Computational search for redox isomerism
in Ge and Sn bis-chelates with α-diimine ligands

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**Table S1**. Spin states (S), total energies without (E) and with (E^{ZPE}) zero-point harmonic vibrations, relative energies without (ΔE) and with (ΔE^{ZPE}) zero-point harmonic vibrations of the isomers of the germanium complexes calculated by the DFT B3LYP/Def2-TZVP method.

Structure	S	E, a.u.	ΔE, kcal mol^{-1}	E^{ZPE}, a.u.	ΔE^{ZPE}, kcal mol^{-1}
Ge(R-L1)$_2$ (R = H, Me, Ph, Bu^t)					
1a Ge^{II}(H-L1)$_2$	1	-3223.09747	29.6	-3222.71432	28.6
2a Ge^{IV}(H-L1)$_2$	0	-3223.14467	0.0	-3222.75988	0.0
1b Ge^{II}(Me-L1)$_2$	1	-3301.72451	37.1	-3301.28578	35.7
2b Ge^{IV}(Me-L1)$_2$	0	-3301.78368	0.0	-3301.34269	0.0
1c Ge^{II}(Ph-L1)$_2$	1	-3685.33543	37.5	-3684.79220	35.8
2c Ge^{IV}(Ph-L1)$_2$	0	-3685.39513	0.0	-3684.84923	0.0
1d Ge^{II}(Bu^t-L1)$_2$	1	-3537.64737	55.8	-3537.04123	53.8
2d Ge^{IV}(Bu^t-L1)$_2$	0	-3537.736269	0.0	-3537.12704	0.0
Ge(R-L2)$_2$ (R = H, Me, Ph, Bu^t)					
3a Ge^{II}(H-L2)$_2$	0	-3372.36493	9.6	-3371.99595	10.0
4a Ge^{IV}(H-L2)$_2$	1	-3372.38020	0.0	-3372.01185	0.0
MECP$_{3a-4a}$	–	-3372.34819	20.1	–	–
3b Ge^{II}(Me-L2)$_2$	0	-3450.98837	19.6	-3450.56388	19.5
4b Ge^{IV}(Me-L2)$_2$	1	-3451.01954	0.0	-3450.59498	0.0
3c Ge^{II}(Ph-L2)$_2$	0	-3834.59911	19.7	-3834.06991	19.7
4c Ge^{IV}(Ph-L2)$_2$	1	-3834.63045	0.0	-3834.10129	0.0
4d Ge^{IV}(Bu^t-L2)$_2$	1	-3686.97253	–	-3686.37986	–

Table S2. Spin states (S), total energies without (E) and with (E^{ZPE}) zero-point harmonic vibrations, relative energies without (ΔE) and with (ΔE^{ZPE}) zero-point harmonic vibrations of the isomers of the tin complexes calculated by the DFT B3LYP/Def2-TZVP method.

Structure	S	E, a.u.	ΔE, kcal mol^{-1}	E^{ZPE}, a.u.	ΔE^{ZPE}, kcal mol^{-1}
Sn(R-L1)$_2$ (R = H, Me, Ph, Bu^t)					
1e Sn^{II}(H-L1)$_2$	1	-1360.43489	0.0	-1360.05318	0.0
2e Sn^{IV}(H-L1)$_2$	0	-1360.42866	3.9	-1360.04547	4.8
MECP$_{1e-2e}$	–	-1360.42631	5.4	–	–
1f Sn^{II}(Me-L1)$_2$	1	-1439.06525	0.0	-1438.62743	0.0
2f Sn^{IV}(Me-L1)$_2$	0	-1439.06416	0.7	-1438.62528	1.3
MECP$_{1f-2f}$	–	-1439.05902	3.9	–	–
1g Sn^{II}(Ph-L1)$_2$	1	-1822.67875	0.2	-1822.13610	0.0
2g Sn^{IV}(Ph-L1)$_2$	0	-1822.67903	0.0	-1822.13569	0.3
MECP$_{1g-2g}$	–	-1822.67025	5.3	–	–
1h Sn^{II}(Bu^t-L1)$_2$	1	-1675.00641	8.8	-1674.40134	7.6
2h Sn^{IV}(Bu^t-L1)$_2$	0	-1675.02039	0.0	-1674.41346	0.0
MECP$_{1h-2h}$	–	-1675.00075	12.3	–	–
Sn(R-L2)$_2$ (R = H, Me, Ph, Bu^t)					
3e Sn^{II}(H-L2)$_2$	0	-1509.70741	0.0	-1509.33956	0.0
4e Sn^{IV}(H-L2)$_2$	1	-1509.66488	26.7	-1509.29875	25.6
3f Sn^{II}(Me-L2)$_2$	0	-1588.33317	0.0	-1587.90923	0.0
4f Sn^{IV}(Me-L2)$_2$	1	-1588.30139	19.9	-1587.87895	19.0
3g Sn^{II}(Ph-L2)$_2$	0	-1971.94470	0.0	-1971.41638	0.0
4g Sn^{IV}(Ph-L2)$_2$	1	-1971.91711	17.3	-1971.39007	16.5
3h Sn^{II}(Bu^t-L2)$_2$	0	-1824.26174	0.0	-1823.67069	0.0
4h Sn^{IV}(Bu^t-L2)$_2$	1	-1824.25818	2.2	-1823.66803	1.7
3′h Sn^{II}(Bu^t-L2)$_2$	0	-1824.25464	4.5	-1823.66428	4.0
MECP$_{4h-3′h}$	–	-1824.24412	11.1	–	–
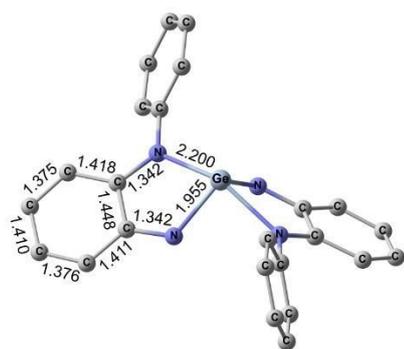
1a Ge^{II}(H-L1)$_2$
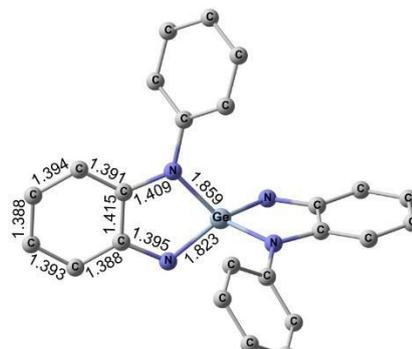
2a Ge^{IV}(H-L1)$_2$
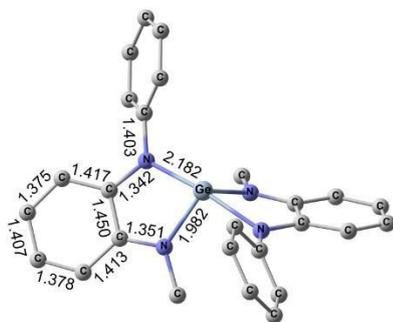
1b Ge^{II}(Me-L1)$_2$
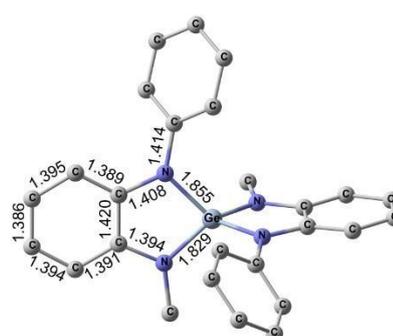
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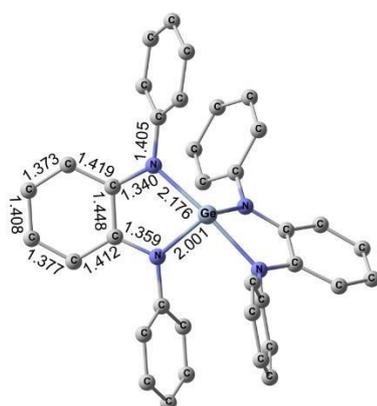
1c Ge^{II}(Ph-L1)$_2$
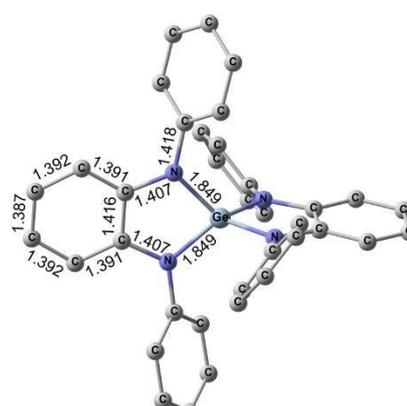
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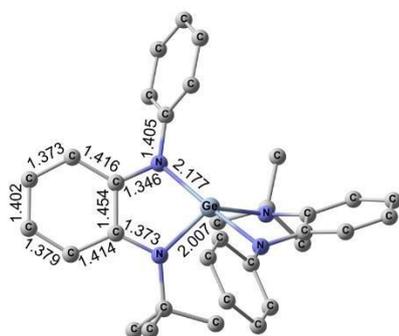
1d Ge^{II}(Bu^t-L1)$_2$
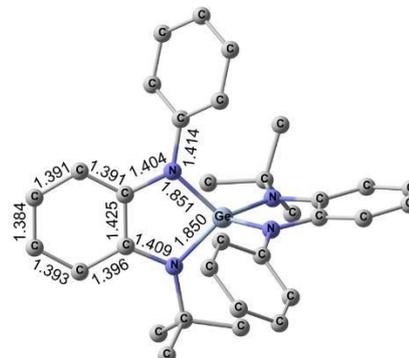
2d Ge^{IV}(Bu^t-L1)$_2$

