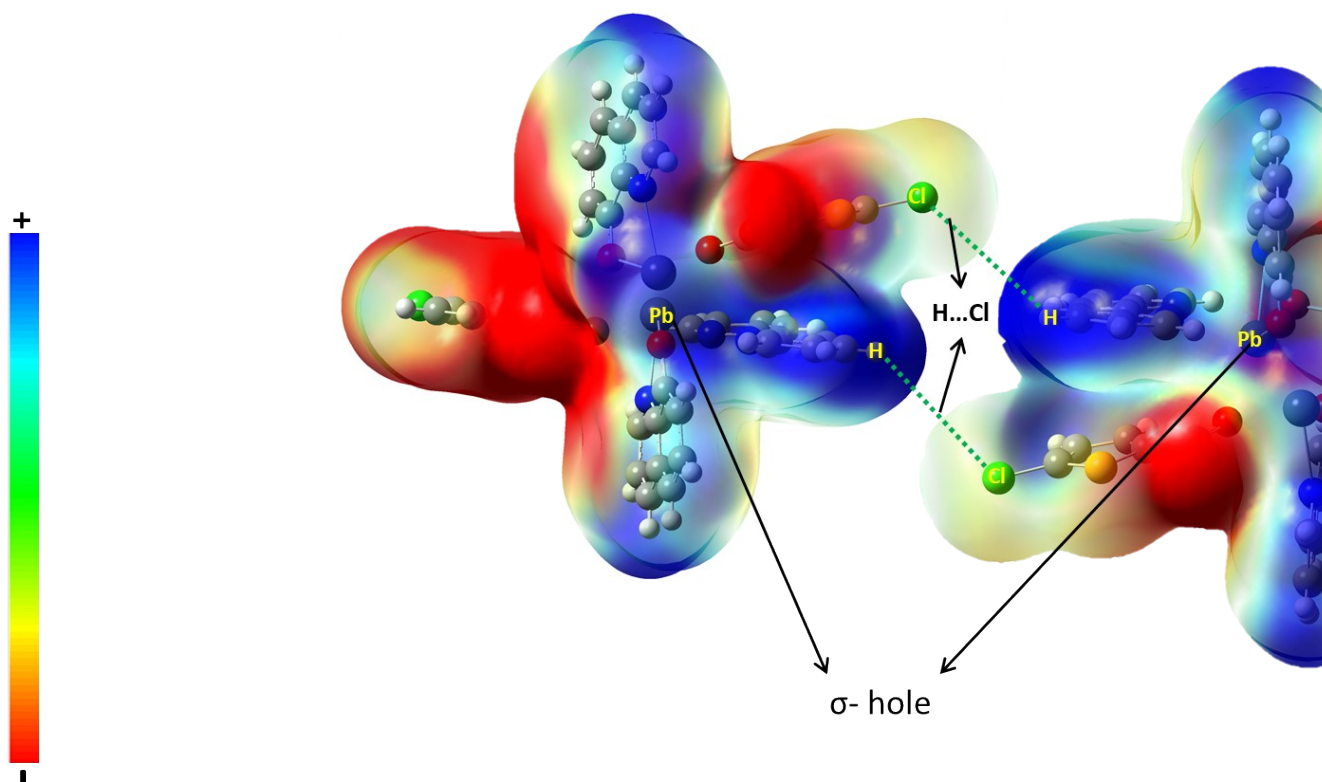


Figure S9: ESP map of asymmetric unit of complex III (computed at BVP86/LanL2DZ basis set using Gaussian 09w suite with isovalue 0.002 a.u.). Other atoms not taking part in intermolecular interactions are removed for clarity. The green dotted lines denote H...Cl hydrogen bonding interactions.

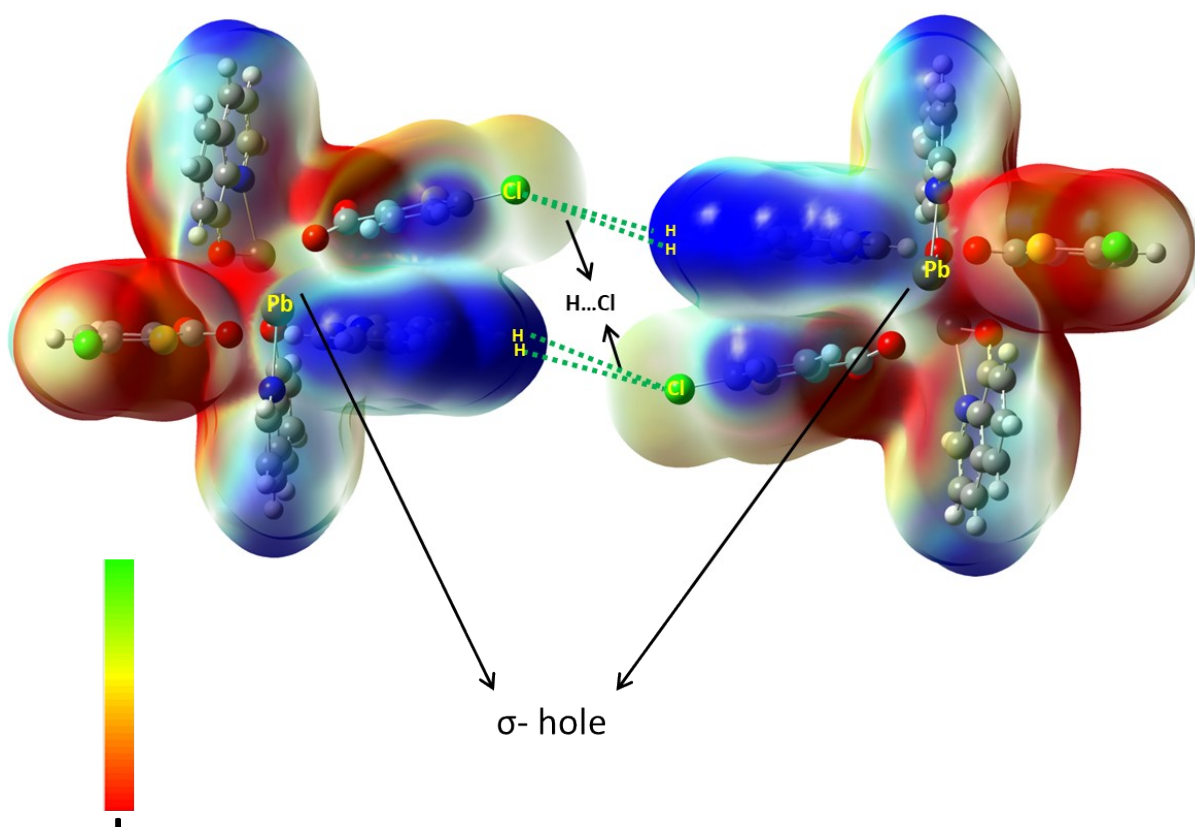


Figure S10: ESP map of asymmetric unit of complex V (computed at BVP86/LanL2DZ basis set using Gaussian 09w suite with isovalue 0.002 a.u.). Other atoms not taking part in intermolecular interactions are removed for clarity. H...Br hydrogen bonding interactions are denoted by green dotted lines.