Figure S1. Optimized geometries of the isomers of the complexes Ge(R-L1)$_2$ (R = H, Me, Ph, Bu^t) calculated by the DFT B3LYP/Def2-TZVP method. Hereafter, hydrogen atoms are omitted for clarity, bond lengths are given in Å.
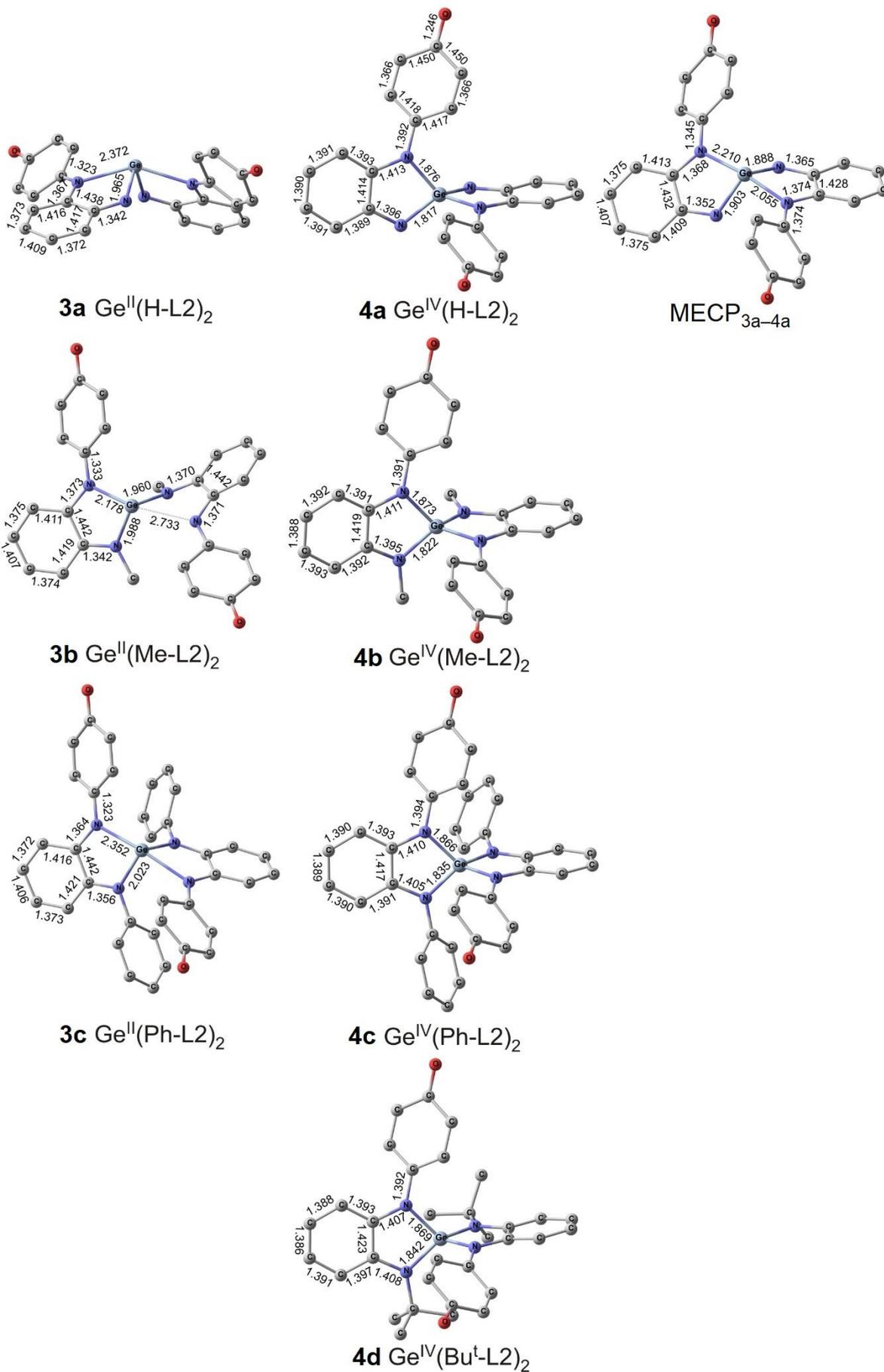
Figure S2. Optimized geometries of the isomers and MECP of the complexes Ge(R-L2)$_2$ (R = H, Me, Ph, Bu^t) calculated by the DFT B3LYP/Def2-TZVP method.
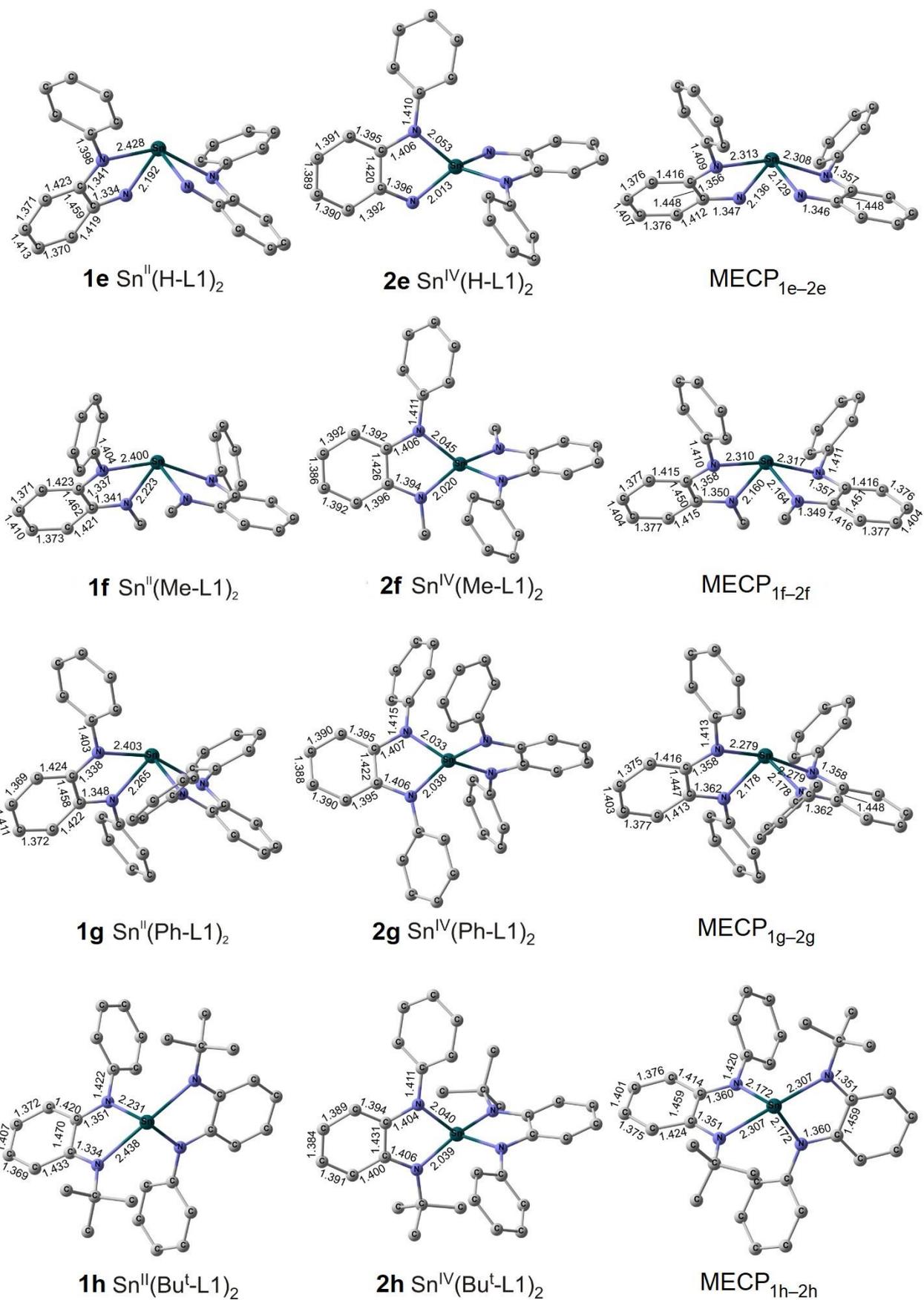
Figure S3. Optimized geometries of the isomers and MECPs of the complexes $Sn(R-L1)_2$ (R = H, Me, Ph, Bu^t) calculated by the DFT B3LYP/Def2-TZVP method.
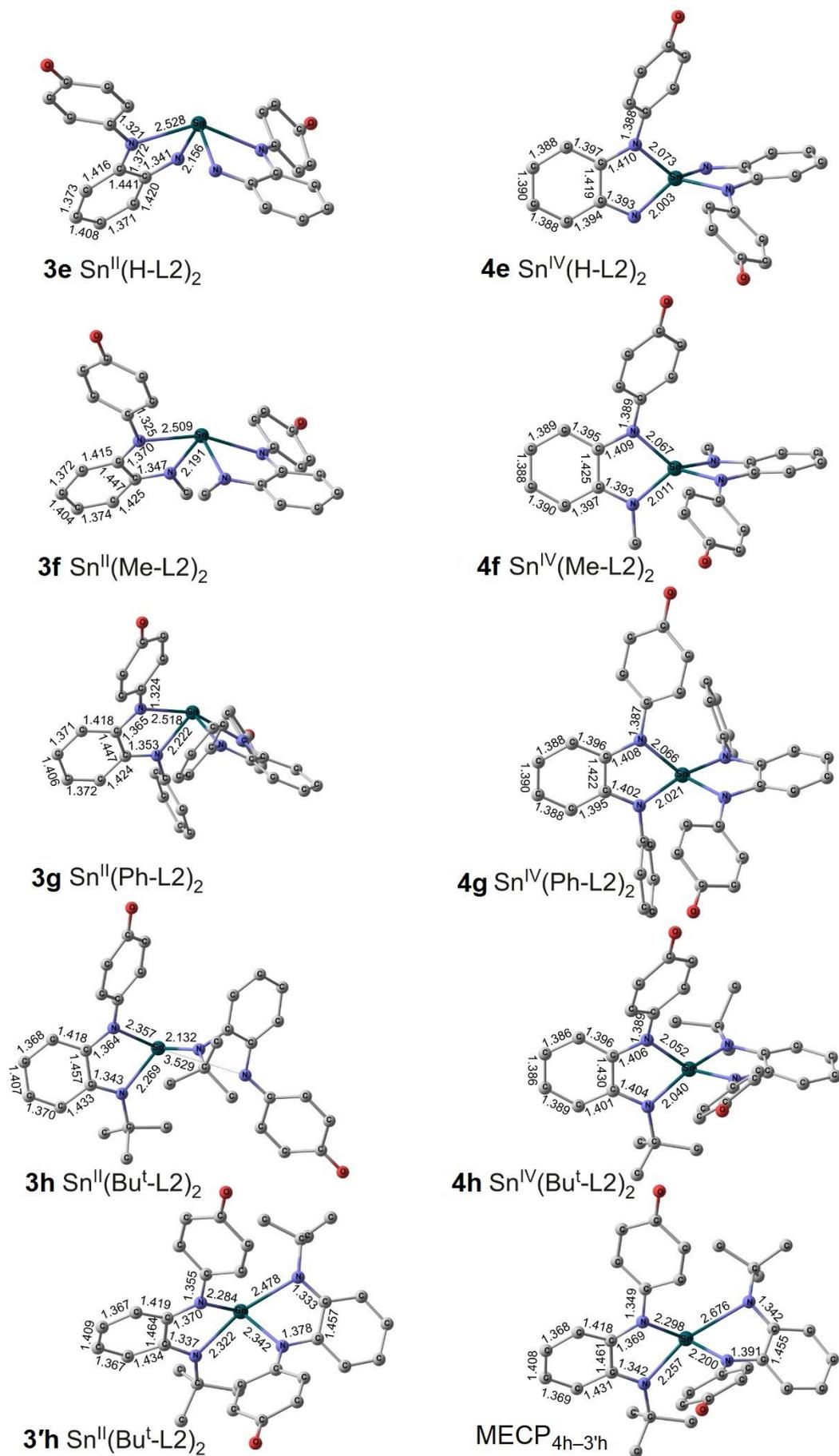
Figure S4. Optimized geometries of the isomers and MECP of the complexes $Sn(R-L2)_2$ (R = H, Me, Ph, Bu^t) calculated by the DFT B3LYP/Def2-TZVP method.

Cartesian coordinates of the isomers and MECPs of the complexes Ge(R-L1)₂, Ge(R-L2)₂ Sn(R-L1)₂, Sn(R-L2)₂ (R = H, Me, Ph, Buᵗ) calculated by DFT B3LYP/Def2-TZVP method

1a Ge^{II}(H-L1)₂

7	-0.115758000	1.543750000	-0.476470000
7	2.096579000	0.392281000	0.180784000
6	2.246409000	1.585613000	-0.414591000
6	3.457726000	2.279404000	-0.662167000
6	3.444505000	3.514321000	-1.265882000
6	2.227870000	4.121508000	-1.640245000
6	1.028069000	3.496170000	-1.391932000
6	0.999238000	2.227563000	-0.775346000
1	4.393089000	1.831074000	-0.359200000
1	2.239184000	5.094586000	-2.114376000
6	3.144918000	-0.474034000	0.495160000
6	3.174356000	-1.094462000	1.753191000
6	4.124937000	-0.829319000	-0.447208000
6	4.160362000	-2.021931000	2.061094000
6	5.103802000	-1.759810000	-0.130123000
6	5.132202000	-2.359333000	1.125640000
1	2.424901000	-0.826415000	2.485983000
1	4.095555000	-0.387183000	-1.434223000
7	0.115861000	-1.543494000	-0.476523000
7	-2.096614000	-0.392199000	0.180675000
6	-2.246316000	-1.585578000	-0.414635000
6	-3.457561000	-2.279505000	-0.662171000
6	-3.444219000	-3.514426000	-1.265873000
6	-2.227527000	-4.121480000	-1.640262000
6	-1.027789000	-3.496009000	-1.391977000
6	-0.999080000	-2.227396000	-0.775399000
1	-4.392968000	-1.831267000	-0.359200000
1	-2.238744000	-5.094563000	-2.114386000
6	-3.145050000	0.473991000	0.495066000
6	-3.174433000	1.094565000	1.753026000
6	-4.125246000	0.829000000	-0.447224000
6	-4.160547000	2.021918000	2.060935000
6	-5.104220000	1.759373000	-0.130132000
6	-5.132558000	2.359050000	1.125560000
1	-2.424844000	0.826729000	2.485757000
1	-4.095920000	0.386739000	-1.434185000
32	0.000016000	0.000105000	0.717722000
1	4.169498000	-2.480984000	3.041947000
1	5.846270000	-2.023469000	-0.873441000
1	4.377385000	4.032927000	-1.446323000
1	0.091170000	3.968274000	-1.662654000

1	-0.995544000	2.003537000	-0.663369000
1	0.995673000	-2.003231000	-0.663419000
1	-0.090845000	-3.968017000	-1.662708000
1	-4.377048000	-4.033133000	-1.446294000
1	-5.846826000	2.022816000	-0.873390000
1	-4.169632000	2.481093000	3.041732000
1	5.899395000	-3.082728000	1.369223000
1	-5.899836000	3.082355000	1.369148000

2a $Ge^{IV}(H-L1)_2$

7	0.813839000	1.384054000	-1.741184000
7	1.609854000	-0.348147000	-0.015764000
6	2.562676000	0.640747000	-0.332647000
6	3.827654000	0.782595000	0.227742000
6	4.648464000	1.840913000	-0.158464000
6	4.208417000	2.767222000	-1.094154000
6	2.936125000	2.649043000	-1.648189000
6	2.110778000	1.597596000	-1.272456000
1	4.171026000	0.075938000	0.970082000
1	4.848115000	3.587315000	-1.393365000
6	1.893016000	-1.541943000	0.686249000
6	0.987857000	-2.015795000	1.640000000
6	3.035826000	-2.301236000	0.408724000
6	1.216606000	-3.219410000	2.295943000
6	3.266606000	-3.493004000	1.081298000
6	2.359911000	-3.961218000	2.027288000
1	0.102134000	-1.436323000	1.869240000
1	3.734473000	-1.959410000	-0.342721000
7	-0.813933000	-1.384083000	-1.741120000
7	-1.609855000	0.348144000	-0.015681000
6	-2.562691000	-0.640758000	-0.332494000
6	-3.827637000	-0.782601000	0.227970000
6	-4.648465000	-1.840929000	-0.158171000
6	-4.208469000	-2.767253000	-1.093871000
6	-2.936208000	-2.649078000	-1.647980000
6	-2.110843000	-1.597622000	-1.272311000
1	-4.170969000	-0.075933000	0.970317000
1	-4.848180000	-3.587353000	-1.393031000
6	-1.892982000	1.541957000	0.686316000
6	-0.987767000	2.015843000	1.639997000
6	-3.035814000	2.301234000	0.408841000
6	-1.216482000	3.219476000	2.295920000
6	-3.266560000	3.493021000	1.081396000
6	-2.359809000	3.961268000	2.027315000
1	-0.102025000	1.436384000	1.869197000
1	-3.734508000	1.959382000	-0.342550000

32	-0.000024000	-0.000007000	-0.876983000
1	0.499489000	-3.569682000	3.027650000
1	4.156714000	-4.066565000	0.853645000
1	5.632337000	1.936903000	0.282093000
1	2.581917000	3.375129000	-2.370556000
1	0.369200000	2.103018000	-2.285292000
1	-0.369318000	-2.103062000	-2.285227000
1	-2.582039000	-3.375175000	-2.370355000
1	-5.632313000	-1.936915000	0.282443000
1	-4.156687000	4.066568000	0.853782000
1	-0.499322000	3.569773000	3.027571000
1	2.542382000	-4.893566000	2.545595000
1	-2.542254000	4.893630000	2.545605000

1b Ge^{II}(Me-L1)$_2$

7	0.175244000	1.513355000	-0.949906000
7	2.164231000	0.178398000	0.105674000
6	2.484668000	1.391037000	-0.372121000
6	3.750149000	2.022374000	-0.290154000
6	3.958832000	3.253679000	-0.865184000
6	2.910968000	3.917475000	-1.528500000
6	1.651000000	3.361825000	-1.587470000
6	1.387908000	2.106273000	-0.995063000
1	4.554558000	1.517458000	0.224976000
1	3.089711000	4.884461000	-1.981206000
6	3.084289000	-0.686702000	0.716999000
6	2.813198000	-1.217446000	1.984617000
6	4.239453000	-1.116373000	0.045909000
6	3.674738000	-2.141354000	2.562497000
6	5.095006000	-2.038075000	0.631769000
6	4.820172000	-2.556198000	1.893656000
1	1.929670000	-0.887487000	2.513789000
1	4.450018000	-0.734295000	-0.944524000
7	-0.175266000	-1.513356000	-0.950072000
7	-2.164213000	-0.178446000	0.105601000
6	-2.484706000	-1.391004000	-0.372380000
6	-3.750217000	-2.022290000	-0.290543000
6	-3.958935000	-3.253512000	-0.865745000
6	-2.911078000	-3.917271000	-1.529108000
6	-1.651080000	-3.361673000	-1.587949000
6	-1.387958000	-2.106212000	-0.995368000
1	-4.554622000	-1.517410000	0.224628000
1	-3.089852000	-4.884186000	-1.981953000
6	-3.084239000	0.686649000	0.716984000
6	-2.813137000	1.217270000	1.984650000
6	-4.239368000	1.116446000	0.045911000

6	-3.674631000	2.141181000	2.562597000
6	-5.094876000	2.038148000	0.631838000
6	-4.820033000	2.556145000	1.893774000
1	-1.929637000	0.887217000	2.513810000
1	-4.449936000	0.734476000	-0.944562000
32	-0.000031000	-0.000074000	0.318490000
1	3.448941000	-2.534135000	3.546210000
1	5.979132000	-2.358878000	0.094482000
1	4.934880000	3.717708000	-0.802894000
1	0.852476000	3.902355000	-2.073581000
1	-0.852561000	-3.902174000	-2.074102000
1	-4.935008000	-3.717502000	-0.803555000
1	-5.978973000	2.359050000	0.094566000
1	-3.448827000	2.533863000	3.546346000
1	5.489928000	-3.275034000	2.347583000
1	-5.489755000	3.274981000	2.347752000
6	0.936935000	-2.148637000	-1.635968000
1	1.208018000	-3.107617000	-1.181028000
1	0.685990000	-2.330442000	-2.685283000
1	1.801814000	-1.496294000	-1.602427000
6	-0.936924000	2.148626000	-1.635865000
1	-0.685841000	2.330622000	-2.685113000
1	-1.801740000	1.496190000	-1.602555000
1	-1.208180000	3.107507000	-1.180817000

2b Ge^{IV}(Me-L1)$_2$

7	-0.816126000	-1.384291000	-1.556317000
7	-1.600038000	0.364128000	0.182909000
6	-2.566554000	-0.602746000	-0.154834000
6	-3.836063000	-0.723578000	0.395443000
6	-4.682932000	-1.754238000	-0.013066000
6	-4.260556000	-2.672231000	-0.961760000
6	-2.979619000	-2.580772000	-1.505270000
6	-2.124911000	-1.557684000	-1.108049000
1	-4.166009000	-0.021091000	1.147634000
1	-4.918418000	-3.470544000	-1.280233000
6	-1.863736000	1.557515000	0.893407000
6	-0.942177000	2.016278000	1.839188000
6	-3.000349000	2.332131000	0.633039000
6	-1.149519000	3.218768000	2.504086000
6	-3.209422000	3.522854000	1.314576000
6	-2.287071000	3.975456000	2.252821000
1	-0.060170000	1.426049000	2.054700000
1	-3.711687000	2.004056000	-0.112354000
7	0.816178000	1.384355000	-1.556262000
7	1.600030000	-0.364087000	0.182968000

6	2.566575000	0.602759000	-0.154767000
6	3.836083000	0.723559000	0.395515000
6	4.682977000	1.754206000	-0.012974000
6	4.260624000	2.672227000	-0.961651000
6	2.979687000	2.580801000	-1.505170000
6	2.124961000	1.557719000	-1.107979000
1	4.166012000	0.021058000	1.147701000
1	4.918500000	3.470536000	-1.280104000
6	1.863700000	-1.557522000	0.893399000
6	0.942109000	-2.016321000	1.839132000
6	3.000299000	-2.332148000	0.633011000
6	1.149407000	-3.218852000	2.503966000
6	3.209330000	-3.522918000	1.314486000
6	2.286950000	-3.975551000	2.252684000
1	0.060111000	-1.426083000	2.054659000
1	3.711664000	-2.004052000	-0.112346000
32	0.000011000	0.000026000	-0.682266000
1	-0.419914000	3.556593000	3.229283000
1	-4.095296000	4.107850000	1.099816000
1	-5.671311000	-1.832272000	0.420907000
1	-2.649490000	-3.310337000	-2.232062000
1	2.649572000	3.310395000	-2.231939000
1	5.671357000	1.832210000	0.421004000
1	4.095198000	-4.107918000	1.099711000
1	0.419779000	-3.556704000	3.229126000
1	-2.452832000	4.906783000	2.778491000
1	2.452676000	-4.906911000	2.778305000
6	-0.206637000	-2.313795000	-2.484599000
1	-0.749528000	-2.340504000	-3.434958000
1	0.816752000	-2.003451000	-2.692470000
1	-0.176467000	-3.330419000	-2.079214000
6	0.206728000	2.313856000	-2.484573000
1	-0.816608000	2.003434000	-2.692593000
1	0.176423000	3.330462000	-2.079148000
1	0.749739000	2.340651000	-3.434860000

1c Ge^{II}(Ph-L1)$_2$

7	-0.432496000	1.464722000	-0.466102000
7	1.924877000	0.986966000	0.595629000
6	1.795008000	2.186637000	0.011954000
6	2.764253000	3.222954000	-0.001992000
6	2.537364000	4.387675000	-0.692634000
6	1.327521000	4.578421000	-1.386782000
6	0.335232000	3.624675000	-1.346852000
6	0.515155000	2.425642000	-0.622263000
1	3.692355000	3.075291000	0.530393000

1	1.167002000	5.491144000	-1.946366000
6	3.078777000	0.586487000	1.289817000
6	2.976675000	0.155767000	2.618581000
6	4.331508000	0.537040000	0.663289000
6	4.097553000	-0.301037000	3.300659000
6	5.445292000	0.081575000	1.352794000
6	5.337788000	-0.338444000	2.675221000
1	2.015819000	0.199531000	3.112791000
1	4.416518000	0.830718000	-0.373935000
7	0.432538000	-1.464640000	-0.466295000
7	-1.924918000	-0.987020000	0.595291000
6	-1.795023000	-2.186593000	0.011426000
6	-2.764296000	-3.222876000	-0.002799000
6	-2.537348000	-4.387501000	-0.693585000
6	-1.327418000	-4.578181000	-1.387603000
6	-0.335114000	-3.624462000	-1.347418000
6	-0.515109000	-2.425522000	-0.622694000
1	-3.692462000	-3.075268000	0.529493000
1	-1.166850000	-5.490834000	-1.947286000
6	-3.078865000	-0.586627000	1.289445000
6	-2.976857000	-0.156030000	2.618260000
6	-4.331564000	-0.537182000	0.662857000
6	-4.097786000	0.300679000	3.300314000
6	-5.445402000	-0.081814000	1.352341000
6	-5.337987000	0.338100000	2.674807000
1	-2.016029000	-0.199811000	3.112521000
1	-4.416513000	-0.830784000	-0.374393000
32	-0.000034000	-0.000062000	0.827018000
1	3.998478000	-0.622419000	4.330194000
1	6.403409000	0.045784000	0.848913000
1	3.293299000	5.162440000	-0.704863000
1	-0.598312000	3.793965000	-1.862505000
1	0.598496000	-3.793696000	-1.862972000
1	-3.293304000	-5.162242000	-0.706030000
1	-6.403491000	-0.046014000	0.848409000
1	-3.998780000	0.621967000	4.329885000
1	6.210266000	-0.691913000	3.209544000
1	-6.210511000	0.691489000	3.209108000
6	1.716702000	-1.661214000	-1.051368000
6	2.623726000	-2.564913000	-0.496159000
6	2.074375000	-0.954334000	-2.198768000
6	3.863242000	-2.767704000	-1.089369000
6	3.316515000	-1.158045000	-2.788311000
6	4.212961000	-2.068303000	-2.239132000
1	2.349890000	-3.104494000	0.401301000
1	1.373626000	-0.248041000	-2.623769000

1	4.559253000	-3.468977000	-0.646609000
1	3.581274000	-0.605622000	-3.681376000
1	5.178966000	-2.227785000	-2.701150000
6	-1.716600000	1.661350000	-1.051280000
6	-2.074175000	0.954558000	-2.198765000
6	-2.623706000	2.564956000	-0.496048000
6	-3.316272000	1.158293000	-2.788388000
6	-3.863178000	2.767774000	-1.089337000
6	-4.212784000	2.068481000	-2.239201000
1	-1.373379000	0.248315000	-2.623773000
1	-2.349968000	3.104436000	0.401504000
1	-3.580948000	0.605940000	-3.681521000
1	-4.559243000	3.468984000	-0.646562000
1	-5.178755000	2.227983000	-2.701283000

2c Ge^{IV}(Ph-L1)$_2$

7	0.961863000	0.821423000	-1.348849000
7	-1.098971000	-0.757929000	-1.278153000
6	-0.701815000	-0.362096000	-2.568767000
6	-1.295402000	-0.768874000	-3.758859000
6	-0.813254000	-0.300430000	-4.978315000
6	0.259001000	0.579226000	-5.013374000
6	0.877788000	0.976815000	-3.830969000
6	0.421822000	0.498364000	-2.607398000
1	-2.131060000	-1.453731000	-3.734868000
1	0.624319000	0.959552000	-5.958477000
6	-2.304172000	-1.455284000	-1.007990000
6	-2.279206000	-2.601264000	-0.212111000
6	-3.533405000	-0.994256000	-1.491915000
6	-3.459192000	-3.264451000	0.105275000
6	-4.705935000	-1.671079000	-1.186043000
6	-4.676545000	-2.806410000	-0.382139000
1	-1.329244000	-2.978155000	0.143296000
1	-3.564219000	-0.105056000	-2.107472000
7	-0.719468000	1.001437000	1.377912000
7	0.855782000	-1.059714000	1.250124000
6	0.568021000	-0.615678000	2.554109000
6	1.077905000	-1.163455000	3.726180000
6	0.712791000	-0.636617000	4.962336000
6	-0.165382000	0.435135000	5.032223000
6	-0.664874000	1.009116000	3.865912000
6	-0.290760000	0.507820000	2.623799000
1	1.762527000	-1.998056000	3.674616000
1	-0.464544000	0.835716000	5.992128000
6	1.526575000	-2.276305000	0.965480000
6	1.109690000	-3.484687000	1.534676000

6	2.596576000	-2.286199000	0.069626000
6	1.755766000	-4.670516000	1.214090000
6	3.227999000	-3.479909000	-0.260812000
6	2.814809000	-4.676159000	0.311559000
1	0.278078000	-3.489341000	2.226719000
1	2.941348000	-1.351586000	-0.352908000
32	0.000740000	0.000109000	0.000215000
1	-3.421394000	-4.149870000	0.727417000
1	-5.649343000	-1.301885000	-1.568828000
1	-1.284990000	-0.625274000	-5.896615000
1	1.712428000	1.662794000	-3.861616000
1	-1.348366000	1.844373000	3.923842000
1	1.117149000	-1.072778000	5.866540000
1	4.054883000	-3.469016000	-0.959779000
1	1.421352000	-5.597327000	1.663567000
1	-5.593655000	-3.327698000	-0.140243000
1	3.312244000	-5.603680000	0.059370000
6	-1.417646000	2.225333000	1.216329000
6	-0.940524000	3.414473000	1.778717000
6	-2.582347000	2.261949000	0.448741000
6	-1.618761000	4.608208000	1.574279000
6	-3.247585000	3.463667000	0.233625000
6	-2.772227000	4.641010000	0.796628000
1	-0.037052000	3.397863000	2.373821000
1	-2.971512000	1.341371000	0.034208000
1	-1.236524000	5.520131000	2.016036000
1	-4.147567000	3.473796000	-0.368364000
1	-3.294675000	5.574864000	0.634360000
6	2.196269000	1.496247000	-1.172699000
6	3.357952000	1.067940000	-1.824599000
6	2.273703000	2.583947000	-0.301639000
6	4.563984000	1.720504000	-1.609240000
6	3.488101000	3.222035000	-0.076860000
6	4.637404000	2.797562000	-0.731374000
1	3.310045000	0.223258000	-2.498982000
1	1.374353000	2.936048000	0.186093000
1	5.453888000	1.377252000	-2.122186000
1	3.529818000	4.062446000	0.604633000
1	5.580857000	3.299875000	-0.561313000

1d Ge^{II}(Bu^t-L1)$_2$

7	0.168067000	-1.630304000	0.898885000
7	2.142226000	-0.382170000	-0.364599000
6	2.278777000	-1.716582000	-0.258228000
6	3.351912000	-2.458095000	-0.809665000
6	3.429047000	-3.819309000	-0.650446000

6	2.410240000	-4.493209000	0.038209000
6	1.331095000	-3.808544000	0.557494000
6	1.207561000	-2.404281000	0.444276000
1	4.116768000	-1.927203000	-1.358067000
1	2.451893000	-5.569778000	0.145694000
7	-0.165367000	1.626566000	0.901095000
7	-2.144241000	0.383624000	-0.363022000
6	-2.277018000	1.717795000	-0.255345000
6	-3.348954000	2.462568000	-0.805385000
6	-3.423203000	3.823579000	-0.644339000
6	-2.402789000	4.494393000	0.045189000
6	-1.324959000	3.806840000	0.563242000
6	-1.203801000	2.402513000	0.447680000
1	-4.115123000	1.933876000	-1.354105000
1	-2.442228000	5.570891000	0.154251000
32	0.001015000	-0.001312000	-0.262331000
1	4.261092000	-4.370224000	-1.069775000
1	0.557438000	-4.381988000	1.034104000
1	-0.550187000	4.378090000	1.040656000
1	-4.254155000	4.376871000	-1.062713000
6	0.821034000	2.154559000	1.906290000
6	1.817651000	3.142111000	1.266248000
6	1.638671000	0.996590000	2.499566000
1	1.004829000	0.300616000	3.045472000
1	2.179159000	0.444115000	1.737997000
1	2.364845000	1.407630000	3.202404000
1	2.411124000	2.642159000	0.502110000
1	2.502639000	3.518188000	2.029212000
1	1.335319000	3.998166000	0.801022000
6	0.086050000	2.789822000	3.108641000
1	-0.632973000	2.082852000	3.524680000
1	0.819185000	3.018232000	3.884025000
1	-0.446111000	3.707417000	2.880572000
6	-0.819518000	-2.161608000	1.900895000
6	-1.814052000	-3.148230000	1.256257000
6	-1.638858000	-1.005670000	2.495810000
1	-1.006252000	-0.310873000	3.044688000
1	-2.178241000	-0.451327000	1.734803000
1	-2.366101000	-1.418935000	3.196233000
1	-2.406841000	-2.646526000	0.492693000
1	-2.499885000	-3.527594000	2.016837000
1	-1.329769000	-4.002159000	0.789106000
6	-0.086299000	-2.799487000	3.102957000
1	0.631583000	-2.093158000	3.522034000
1	-0.820744000	-3.030172000	3.876427000
1	0.446746000	-3.716236000	2.873649000

6	3.075959000	0.429890000	-1.030942000
6	2.715013000	1.137210000	-2.183361000
6	4.361348000	0.617697000	-0.503426000
6	3.614173000	2.009189000	-2.785416000
6	5.254727000	1.486124000	-1.114462000
6	4.887235000	2.188690000	-2.257960000
1	1.729522000	0.990292000	-2.604081000
1	4.645535000	0.086515000	0.395792000
1	3.316057000	2.546239000	-3.677441000
1	6.242115000	1.619365000	-0.689572000
1	5.585241000	2.867337000	-2.730854000
6	-3.080249000	-0.425673000	-1.029216000
6	-4.365174000	-0.612399000	-0.500178000
6	-2.721852000	-1.131854000	-2.183171000
6	-5.260678000	-1.478573000	-1.111331000
6	-3.623196000	-2.001433000	-2.785400000
6	-4.895826000	-2.179834000	-2.256467000
1	-4.647308000	-0.082109000	0.400225000
1	-1.736558000	-0.986016000	-2.604732000
1	-6.247682000	-1.611017000	-0.685297000
1	-3.327107000	-2.537603000	-3.678631000
1	-5.595491000	-2.856706000	-2.729453000

2d Ge^{IV}(Bu^t-L1)$_2$

7	-1.508867000	0.674770000	1.129774000
7	-1.054290000	-1.180476000	-0.659898000
6	-2.408935000	-0.975675000	-0.353525000
6	-3.469215000	-1.626379000	-0.975046000
6	-4.783854000	-1.334678000	-0.625721000
6	-5.036135000	-0.380935000	0.345405000
6	-3.985003000	0.299057000	0.956672000
6	-2.655635000	0.033144000	0.621478000
1	-3.266417000	-2.357172000	-1.744583000
1	-6.052783000	-0.145095000	0.632726000
7	1.510690000	-0.674182000	1.127834000
7	1.054167000	1.181614000	-0.660200000
6	2.409008000	0.977213000	-0.355540000
6	3.468386000	1.629321000	-0.977189000
6	4.783408000	1.337655000	-0.629369000
6	5.036841000	0.382948000	0.340477000
6	3.986554000	-0.297943000	0.952288000
6	2.656800000	-0.032175000	0.618662000
1	3.264201000	2.360883000	-1.745607000
1	6.053878000	0.147018000	0.626364000
32	0.000401000	0.000425000	0.298990000
1	-5.597424000	-1.852109000	-1.117158000

1	-4.226697000	1.047185000	1.691482000
1	4.229334000	-1.046552000	1.686260000
1	5.596560000	1.855524000	-1.121041000
6	-1.538829000	1.787398000	2.121516000
6	-2.145595000	1.317598000	3.458260000
6	-2.285961000	3.010849000	1.556247000
1	-1.806189000	3.350985000	0.637794000
1	-3.329547000	2.808757000	1.330545000
1	-2.253001000	3.827755000	2.279981000
1	-3.157800000	0.935140000	3.360717000
1	-2.168441000	2.149805000	4.164414000
1	-1.533434000	0.525894000	3.893457000
6	-0.099377000	2.234543000	2.415764000
1	0.387393000	2.641664000	1.529983000
1	-0.117293000	3.021160000	3.170545000
1	0.508696000	1.417700000	2.805763000
6	1.541991000	-1.787008000	2.119336000
6	2.152205000	-1.318006000	3.454699000
6	2.287012000	-3.011144000	1.552544000
1	1.805171000	-3.351021000	0.635076000
1	3.330298000	-2.809820000	1.324736000
1	2.254972000	-3.827990000	2.276385000
1	3.164854000	-0.937325000	3.354649000
1	2.175328000	-2.150165000	4.160907000
1	1.542421000	-0.525216000	3.891225000
6	0.102918000	-2.233099000	2.416565000
1	-0.385804000	-2.639879000	1.531661000
1	0.121619000	-3.019856000	3.171178000
1	-0.503834000	-1.415854000	2.807827000
6	0.547296000	2.273373000	-1.401941000
6	-0.490274000	2.062487000	-2.315376000
6	1.010436000	3.580583000	-1.204568000
6	-1.050129000	3.127952000	-3.009660000
6	0.456912000	4.637578000	-1.913749000
6	-0.576577000	4.420023000	-2.819424000
1	-0.858272000	1.058143000	-2.479775000
1	1.799820000	3.765905000	-0.489353000
1	-1.854751000	2.940826000	-3.709555000
1	0.828968000	5.640988000	-1.747050000
1	-1.007292000	5.247997000	-3.367375000
6	-0.548868000	-2.274227000	-1.399253000
6	-1.015393000	-3.580310000	-1.202402000
6	0.489707000	-2.066574000	-2.312667000
6	-0.464034000	-4.638884000	-1.911179000
6	1.047452000	-3.133511000	-3.006100000
6	0.570697000	-4.424563000	-2.816024000

1	-1.805814000	-3.764245000	-0.487997000
1	0.860514000	-1.063362000	-2.477845000
1	-0.839411000	-5.641093000	-1.744542000
1	1.853065000	-2.948267000	-3.705393000
1	0.999520000	-5.253655000	-3.363718000

3a Ge^{II}(H-L2)$_2$

7	-0.402257000	-1.418902000	0.396220000
7	2.105838000	-0.856675000	-0.225086000
6	1.910634000	-2.017462000	0.469713000
6	2.896590000	-2.981559000	0.789521000
6	2.565789000	-4.144407000	1.440082000
6	1.224519000	-4.390415000	1.795307000
6	0.231699000	-3.505690000	1.458803000
6	0.534047000	-2.304361000	0.770639000
1	3.912028000	-2.831851000	0.455085000
1	0.968573000	-5.307229000	2.311788000
6	3.239141000	-0.194428000	-0.388948000
6	3.289950000	0.802280000	-1.439020000
6	4.420214000	-0.337604000	0.439285000
6	4.404927000	1.515306000	-1.696392000
6	5.526015000	0.402310000	0.219166000
6	5.618851000	1.361926000	-0.888957000
1	2.412926000	0.906122000	-2.066158000
1	4.369855000	-0.984852000	1.302473000
8	6.639256000	2.009032000	-1.105491000
7	0.402381000	1.418704000	0.396262000
7	-2.105782000	0.856514000	-0.224937000
6	-1.910505000	2.017303000	0.469818000
6	-2.896423000	2.981441000	0.789627000
6	-2.565577000	4.144279000	1.440175000
6	-1.224290000	4.390245000	1.795385000
6	-0.231505000	3.505494000	1.458869000
6	-0.533896000	2.304163000	0.770714000
1	-3.911874000	2.831750000	0.455218000
1	-0.968312000	5.307056000	2.311856000
6	-3.239182000	0.194420000	-0.388851000
6	-3.290075000	-0.802342000	-1.438855000
6	-4.420305000	0.337907000	0.439243000
6	-4.405148000	-1.515222000	-1.696235000
6	-5.526211000	-0.401854000	0.219122000
6	-5.619060000	-1.361681000	-0.888813000
1	-2.413044000	-0.906354000	-2.065954000
1	-4.369927000	0.985285000	1.302333000
8	-6.639640000	-2.008455000	-1.105531000
32	0.000012000	-0.000080000	-0.902136000

1	4.452696000	2.217300000	-2.519027000
1	6.383597000	0.343790000	0.877717000
1	3.325560000	-4.885525000	1.647706000
1	-0.801951000	-3.718919000	1.702759000
1	-1.357135000	-1.711802000	0.548863000
1	1.357262000	1.711579000	0.548936000
1	0.802158000	3.718698000	1.702799000
1	-3.325318000	4.885427000	1.647801000
1	-6.383855000	-0.343077000	0.877566000
1	-4.452986000	-2.217240000	-2.518846000

4a Ge^{IV}(H-L2)$_2$

7	0.125976000	-1.586718000	-1.879936000
7	-1.521146000	-0.655740000	-0.122376000
6	-1.688841000	-2.026429000	-0.419660000
6	-2.579990000	-2.901156000	0.197640000
6	-2.596569000	-4.244552000	-0.162138000
6	-1.714105000	-4.726546000	-1.121845000
6	-0.793555000	-3.872612000	-1.719302000
6	-0.770409000	-2.528268000	-1.370572000
1	-3.244791000	-2.542659000	0.969884000
1	-1.729516000	-5.772448000	-1.398635000
6	-2.454066000	0.166292000	0.502941000
6	-1.997558000	1.282802000	1.246857000
6	-3.851377000	-0.035979000	0.368697000
6	-2.874094000	2.142867000	1.844306000
6	-4.741274000	0.816676000	0.957371000
6	-4.308028000	1.957269000	1.740629000
1	-0.930645000	1.434544000	1.366934000
1	-4.209308000	-0.856083000	-0.237743000
8	-5.117551000	2.735339000	2.281863000
7	-0.126001000	1.586995000	-1.879749000
7	1.521215000	0.655774000	-0.122406000
6	1.688978000	2.026469000	-0.419600000
6	2.580243000	2.901098000	0.197676000
6	2.596877000	4.244518000	-0.162008000
6	1.714360000	4.726638000	-1.121603000
6	0.793699000	3.872807000	-1.719033000
6	0.770494000	2.528439000	-1.370396000
1	3.245083000	2.542510000	0.969843000
1	1.729813000	5.772558000	-1.398321000
6	2.454031000	-0.166340000	0.502935000
6	1.997402000	-1.282830000	1.246820000
6	3.851368000	0.035808000	0.368766000
6	2.873835000	-2.142970000	1.844302000
6	4.741166000	-0.816929000	0.957471000

6	4.307790000	-1.957484000	1.740704000
1	0.930470000	-1.434481000	1.366844000
1	4.209406000	0.855881000	-0.237654000
8	5.117223000	-2.735647000	2.281946000
32	-0.000014000	0.000088000	-1.003082000
1	-2.524683000	2.984590000	2.427946000
1	-5.808473000	0.679079000	0.838810000
1	-3.295490000	-4.914540000	0.320430000
1	-0.089245000	-4.248375000	-2.451507000
1	0.910733000	-1.910411000	-2.419883000
1	-0.910821000	1.910789000	-2.419546000
1	0.089348000	4.248665000	-2.451149000
1	3.295889000	4.914425000	0.320541000
1	5.808381000	-0.679420000	0.838958000
1	2.524325000	-2.984673000	2.427914000

MECP$_{3a-4a}$

7	-0.362274000	1.542953000	-0.764369000
7	1.942559000	0.776471000	0.065860000
6	1.904705000	2.076848000	-0.375104000
6	2.940714000	3.025807000	-0.312055000
6	2.728575000	4.315810000	-0.758686000
6	1.471240000	4.706428000	-1.239493000
6	0.417158000	3.814606000	-1.248224000
6	0.614552000	2.493891000	-0.823463000
1	3.901312000	2.747148000	0.095975000
1	1.318685000	5.718832000	-1.589546000
6	3.078723000	0.061686000	0.358872000
6	3.049048000	-0.918397000	1.389927000
6	4.278780000	0.200836000	-0.398115000
6	4.137435000	-1.691442000	1.669978000
6	5.368962000	-0.576206000	-0.140200000
6	5.375296000	-1.568075000	0.920925000
1	2.150218000	-1.007835000	1.988589000
1	4.298092000	0.904423000	-1.219021000
8	6.372220000	-2.270492000	1.166357000
7	0.339147000	-1.474780000	-0.835270000
7	-2.000038000	-0.779154000	0.041101000
6	-1.913759000	-2.072792000	-0.395737000
6	-2.904606000	-3.075831000	-0.295242000
6	-2.649520000	-4.354497000	-0.731813000
6	-1.386385000	-4.687641000	-1.255069000
6	-0.375344000	-3.757071000	-1.297132000
6	-0.610503000	-2.437267000	-0.864821000
1	-3.855964000	-2.846709000	0.160578000
1	-1.197867000	-5.696265000	-1.599323000

6	-3.123484000	-0.098755000	0.328641000
6	-3.043338000	1.029181000	1.216801000
6	-4.402083000	-0.378421000	-0.270376000
6	-4.124373000	1.790240000	1.506896000
6	-5.481441000	0.402106000	-0.021466000
6	-5.429208000	1.533926000	0.901464000
1	-2.097873000	1.216150000	1.710762000
1	-4.471516000	-1.169569000	-1.002803000
8	-6.417463000	2.229981000	1.145767000
32	0.040996000	0.030170000	0.291266000
1	4.119761000	-2.413073000	2.476749000
1	6.268466000	-0.490432000	-0.737038000
1	3.537606000	5.033225000	-0.723189000
1	-0.564539000	4.120089000	-1.589113000
1	-1.309380000	1.861099000	-0.910200000
1	1.285152000	-1.783144000	-1.013869000
1	0.609298000	-4.023891000	-1.660623000
1	-3.413874000	-5.114985000	-0.647269000
1	-6.424118000	0.230699000	-0.526363000
1	-4.066000000	2.604618000	2.217889000

3b Ge^{II}(Me-L2)$_2$

7	0.254807000	1.995005000	-0.724098000
7	2.273834000	0.663225000	0.278049000
6	2.528123000	1.977065000	-0.031043000
6	3.719488000	2.682807000	0.239838000
6	3.844891000	4.009928000	-0.096169000
6	2.771080000	4.679452000	-0.710551000
6	1.570577000	4.048024000	-0.931270000
6	1.397315000	2.684665000	-0.579891000
1	4.519784000	2.191358000	0.771839000
1	2.878609000	5.722776000	-0.980613000
6	3.166611000	-0.295312000	0.524791000
6	2.716123000	-1.499951000	1.180484000
6	4.550812000	-0.249250000	0.112880000
6	3.555230000	-2.517853000	1.463117000
6	5.390521000	-1.280066000	0.349979000
6	4.967718000	-2.481918000	1.075724000
1	1.685029000	-1.540969000	1.509616000
1	4.886545000	0.584763000	-0.485031000
8	5.742055000	-3.403214000	1.323132000
7	0.004154000	-0.875286000	-1.088605000
7	-2.427342000	-0.575291000	0.131566000
6	-2.108278000	-1.826491000	-0.328958000
6	-2.903571000	-2.973808000	-0.135869000
6	-2.531824000	-4.203881000	-0.635962000

6	-1.341827000	-4.310672000	-1.360127000
6	-0.507871000	-3.220423000	-1.519975000
6	-0.826101000	-1.959349000	-0.974217000
1	-3.797693000	-2.889259000	0.465426000
1	-1.042657000	-5.268591000	-1.767480000
6	-3.619696000	-0.081442000	0.332871000
6	-3.690611000	1.174053000	1.065728000
6	-4.879314000	-0.630650000	-0.154092000
6	-4.861384000	1.757904000	1.375752000
6	-6.052856000	-0.027523000	0.109628000
6	-6.141187000	1.191056000	0.930319000
1	-2.749230000	1.585773000	1.407344000
1	-4.847767000	-1.493498000	-0.803654000
8	-7.216784000	1.714626000	1.196980000
32	0.119599000	0.373291000	0.418017000
1	3.220086000	-3.392469000	2.005555000
1	6.406346000	-1.274148000	-0.024630000
1	4.753378000	4.545940000	0.142388000
1	0.745785000	4.596237000	-1.362137000
1	0.431352000	-3.350874000	-2.036891000
1	-3.144318000	-5.076398000	-0.452534000
1	-6.985404000	-0.397673000	-0.298137000
1	-4.911811000	2.664623000	1.965203000
6	-0.929885000	2.639110000	-1.261538000
1	-1.729631000	1.905464000	-1.337831000
1	-1.282015000	3.470658000	-0.639748000
1	-0.738456000	3.026925000	-2.266360000
6	1.045831000	-0.913648000	-2.103336000
1	0.637928000	-1.277224000	-3.050431000
1	1.417814000	0.096225000	-2.266844000
1	1.899303000	-1.550752000	-1.839563000

4b Ge^{IV}(Me-L2)$_2$

7	0.343858000	-1.559287000	-1.690307000
7	-1.423525000	-0.836857000	0.072317000
6	-1.421880000	-2.213891000	-0.235361000
6	-2.201619000	-3.188897000	0.377938000
6	-2.067292000	-4.524207000	0.008539000
6	-1.142799000	-4.891764000	-0.958930000
6	-0.325246000	-3.933867000	-1.553215000
6	-0.449382000	-2.594822000	-1.195377000
1	-2.899591000	-2.913455000	1.155061000
1	-1.039049000	-5.929977000	-1.245864000
6	-2.450353000	-0.135881000	0.697201000
6	-2.133894000	1.031589000	1.436071000
6	-3.812547000	-0.508945000	0.566950000

6	-3.108848000	1.779911000	2.031315000
6	-4.799773000	0.230328000	1.153581000
6	-4.509350000	1.419533000	1.930551000
1	-1.093507000	1.313372000	1.553461000
1	-4.068141000	-1.369626000	-0.034852000
8	-5.407821000	2.095263000	2.468958000
7	-0.344428000	1.557835000	-1.690680000
7	1.423892000	0.836761000	0.071614000
6	1.421391000	2.213784000	-0.236455000
6	2.200658000	3.189381000	0.376498000
6	2.065515000	4.524521000	0.006801000
6	1.140673000	4.891286000	-0.960642000
6	0.323570000	3.932790000	-1.554545000
6	0.448432000	2.593890000	-1.196347000
1	2.898867000	2.914547000	1.153612000
1	1.036307000	5.929362000	-1.247854000
6	2.451103000	0.136437000	0.696621000
6	2.135157000	-1.030960000	1.435812000
6	3.813170000	0.509916000	0.566067000
6	3.110430000	-1.778752000	2.031210000
6	4.800699000	-0.228811000	1.152854000
6	4.510766000	-1.417772000	1.930390000
1	1.094885000	-1.313123000	1.553371000
1	4.068406000	1.370396000	-0.036158000
8	5.409560000	-2.093164000	2.468676000
32	0.000318000	-0.000507000	-0.811469000
1	-2.864786000	2.660628000	2.611012000
1	-5.842071000	-0.038179000	1.037515000
1	-2.682230000	-5.273103000	0.489422000
1	0.411808000	-4.233405000	-2.284948000
1	-0.413778000	4.231730000	-2.286231000
1	2.680015000	5.273908000	0.487474000
1	5.842899000	0.039965000	1.036535000
1	2.866752000	-2.659432000	2.611125000
6	1.436631000	-1.816983000	-2.610120000
1	2.178273000	-2.495735000	-2.178251000
1	1.067955000	-2.254415000	-3.542211000
1	1.935501000	-0.880397000	-2.855654000
6	-1.437795000	1.814611000	-2.610032000
1	-1.069844000	2.251692000	-3.542584000
1	-1.936404000	0.877691000	-2.854834000
1	-2.179438000	2.493290000	-2.178076000

3c $Ge^{II}(Ph-L2)_2$

7	-0.418117000	1.407453000	-0.475087000
7	2.035096000	1.141155000	0.618556000

6	1.817392000	2.266524000	-0.121521000
6	2.714441000	3.356274000	-0.240587000
6	2.412816000	4.452736000	-1.007576000
6	1.185010000	4.495061000	-1.691205000
6	0.253320000	3.497788000	-1.539716000
6	0.505859000	2.371976000	-0.710653000
1	3.628712000	3.347228000	0.332257000
1	0.950177000	5.344820000	-2.320484000
6	3.185281000	0.693822000	1.096611000
6	3.137191000	-0.254868000	2.190191000
6	4.498056000	1.043394000	0.591156000
6	4.253621000	-0.715638000	2.788223000
6	5.620832000	0.543419000	1.144991000
6	5.589090000	-0.344142000	2.314013000
1	2.160253000	-0.520908000	2.572346000
1	4.562148000	1.631781000	-0.311866000
8	6.615951000	-0.767299000	2.838287000
7	0.418134000	-1.407153000	-0.475450000
7	-2.035266000	-1.141396000	0.618044000
6	-1.817269000	-2.266680000	-0.122053000
6	-2.714021000	-3.356675000	-0.241185000
6	-2.412165000	-4.452951000	-1.008345000
6	-1.184402000	-4.494843000	-1.692075000
6	-0.252953000	-3.497360000	-1.540483000
6	-0.505711000	-2.371751000	-0.711208000
1	-3.628254000	-3.347955000	0.331726000
1	-0.949391000	-5.344443000	-2.321502000
6	-3.185524000	-0.694272000	1.096096000
6	-3.137544000	0.254433000	2.189679000
6	-4.498283000	-1.044169000	0.590797000
6	-4.254014000	0.714984000	2.787798000
6	-5.621113000	-0.544442000	1.144740000
6	-5.589445000	0.343317000	2.313616000
1	-2.160624000	0.520664000	2.571745000
1	-4.562348000	-1.632613000	-0.312188000
8	-6.616353000	0.765971000	2.838205000
32	0.000036000	-0.000009000	0.916172000
1	4.207234000	-1.369716000	3.649668000
1	6.596422000	0.745528000	0.720752000
1	3.100493000	5.285555000	-1.064692000
1	-0.698804000	3.575131000	-2.041764000
1	0.699176000	-3.574406000	-2.042566000
1	-3.099618000	-5.285950000	-1.065520000
1	-6.596709000	-0.746847000	0.720654000
1	-4.207696000	1.369062000	3.649247000
6	-1.710577000	1.542935000	-1.064065000

6	-2.662058000	2.402307000	-0.512447000
6	-2.037505000	0.812393000	-2.206963000
6	-3.915721000	2.533216000	-1.097634000
6	-3.292506000	0.944778000	-2.789935000
6	-4.234602000	1.806774000	-2.239331000
1	-2.410626000	2.970137000	0.374135000
1	-1.302588000	0.143578000	-2.634383000
1	-4.645208000	3.200656000	-0.656590000
1	-3.531863000	0.374286000	-3.678714000
1	-5.211494000	1.909046000	-2.694133000
6	1.710563000	-1.542340000	-1.064558000
6	2.037289000	-0.811601000	-2.207388000
6	2.662238000	-2.401595000	-0.513095000
6	3.292282000	-0.943672000	-2.790441000
6	3.915900000	-2.532185000	-1.098358000
6	4.234580000	-1.805546000	-2.239983000
1	1.302220000	-0.142873000	-2.634685000
1	2.410974000	-2.969564000	0.373445000
1	3.531478000	-0.373026000	-3.679164000
1	4.645540000	-3.199531000	-0.657427000
1	5.211472000	-1.907565000	-2.694842000

4c Ge^{IV}(Ph-L2)$_2$

7	0.999044000	1.275348000	0.995807000
7	-0.955521000	1.347385000	-0.734282000
6	-0.439777000	2.606965000	-0.364671000
6	-0.833444000	3.831914000	-0.898261000
6	-0.237648000	5.008405000	-0.459326000
6	0.758104000	4.966955000	0.508333000
6	1.193042000	3.748910000	1.018867000
6	0.619423000	2.561501000	0.575257000
1	-1.592842000	3.866838000	-1.665477000
1	1.212965000	5.883078000	0.861626000
6	-2.163445000	1.115121000	-1.389152000
6	-2.278274000	-0.022191000	-2.226202000
6	-3.301017000	1.939878000	-1.199534000
6	-3.451585000	-0.320433000	-2.858689000
6	-4.482044000	1.654423000	-1.822297000
6	-4.630649000	0.507363000	-2.696753000
1	-1.405522000	-0.645154000	-2.386633000
1	-3.236216000	2.777917000	-0.520176000
8	-5.708401000	0.241817000	-3.264186000
7	-0.999136000	-1.275416000	0.995626000
7	0.955583000	-1.347330000	-0.734295000
6	0.439810000	-2.606936000	-0.364815000
6	0.833527000	-3.831848000	-0.898453000

6	0.237697000	-5.008371000	-0.459649000
6	-0.758138000	-4.966989000	0.507927000
6	-1.193124000	-3.748980000	1.018506000
6	-0.619471000	-2.561540000	0.575025000
1	1.592992000	-3.866719000	-1.665604000
1	-1.213026000	-5.883138000	0.861120000
6	2.163565000	-1.115018000	-1.389041000
6	2.278468000	0.022357000	-2.225996000
6	3.301120000	-1.939789000	-1.199383000
6	3.451836000	0.320646000	-2.858356000
6	4.482202000	-1.654288000	-1.822021000
6	4.630886000	-0.507162000	-2.696377000
1	1.405731000	0.645332000	-2.386457000
1	3.236259000	-2.777878000	-0.520093000
8	5.708689000	-0.241572000	-3.263692000
32	-0.000007000	-0.000003000	0.134454000
1	-3.534646000	-1.177559000	-3.514334000
1	-5.360855000	2.265347000	-1.660180000
1	-0.553492000	5.953940000	-0.879477000
1	1.981873000	3.719256000	1.756885000
1	-1.982019000	-3.719378000	1.756458000
1	0.553580000	-5.953877000	-0.879836000
1	5.360999000	-2.265225000	-1.659871000
1	3.534956000	1.177822000	-3.513929000
6	2.192451000	1.003199000	1.726389000
6	3.434295000	1.452975000	1.271159000
6	2.129274000	0.239143000	2.890977000
6	4.587506000	1.152131000	1.981901000
6	3.290096000	-0.073229000	3.590163000
6	4.521438000	0.387465000	3.142793000
1	3.493731000	2.025986000	0.355706000
1	1.169827000	-0.111160000	3.247894000
1	5.544130000	1.503190000	1.616521000
1	3.226124000	-0.671353000	4.490192000
1	5.424412000	0.149542000	3.689828000
6	-2.192606000	-1.003324000	1.726124000
6	-2.129534000	-0.239344000	2.890769000
6	-3.434408000	-1.453083000	1.270763000
6	-3.290416000	0.072966000	3.589881000
6	-4.587680000	-1.152301000	1.981430000
6	-4.521716000	-0.387714000	3.142380000
1	-1.170120000	0.110946000	3.247788000
1	-3.493761000	-2.026035000	0.355268000
1	-3.226525000	0.671031000	4.489956000
1	-5.544270000	-1.503348000	1.615949000
1	-5.424738000	-0.149839000	3.689358000

4d Ge^{IV}(Bu^t-L2)$_2$

7	-1.038453000	-1.272113000	1.273406000
7	0.866529000	-1.335454000	-0.539818000
6	0.291671000	-2.582021000	-0.232897000
6	0.595408000	-3.771402000	-0.891168000
6	-0.043912000	-4.953649000	-0.544241000
6	-1.001331000	-4.941084000	0.458140000
6	-1.349408000	-3.752544000	1.091333000
6	-0.733351000	-2.544514000	0.754093000
1	1.319842000	-3.767247000	-1.692028000
1	-1.503556000	-5.855532000	0.746001000
6	2.063647000	-1.135436000	-1.221621000
6	2.232032000	0.048853000	-1.983115000
6	3.151310000	-2.042572000	-1.131165000
6	3.400797000	0.309829000	-2.639529000
6	4.328829000	-1.793306000	-1.777019000
6	4.525009000	-0.603313000	-2.581842000
1	1.402514000	0.740565000	-2.066177000
1	3.051704000	-2.924714000	-0.514531000
8	5.596816000	-0.374682000	-3.175774000
7	1.038390000	1.272227000	1.273378000
7	-0.866603000	1.335609000	-0.539816000
6	-0.291739000	2.582175000	-0.232886000
6	-0.595390000	3.771582000	-0.891156000
6	0.043996000	4.953794000	-0.544228000
6	1.001405000	4.941203000	0.458152000
6	1.349432000	3.752639000	1.091334000
6	0.733302000	2.544645000	0.754087000
1	-1.319762000	3.767504000	-1.692065000
1	1.503695000	5.855626000	0.745977000
6	-2.063691000	1.135494000	-1.221634000
6	-2.231872000	-0.048767000	-1.983237000
6	-3.151495000	2.042464000	-1.131215000
6	-3.400552000	-0.309875000	-2.639741000
6	-4.328943000	1.793053000	-1.777152000
6	-4.524990000	0.602972000	-2.581867000
1	-1.402237000	-0.740330000	-2.066365000
1	-3.052104000	2.924569000	-0.514502000
8	-5.596582000	0.374436000	-3.176230000
32	-0.000038000	0.000062000	0.438962000
1	3.519962000	1.203871000	-3.237731000
1	5.167991000	-2.471751000	-1.690178000
1	0.203064000	-5.870791000	-1.061837000
1	-2.117980000	-3.784745000	1.843107000
1	2.118023000	3.784782000	1.843082000

1	-0.202960000	5.870946000	-1.061819000
1	-5.168184000	2.471410000	-1.690376000
1	-3.519508000	-1.203860000	-3.238071000
6	-2.126568000	-1.000927000	2.264250000
6	-1.826737000	-1.699205000	3.603671000
6	-3.502167000	-1.408340000	1.704178000
1	-3.699878000	-0.886159000	0.767714000
1	-3.593278000	-2.474036000	1.513928000
1	-4.281066000	-1.131533000	2.416832000
1	-1.719922000	-2.776628000	3.512344000
1	-2.636658000	-1.502928000	4.308291000
1	-0.904114000	-1.310306000	4.037506000
6	-2.181749000	0.507919000	2.542515000
1	-2.464916000	1.074863000	1.655615000
1	-2.937396000	0.701553000	3.303752000
1	-1.232431000	0.889747000	2.919165000
6	2.126547000	1.000895000	2.264097000
6	1.826876000	1.699152000	3.603588000
6	3.502150000	1.408116000	1.703850000
1	3.699830000	0.885617000	0.767550000
1	3.593321000	2.473737000	1.513188000
1	4.281053000	1.131509000	2.416580000
1	1.719799000	2.776539000	3.512258000
1	2.636952000	1.503037000	4.308063000
1	0.904404000	1.310074000	4.037589000
6	2.181516000	-0.507982000	2.542220000
1	2.464695000	-1.074903000	1.655312000
1	2.937089000	-0.701734000	3.303497000
1	1.232120000	-0.889742000	2.918756000

1e Sn^{II}(H-L1)$_2$

7	2.314513000	0.049194000	-0.020057000
7	0.250489000	1.553925000	0.774420000
6	1.439354000	1.803696000	1.325259000
6	2.578854000	1.011817000	0.875992000
7	-2.314519000	-0.049175000	-0.019977000
7	-0.250393000	-1.553416000	0.775156000
6	-1.439218000	-1.802957000	1.326189000
6	-2.578778000	-1.011385000	0.876540000
50	-0.000004000	-0.000093000	-0.751009000
6	-3.846463000	-1.273452000	1.467826000
6	-1.650845000	-2.798155000	2.315884000
6	-3.998497000	-2.239007000	2.429142000
6	-2.894219000	-3.014217000	2.850120000
1	-4.690640000	-0.666435000	1.174326000
1	-0.800538000	-3.384773000	2.643918000

1	-4.968946000	-2.400132000	2.880815000
1	-3.031262000	-3.775838000	3.607293000
6	1.651083000	2.799414000	2.314409000
6	2.894482000	3.015662000	2.848512000
6	3.846560000	1.274076000	1.467142000
6	3.998688000	2.240127000	2.427945000
1	0.800830000	3.386278000	2.642146000
1	3.031597000	3.777683000	3.605269000
1	4.690680000	0.666826000	1.173963000
1	4.969152000	2.401403000	2.879530000
1	-0.517083000	2.087435000	1.159684000
1	0.517242000	-2.086626000	1.160713000
6	3.304670000	-0.607985000	-0.755716000
6	3.167665000	-1.983966000	-0.993414000
6	4.381256000	0.063332000	-1.359071000
6	4.089484000	-2.667911000	-1.772555000
6	5.294038000	-0.625272000	-2.144012000
6	5.161054000	-1.995201000	-2.350112000
1	2.331991000	-2.513158000	-0.553671000
1	4.478079000	1.132937000	-1.230135000
1	3.967105000	-3.731970000	-1.932586000
1	6.110593000	-0.084925000	-2.607144000
1	5.876096000	-2.528411000	-2.963003000
6	-3.304756000	0.607555000	-0.755934000
6	-4.381223000	-0.064189000	-1.359022000
6	-3.167963000	1.983455000	-0.994204000
6	-5.294096000	0.623937000	-2.144276000
6	-4.089874000	2.666924000	-1.773657000
6	-5.161321000	1.993800000	-2.350954000
1	-4.477881000	-1.133753000	-1.229616000
1	-2.332390000	2.512965000	-0.554653000
1	-6.110559000	0.083266000	-2.607194000
1	-3.967662000	3.730935000	-1.934133000
1	-5.876433000	2.526638000	-2.964087000

2e Sn^{IV}(H-L1)$_2$

7	-1.846388000	0.292543000	0.040882000
7	-0.963871000	-1.487750000	-1.760353000
6	-2.240567000	-1.701428000	-1.236603000
6	-2.724382000	-0.752648000	-0.297541000
7	1.846389000	-0.292542000	0.040878000
7	0.963858000	1.487689000	-1.760411000
6	2.240557000	1.701387000	-1.236677000
6	2.724379000	0.752639000	-0.297586000
50	-0.000003000	-0.000014000	-0.806493000
6	-3.979911000	-0.954865000	0.275661000

6	-4.763601000	-2.043866000	-0.091814000
6	-3.034708000	-2.790356000	-1.586313000
6	-4.294898000	-2.959563000	-1.024869000
1	-4.342993000	-0.259632000	1.019311000
1	-5.738086000	-2.174183000	0.360760000
1	-2.656854000	-3.507461000	-2.306176000
1	-4.901350000	-3.808206000	-1.313580000
6	3.979911000	0.954878000	0.275601000
6	3.034694000	2.790303000	-1.586431000
6	4.763597000	2.043867000	-0.091916000
6	4.294887000	2.959531000	-1.025000000
1	4.342999000	0.259672000	1.019273000
1	2.656835000	3.507383000	-2.306316000
1	5.738085000	2.174202000	0.360647000
1	4.901336000	3.808165000	-1.313745000
6	-2.212462000	1.448951000	0.759583000
6	-3.381536000	2.162324000	0.462020000
6	-1.362834000	1.947833000	1.752173000
6	-3.685728000	3.329697000	1.147375000
6	-1.664499000	3.127716000	2.421348000
6	-2.830994000	3.822733000	2.129067000
1	-4.041204000	1.802805000	-0.315967000
1	-0.462475000	1.400803000	2.007754000
1	-4.593711000	3.866458000	0.901090000
1	-0.987591000	3.494745000	3.182584000
1	-3.071632000	4.736562000	2.656316000
6	2.212469000	-1.448925000	0.759614000
6	1.362847000	-1.947778000	1.752225000
6	3.381543000	-2.162306000	0.462067000
6	1.664519000	-3.127639000	2.421436000
6	3.685741000	-3.329656000	1.147458000
6	2.831014000	-3.822663000	2.129170000
1	0.462489000	-1.400742000	2.007794000
1	4.041206000	-1.802811000	-0.315935000
1	0.987615000	-3.494646000	3.182687000
1	4.593723000	-3.866423000	0.901185000
1	3.071656000	-4.736475000	2.656447000
1	0.540602000	2.256714000	-2.253412000
1	-0.540620000	-2.256792000	-2.253330000

MECP$_{1e-2e}$
7	-2.267935000	-0.150651000	-0.209108000
7	-0.470544000	1.594345000	-1.112302000
6	-1.765995000	1.938072000	-1.237905000
6	-2.750451000	1.000605000	-0.740276000
7	2.261384000	0.164806000	-0.224249000

7	0.468743000	-1.559843000	-1.173705000
6	1.763833000	-1.912259000	-1.282149000
6	2.745183000	-0.982895000	-0.761372000
50	-0.003979000	-0.005175000	0.212681000
6	4.114813000	-1.322895000	-0.878591000
6	2.207831000	-3.127529000	-1.847672000
6	4.507271000	-2.494002000	-1.484210000
6	3.549836000	-3.407392000	-1.962794000
1	4.858155000	-0.623841000	-0.524617000
1	1.466591000	-3.827103000	-2.215874000
1	5.562038000	-2.709485000	-1.598197000
1	3.871776000	-4.330180000	-2.428553000
6	-2.204160000	3.152491000	-1.808258000
6	-3.544564000	3.422547000	-1.955135000
6	-4.119241000	1.335561000	-0.879407000
6	-4.505696000	2.503833000	-1.496080000
1	-1.458464000	3.857013000	-2.158373000
1	-3.860177000	4.341901000	-2.431507000
1	-4.866884000	0.633820000	-0.537637000
1	-5.558520000	2.713136000	-1.635098000
1	0.191169000	2.309668000	-1.380065000
1	-0.194569000	-2.262095000	-1.472632000
6	-3.065933000	-0.976231000	0.605560000
6	-3.023563000	-2.361258000	0.408420000
6	-3.825463000	-0.477834000	1.674804000
6	-3.727975000	-3.219958000	1.242017000
6	-4.523420000	-1.339588000	2.507302000
6	-4.482222000	-2.714944000	2.294806000
1	-2.435984000	-2.754442000	-0.410661000
1	-3.835828000	0.587468000	1.864695000
1	-3.680871000	-4.288032000	1.069970000
1	-5.089157000	-0.937121000	3.338408000
1	-5.022259000	-3.384599000	2.951503000
6	3.062164000	0.976450000	0.603463000
6	3.800176000	0.457149000	1.676598000
6	3.052550000	2.362671000	0.410369000
6	4.505862000	1.299307000	2.521623000
6	3.764283000	3.202739000	1.257597000
6	4.492781000	2.676765000	2.317942000
1	3.795422000	-0.610421000	1.852601000
1	2.495088000	2.771465000	-0.422734000
1	5.061129000	0.878594000	3.351002000
1	3.749084000	4.272020000	1.087691000
1	5.042297000	3.331938000	2.981682000

1f Sn^{II}(Me-L1)$_2$

7	2.332700000	0.238213000	-0.153658000
7	0.238586000	1.611818000	0.846430000
6	1.469273000	2.103465000	1.051241000
6	2.607223000	1.378391000	0.487607000
7	-2.332669000	-0.238228000	-0.153645000
7	-0.238586000	-1.611870000	0.846438000
6	-1.469287000	-2.103452000	1.051317000
6	-2.607221000	-1.378358000	0.487684000
50	-0.000002000	-0.000023000	-0.665438000
6	-3.903676000	-1.948750000	0.623822000
6	-1.736166000	-3.291822000	1.784103000
6	-4.103292000	-3.109348000	1.325257000
6	-3.013932000	-3.776136000	1.922419000
1	-4.739450000	-1.446855000	0.158340000
1	-0.915135000	-3.834621000	2.227599000
1	-5.100887000	-3.520194000	1.414895000
1	-3.182987000	-4.688475000	2.480368000
6	1.736124000	3.291896000	1.783937000
6	3.013872000	3.776283000	1.922176000
6	3.903654000	1.948864000	0.623656000
6	4.103241000	3.109515000	1.325012000
1	0.915085000	3.834694000	2.227417000
1	3.182900000	4.688670000	2.480052000
1	4.739435000	1.446994000	0.158159000
1	5.100817000	3.520423000	1.414575000
6	3.327447000	-0.596263000	-0.687723000
6	4.335523000	-1.152225000	0.115023000
6	3.270627000	-0.970331000	-2.036689000
6	5.256654000	-2.041159000	-0.420426000
6	4.198126000	-1.859043000	-2.565709000
6	5.196431000	-2.399210000	-1.763645000
1	4.380618000	-0.891006000	1.164423000
1	2.502249000	-0.544959000	-2.668475000
1	6.023579000	-2.461500000	0.218688000
1	4.139407000	-2.127207000	-3.613369000
1	5.916916000	-3.092563000	-2.177798000
6	-3.327402000	0.596255000	-0.687718000
6	-3.270625000	0.970256000	-2.036703000
6	-4.335455000	1.152247000	0.115031000
6	-4.198131000	1.858955000	-2.565734000
6	-5.256596000	2.041164000	-0.420427000
6	-5.196404000	2.399167000	-1.763661000
1	-2.502276000	0.544844000	-2.668496000
1	-4.380529000	0.891059000	1.164438000
1	-4.139442000	2.127074000	-3.613408000
1	-6.023504000	2.461532000	0.218690000

1	-5.916899000	3.092508000	-2.177821000
6	-0.891155000	2.294383000	1.453122000
1	-0.771063000	2.363911000	2.539325000
1	-1.018090000	3.311135000	1.063755000
1	-1.799319000	1.737395000	1.251121000
6	0.891146000	-2.294484000	1.453093000
1	1.799344000	-1.737594000	1.250975000
1	0.771136000	-2.363917000	2.539313000
1	1.017956000	-3.311277000	1.063794000

2f $Sn^{IV}(Me-L1)_2$

7	1.840521000	-0.291908000	0.231517000
7	0.931889000	1.532723000	-1.537815000
6	2.231866000	1.701206000	-1.062978000
6	2.722851000	0.741031000	-0.130130000
7	-1.840522000	0.291867000	0.231557000
7	-0.931879000	-1.532652000	-1.537876000
6	-2.231859000	-1.701171000	-1.063051000
6	-2.722844000	-0.741042000	-0.130149000
50	0.000002000	0.000021000	-0.609893000
6	3.993622000	0.913076000	0.412426000
6	4.800416000	1.979000000	0.023079000
6	3.055406000	2.764507000	-1.435684000
6	4.335162000	2.897980000	-0.904200000
1	4.354219000	0.210400000	1.150185000
1	5.787635000	2.084554000	0.453947000
1	2.695861000	3.497570000	-2.144115000
1	4.956670000	3.728413000	-1.213655000
6	-3.993622000	-0.913119000	0.412389000
6	-3.055395000	-2.764451000	-1.435816000
6	-4.800411000	-1.979021000	0.022979000
6	-4.335153000	-2.897954000	-0.904344000
1	-4.354219000	-0.210478000	1.150185000
1	-2.695842000	-3.497479000	-2.144280000
1	-5.787632000	-2.084600000	0.453835000
1	-4.956661000	-3.728369000	-1.213843000
6	2.208549000	-1.457664000	0.935587000
6	3.360915000	-2.185990000	0.610803000
6	1.373134000	-1.948779000	1.943871000
6	3.663521000	-3.359888000	1.285754000
6	1.672717000	-3.134765000	2.603010000
6	2.823249000	-3.844480000	2.283937000
1	4.009607000	-1.832488000	-0.179023000
1	0.485185000	-1.391004000	2.218529000
1	4.558650000	-3.908096000	1.018494000
1	1.006972000	-3.495337000	3.377068000

1	3.062534000	-4.763257000	2.803174000
6	-2.208544000	1.457614000	0.935651000
6	-1.373148000	1.948713000	1.943936000
6	-3.360928000	2.185940000	0.610863000
6	-1.672747000	3.134703000	2.603093000
6	-3.663541000	3.359817000	1.285820000
6	-2.823268000	3.844408000	2.284024000
1	-0.485196000	1.390954000	2.218611000
1	-4.009602000	1.832421000	-0.178969000
1	-1.006995000	3.495249000	3.377156000
1	-4.558666000	3.908039000	1.018576000
1	-3.062582000	4.763179000	2.803256000
6	0.334269000	2.517352000	-2.418074000
1	0.887508000	2.596130000	-3.360036000
1	-0.687719000	2.225338000	-2.658062000
1	0.301930000	3.511447000	-1.958670000
6	-0.334242000	-2.517241000	-2.418180000
1	-0.301869000	-3.511345000	-1.958803000
1	-0.887499000	-2.596000000	-3.360131000
1	0.687731000	-2.225182000	-2.658175000

MECP$_{1f-2f}$

7	-2.282792000	-0.247441000	-0.074085000
7	-0.618771000	1.510888000	-1.245891000
6	-1.938465000	1.794862000	-1.272209000
6	-2.841417000	0.859754000	-0.628631000
7	2.286282000	0.254787000	-0.088821000
7	0.599160000	-1.450438000	-1.301746000
6	1.913262000	-1.753945000	-1.334057000
6	2.827831000	-0.850008000	-0.661351000
50	-0.001559000	0.009194000	0.179161000
6	4.211757000	-1.146420000	-0.691420000
6	2.449150000	-2.898909000	-1.970986000
6	4.693429000	-2.245399000	-1.365647000
6	3.806371000	-3.130572000	-1.999220000
1	4.899780000	-0.460421000	-0.218811000
1	1.781716000	-3.594027000	-2.459005000
1	5.760359000	-2.421972000	-1.414197000
1	4.190479000	-3.999312000	-2.518828000
6	-2.489056000	2.948648000	-1.879134000
6	-3.850225000	3.155648000	-1.916087000
6	-4.230374000	1.127519000	-0.670019000
6	-4.726542000	2.234538000	-1.320963000
1	-1.829183000	3.670087000	-2.338100000
1	-4.245113000	4.032136000	-2.414062000
1	-4.910470000	0.414258000	-0.226930000

1	-5.796490000	2.388930000	-1.380919000
6	-2.989069000	-1.022805000	0.868515000
6	-2.912211000	-2.417989000	0.786542000
6	-3.695460000	-0.456615000	1.940772000
6	-3.539315000	-3.221292000	1.730410000
6	-4.316859000	-1.263053000	2.882283000
6	-4.246854000	-2.650030000	2.781589000
1	-2.366439000	-2.864521000	-0.033270000
1	-3.736070000	0.620343000	2.039305000
1	-3.474293000	-4.298581000	1.641932000
1	-4.850797000	-0.806332000	3.706691000
1	-4.730336000	-3.276593000	3.520200000
6	3.008547000	0.998291000	0.868873000
6	3.670364000	0.396933000	1.950074000
6	2.996483000	2.395043000	0.789910000
6	4.311998000	1.171183000	2.905080000
6	3.644741000	3.166068000	1.746679000
6	4.307489000	2.560061000	2.807515000
1	3.660809000	-0.681266000	2.043402000
1	2.484432000	2.868449000	-0.036816000
1	4.809817000	0.688009000	3.737098000
1	3.630835000	4.245482000	1.661198000
1	4.807085000	3.161966000	3.555779000
6	-0.339625000	-2.285767000	-2.025868000
1	-0.041518000	-2.374047000	-3.075887000
1	-0.414044000	-3.302285000	-1.619229000
1	-1.325272000	-1.828246000	-1.988648000
6	0.308259000	2.379661000	-1.945988000
1	0.368277000	3.385336000	-1.511865000
1	1.300665000	1.934479000	-1.919506000
1	0.011307000	2.491421000	-2.993741000

1g Sn^{II}(Ph-L1)$_2$

7	2.242954000	-0.716643000	0.486943000
7	-0.073547000	-1.626714000	-0.606513000
6	1.086643000	-2.198350000	-0.987650000
6	2.326215000	-1.740545000	-0.370466000
7	-2.242954000	0.716712000	0.487138000
7	0.073541000	1.626940000	-0.606210000
6	-1.086666000	2.198567000	-0.987323000
6	-2.326235000	1.740675000	-0.370207000
50	-0.000001000	-0.000056000	0.968397000
6	-3.545474000	2.368174000	-0.755680000
6	-1.172318000	3.229765000	-1.962111000
6	-3.573236000	3.359680000	-1.699263000
6	-2.374927000	3.793045000	-2.305608000

1	-4.465097000	2.010795000	-0.315421000
1	-0.265661000	3.564809000	-2.443439000
1	-4.517739000	3.797532000	-1.995956000
1	-2.404482000	4.569608000	-3.059570000
6	1.172262000	-3.229556000	-1.962426000
6	2.374852000	-3.792914000	-2.305866000
6	3.545429000	-2.368132000	-0.755873000
6	3.573163000	-3.359633000	-1.699461000
1	0.265593000	-3.564558000	-2.443772000
1	2.404385000	-4.569499000	-3.059806000
1	4.465048000	-2.010843000	-0.315534000
1	4.517648000	-3.797560000	-1.996098000
6	3.268638000	-0.415529000	1.395045000
6	3.648842000	0.918476000	1.587112000
6	3.859782000	-1.401458000	2.201760000
6	4.608644000	1.250364000	2.533688000
6	4.811528000	-1.060526000	3.151063000
6	5.196725000	0.266110000	3.320393000
1	3.203261000	1.686566000	0.970638000
1	3.549538000	-2.432184000	2.090732000
1	4.897489000	2.286920000	2.656345000
1	5.248178000	-1.835196000	3.769484000
1	5.939632000	0.529093000	4.062337000
6	-3.268608000	0.415412000	1.395190000
6	-3.860012000	1.401192000	2.201911000
6	-3.648501000	-0.918689000	1.587252000
6	-4.811709000	1.060019000	3.151175000
6	-4.608256000	-1.250816000	2.533786000
6	-5.196600000	-0.266710000	3.320478000
1	-3.549989000	2.431990000	2.090938000
1	-3.202723000	-1.686662000	0.970769000
1	-5.248561000	1.834576000	3.769597000
1	-4.896853000	-2.287443000	2.656429000
1	-5.939468000	-0.529873000	4.062398000
6	1.293716000	2.153521000	-1.109491000
6	2.023501000	1.457926000	-2.073254000
6	1.794364000	3.365432000	-0.623765000
6	3.230368000	1.964223000	-2.541710000
6	2.999724000	3.869204000	-1.096465000
6	3.723467000	3.170329000	-2.057062000
1	1.639597000	0.519746000	-2.450487000
1	1.230024000	3.905771000	0.126013000
1	3.786476000	1.410648000	-3.287840000
1	3.375552000	4.808481000	-0.709718000
1	4.664444000	3.561455000	-2.422093000
6	-1.293743000	-2.153261000	-1.109785000

6	-1.794177000	-3.365385000	-0.624373000
6	-2.023731000	-1.457452000	-2.073242000
6	-2.999548000	-3.869151000	-1.097063000
6	-3.230608000	-1.963737000	-2.541674000
6	-3.723504000	-3.170050000	-2.057330000
1	-1.229664000	-3.905903000	0.125147000
1	-1.639985000	-0.519106000	-2.450229000
1	-3.375211000	-4.808593000	-0.710558000
1	-3.786888000	-1.409995000	-3.287552000
1	-4.664488000	-3.561161000	-2.422357000

2g Sn^{IV}(Ph-L1)$_2$

7	0.877784000	1.709950000	-0.609962000
7	-1.092870000	1.265605000	1.194922000
6	-0.693316000	2.599056000	0.995402000
6	0.340703000	2.831855000	0.046757000
7	1.183322000	-1.525421000	0.890024000
7	-0.747268000	-1.494836000	-1.013318000
6	-0.208998000	-2.744027000	-0.663867000
6	0.806966000	-2.761578000	0.332118000
50	0.064341000	-0.010226000	0.105540000
6	0.822328000	4.128931000	-0.127429000
6	0.292067000	5.191101000	0.595032000
6	-1.192174000	3.675679000	1.728866000
6	-0.713898000	4.964273000	1.523673000
1	1.626625000	4.303992000	-0.827823000
1	0.679294000	6.189324000	0.436742000
1	-1.955521000	3.499219000	2.473102000
1	-1.123398000	5.782916000	2.101233000
6	1.331012000	-3.987469000	0.740359000
6	-0.599832000	-3.945108000	-1.254905000
6	0.912294000	-5.176371000	0.153953000
6	-0.042244000	-5.153270000	-0.852799000
1	2.071794000	-4.009156000	1.527045000
1	-1.346928000	-3.930484000	-2.035787000
1	1.337444000	-6.114057000	0.487633000
1	-0.362928000	-6.071773000	-1.327135000
6	-2.264347000	0.875033000	1.882587000
6	-2.216617000	-0.207443000	2.765943000
6	-3.495935000	1.503076000	1.659338000
6	-3.366983000	-0.654456000	3.405043000
6	-4.636890000	1.063378000	2.314866000
6	-4.582387000	-0.017398000	3.190210000
1	-1.269554000	-0.698419000	2.955816000
1	-3.555184000	2.326667000	0.961024000
1	-3.305579000	-1.497320000	4.081987000

1	-5.580454000	1.560733000	2.126805000
1	-5.476961000	-0.359176000	3.694259000
6	-1.854576000	-1.329319000	-1.885158000
6	-3.094988000	-1.910573000	-1.604303000
6	-1.722586000	-0.529549000	-3.021296000
6	-4.173854000	-1.698725000	-2.451044000
6	-2.811528000	-0.306912000	-3.857182000
6	-4.039043000	-0.894485000	-3.579242000
1	-3.207732000	-2.516963000	-0.715260000
1	-0.758892000	-0.090312000	-3.249367000
1	-5.129749000	-2.151873000	-2.219569000
1	-2.693429000	0.319827000	-4.732174000
1	-4.885418000	-0.726148000	-4.232601000
6	1.725038000	1.782333000	-1.740518000
6	1.393346000	2.565081000	-2.853178000
6	2.892219000	1.015800000	-1.781922000
6	2.217061000	2.581517000	-3.969867000
6	3.703018000	1.022948000	-2.911249000
6	3.374187000	1.808854000	-4.008252000
1	0.485355000	3.153175000	-2.837770000
1	3.170797000	0.423236000	-0.918697000
1	1.945312000	3.193072000	-4.821460000
1	4.601748000	0.419181000	-2.924348000
1	4.010062000	1.820054000	-4.883903000
6	2.368654000	-1.312803000	1.630304000
6	3.599841000	-1.849067000	1.230831000
6	2.334169000	-0.490598000	2.760774000
6	4.752750000	-1.574836000	1.953172000
6	3.495567000	-0.205846000	3.468586000
6	4.710672000	-0.751358000	3.074152000
1	3.648447000	-2.473918000	0.349434000
1	1.388028000	-0.076285000	3.088089000
1	5.694931000	-1.998666000	1.627878000
1	3.443850000	0.437709000	4.337755000
1	5.614044000	-0.536672000	3.629879000

MECP$_{1g–2g}$

7	-2.177379000	0.640824000	0.480026000
7	0.015192000	1.624139000	-0.768935000
6	-1.131968000	2.356008000	-0.831967000
6	-2.292063000	1.849045000	-0.129477000
7	2.177844000	-0.638006000	0.480640000
7	-0.014422000	-1.619621000	-0.771461000
6	1.134155000	-2.349559000	-0.837230000
6	2.293881000	-1.843365000	-0.134421000
50	0.000093000	0.000804000	0.683478000

6	3.490729000	-2.598257000	-0.176065000
6	1.266184000	-3.556153000	-1.561353000
6	3.583363000	-3.753415000	-0.916507000
6	2.464479000	-4.232618000	-1.614060000
1	4.361442000	-2.213780000	0.334975000
1	0.416192000	-3.930644000	-2.110883000
1	4.527298000	-4.279694000	-0.976028000
1	2.541908000	-5.133801000	-2.209063000
6	-1.263735000	3.564649000	-1.552612000
6	-2.460898000	4.242939000	-1.601317000
6	-3.487565000	2.606186000	-0.166293000
6	-3.579492000	3.763689000	-0.902919000
1	-0.413932000	3.940039000	-2.102567000
1	-2.538167000	5.146015000	-2.193523000
1	-4.358006000	2.221176000	0.344813000
1	-4.522644000	4.291807000	-0.959005000
6	-3.100397000	0.244119000	1.473539000
6	-3.622710000	-1.051742000	1.430752000
6	-3.457258000	1.077005000	2.543646000
6	-4.494631000	-1.493881000	2.417931000
6	-4.326935000	0.629856000	3.526704000
6	-4.853314000	-0.657565000	3.468698000
1	-3.349704000	-1.700992000	0.610434000
1	-3.036915000	2.072557000	2.604319000
1	-4.894573000	-2.498702000	2.364209000
1	-4.585637000	1.286192000	4.348452000
1	-5.528877000	-1.006135000	4.239381000
6	3.098704000	-0.247336000	1.478290000
6	3.456522000	-1.088775000	2.541854000
6	3.617849000	1.050158000	1.447564000
6	4.324345000	-0.648241000	3.529230000
6	4.487840000	1.485448000	2.439101000
6	4.847912000	0.640933000	3.482988000
1	3.038045000	-2.085399000	2.593717000
1	3.343626000	1.705814000	0.632587000
1	4.584046000	-1.311021000	4.345510000
1	4.885481000	2.491668000	2.394612000
1	5.521991000	0.984236000	4.257119000
6	-1.203564000	-2.107417000	-1.374284000
6	-1.799510000	-1.367457000	-2.397393000
6	-1.808476000	-3.298142000	-0.959981000
6	-2.965946000	-1.817830000	-3.003124000
6	-2.973943000	-3.745017000	-1.568459000
6	-3.556785000	-3.008246000	-2.594990000
1	-1.341771000	-0.438515000	-2.709831000
1	-1.359623000	-3.866559000	-0.155284000

1	-3.413506000	-1.234261000	-3.797951000
1	-3.431162000	-4.668594000	-1.234964000
1	-4.465213000	-3.357237000	-3.068523000
6	1.204656000	2.109791000	-1.373118000
6	1.810689000	3.301041000	-0.962456000
6	1.799086000	1.366789000	-2.394606000
6	2.975649000	3.745829000	-1.574032000
6	2.965242000	1.814471000	-3.002962000
6	3.556809000	3.005951000	-2.599018000
1	1.363004000	3.871838000	-0.158791000
1	1.340152000	0.437391000	-2.704153000
1	3.433368000	4.670376000	-1.244200000
1	3.411554000	1.228039000	-3.796168000
1	4.464898000	3.353269000	-3.074895000

1h Sn^{II}(Bu^t-L1)$_2$

7	2.376610000	-0.369321000	0.847741000
7	0.212387000	-1.571584000	-0.321125000
6	1.449044000	-2.043607000	-0.590063000
6	2.607161000	-1.438455000	0.084084000
7	-2.376666000	0.369425000	0.847819000
7	-0.212468000	1.571540000	-0.321244000
6	-1.449124000	2.043528000	-0.590225000
6	-2.607242000	1.438477000	0.084026000
50	-0.000028000	0.000058000	1.247963000
6	-3.876544000	2.056582000	-0.161864000
6	-1.674542000	3.101072000	-1.510668000
6	-4.034494000	3.096946000	-1.037966000
6	-2.926535000	3.614786000	-1.734027000
1	-4.750301000	1.678254000	0.336550000
1	-0.829152000	3.510994000	-2.042136000
1	-5.020418000	3.513469000	-1.201946000
1	-3.058540000	4.421961000	-2.443397000
6	1.674478000	-3.101262000	-1.510375000
6	2.926490000	-3.614965000	-1.733682000
6	3.876485000	-2.056526000	-0.161735000
6	4.034452000	-3.096998000	-1.037710000
1	0.829093000	-3.511287000	-2.041773000
1	3.058507000	-4.422230000	-2.442949000
1	4.750230000	-1.678082000	0.336634000
1	5.020389000	-3.513507000	-1.201655000
6	0.907975000	2.187545000	-0.943068000
6	1.562783000	1.556174000	-2.001363000
6	1.378896000	3.427650000	-0.501567000
6	2.658853000	2.156726000	-2.609899000
6	2.475611000	4.024381000	-1.110813000

6	3.119052000	3.392649000	-2.170009000
1	1.208326000	0.592791000	-2.341903000
1	0.869398000	3.923831000	0.315045000
1	3.154888000	1.653540000	-3.430511000
1	2.827255000	4.985668000	-0.756828000
1	3.973075000	3.858001000	-2.645348000
6	-0.908046000	-2.187592000	-0.942965000
6	-1.379010000	-3.427676000	-0.501457000
6	-1.562759000	-1.556255000	-2.001337000
6	-2.475684000	-4.024414000	-1.110769000
6	-2.658782000	-2.156818000	-2.609945000
6	-3.119032000	-3.392715000	-2.170042000
1	-0.869573000	-3.923837000	0.315203000
1	-1.208254000	-0.592894000	-2.341891000
1	-2.827367000	-4.985685000	-0.756783000
1	-3.154739000	-1.653659000	-3.430619000
1	-3.973017000	-3.858080000	-2.645438000
6	3.414257000	0.286792000	1.683637000
6	4.512690000	0.939524000	0.816420000
6	4.008019000	-0.678637000	2.730894000
1	4.563353000	-1.505779000	2.296344000
1	4.685801000	-0.132047000	3.390064000
1	5.096508000	0.224227000	0.243558000
1	5.200551000	1.492849000	1.459532000
1	4.065567000	1.641975000	0.113629000
6	2.743821000	1.428820000	2.467143000
1	3.497121000	1.975642000	3.036729000
1	2.259083000	2.135920000	1.793501000
1	3.209295000	-1.099607000	3.344216000
1	2.002646000	1.052387000	3.172810000
6	-3.414189000	-0.286681000	1.683900000
6	-4.007830000	0.678698000	2.731280000
6	-2.743466000	-1.428565000	2.467355000
1	-2.002056000	-1.052000000	3.172709000
1	-3.496564000	-1.975307000	3.037284000
1	-3.209008000	1.099807000	3.344380000
1	-4.685346000	0.132022000	3.390656000
1	-4.563407000	1.505741000	2.296869000
6	-4.512689000	-0.939671000	0.816946000
1	-5.200303000	-1.493096000	1.460235000
1	-5.096776000	-0.224538000	0.244165000
1	-2.258944000	-2.135758000	1.793658000
1	-4.065575000	-1.642079000	0.114106000

2h $Sn^{IV}(Bu^t\text{-}L1)_2$

7	1.562809000	-0.825610000	0.736730000

7	1.438824000	1.191873000	-1.097029000
6	2.696776000	0.888378000	-0.546493000
6	2.761571000	-0.168651000	0.415871000
7	-1.562726000	0.825628000	0.736807000
7	-1.438812000	-1.191806000	-1.097005000
6	-2.696728000	-0.888345000	-0.546402000
6	-2.761497000	0.168657000	0.415990000
50	0.000024000	0.000021000	-0.281402000
6	1.171772000	2.281510000	-2.072393000
6	1.915324000	2.039541000	-3.400858000
6	1.499481000	3.663673000	-1.472466000
1	0.911757000	3.825749000	-0.567715000
1	2.547975000	3.778237000	-1.211526000
1	1.245283000	4.447990000	-2.188455000
1	2.995339000	2.007616000	-3.288883000
1	1.675853000	2.834397000	-4.109982000
1	1.600355000	1.090395000	-3.838220000
6	-0.329515000	2.278416000	-2.392464000
1	-0.930256000	2.490157000	-1.505455000
1	-0.553793000	3.054614000	-3.124494000
1	-0.649616000	1.326562000	-2.824080000
6	-1.171895000	-2.281430000	-2.072417000
6	0.329345000	-2.278448000	-2.392736000
6	-1.915708000	-2.039406000	-3.400721000
1	-2.995699000	-2.007399000	-3.288483000
1	-1.600765000	-1.090290000	-3.838158000
1	-1.676465000	-2.834292000	-4.109888000
1	0.649455000	-1.326618000	-2.824396000
1	0.553450000	-3.054650000	-3.124809000
1	0.930219000	-2.490250000	-1.505830000
6	-1.499658000	-3.663557000	-1.472456000
1	-2.548158000	-3.778047000	-1.211479000
1	-1.245543000	-4.447894000	-2.188448000
1	-0.911911000	-3.825654000	-0.567726000
6	1.483935000	-2.072196000	1.392854000
6	0.467693000	-2.287845000	2.330686000
6	2.345418000	-3.135876000	1.089463000
6	0.312886000	-3.526057000	2.941135000
6	2.195131000	-4.365233000	1.716212000
6	1.178783000	-4.571386000	2.643945000
1	-0.202079000	-1.474640000	2.583091000
1	3.129043000	-2.995659000	0.357505000
1	-0.484163000	-3.667123000	3.660413000
1	2.872435000	-5.172878000	1.466559000
6	-1.483853000	2.072170000	1.393011000
6	-2.345410000	3.135831000	1.089752000

6	-0.467565000	2.287797000	2.330800000
6	-2.195135000	4.365148000	1.716581000
6	-0.312779000	3.525973000	2.941324000
6	-1.178739000	4.571285000	2.644264000
1	-3.129077000	2.995628000	0.357835000
1	0.202257000	1.474605000	2.583105000
1	-2.872498000	5.172776000	1.467027000
1	0.484310000	3.667022000	3.660565000
6	-3.970860000	0.456521000	1.046847000
6	-3.891712000	-1.552214000	-0.849202000
6	-5.136134000	-0.229089000	0.728675000
6	-5.093995000	-1.227377000	-0.229645000
1	-3.993574000	1.225222000	1.806057000
1	-3.899783000	-2.347006000	-1.574160000
1	-6.061138000	0.018478000	1.232955000
1	-5.989994000	-1.771892000	-0.499107000
6	3.891787000	1.552200000	-0.849338000
6	5.094087000	1.227309000	-0.229840000
6	3.970956000	-0.456565000	1.046666000
6	5.136235000	0.229005000	0.728462000
1	3.899876000	2.346991000	-1.574281000
1	5.990096000	1.771791000	-0.499334000
1	3.993671000	-1.225283000	1.805862000
1	6.061255000	-0.018598000	1.232699000
1	-1.064207000	5.532907000	3.127266000
1	1.064232000	-5.533036000	3.126886000

MECP$_{1h-2h}$

7	-2.285138000	0.233579000	0.800033000
7	-0.277332000	1.570858000	-0.456057000
6	-1.538078000	2.073181000	-0.546893000
6	-2.605919000	1.386387000	0.172933000
7	2.285118000	-0.233565000	0.800072000
7	0.277289000	-1.570825000	-0.456041000
6	1.538140000	-2.073250000	-0.546867000
6	2.605945000	-1.386498000	0.173017000
50	0.000064000	-0.000005000	1.017443000
6	3.893788000	-1.992013000	0.123287000
6	1.855754000	-3.214612000	-1.318046000
6	4.158092000	-3.103792000	-0.641395000
6	3.136253000	-3.713005000	-1.381523000
1	4.712412000	-1.540646000	0.653811000
1	1.070788000	-3.688676000	-1.888318000
1	5.167130000	-3.494453000	-0.681403000
1	3.350074000	-4.570937000	-2.005893000
6	-1.855843000	3.214599000	-1.318136000

6	-3.136345000	3.712926000	-1.381521000
6	-3.893911000	1.991899000	0.123305000
6	-4.158167000	3.103682000	-0.641361000
1	-1.070972000	3.688611000	-1.888298000
1	-3.350212000	4.570867000	-2.005899000
1	-4.712343000	1.540506000	0.653733000
1	-5.167212000	3.494252000	-0.681425000
6	-0.811377000	-2.249369000	-1.064502000
6	-1.536138000	-1.610520000	-2.072202000
6	-1.202024000	-3.531234000	-0.662889000
6	-2.623044000	-2.239676000	-2.666412000
6	-2.290499000	-4.156521000	-1.257540000
6	-3.005715000	-3.513970000	-2.263008000
1	-1.243614000	-0.615976000	-2.380525000
1	-0.643282000	-4.033093000	0.116960000
1	-3.175747000	-1.727511000	-3.443963000
1	-2.583865000	-5.146213000	-0.929597000
1	-3.855369000	-4.001062000	-2.724351000
6	0.811387000	2.249326000	-1.064508000
6	1.201907000	3.531374000	-0.662800000
6	1.536196000	1.610456000	-2.072143000
6	2.290384000	4.156641000	-1.257629000
6	2.622999000	2.239755000	-2.666323000
6	3.005725000	3.514195000	-2.263025000
1	0.643219000	4.033108000	0.116935000
1	1.243622000	0.616045000	-2.380521000
1	2.583771000	5.146301000	-0.929565000
1	3.175806000	1.727612000	-3.443959000
1	3.855288000	4.001162000	-2.724245000
6	-3.208783000	-0.474416000	1.724795000
6	-4.379670000	-1.102102000	0.935000000
6	-3.703929000	0.419893000	2.880662000
1	-4.311695000	1.260381000	2.558449000
1	-4.300457000	-0.176009000	3.575097000
1	-5.004273000	-0.369162000	0.432240000
1	-5.012972000	-1.673804000	1.616713000
1	-3.992320000	-1.783353000	0.177379000
6	-2.454355000	-1.647427000	2.374019000
1	-3.147872000	-2.237869000	2.974382000
1	-2.022584000	-2.307038000	1.621575000
1	-2.848617000	0.819537000	3.428610000
1	-1.660869000	-1.297818000	3.036793000
6	3.208834000	0.474335000	1.724809000
6	3.704116000	-0.419740000	2.880655000
6	2.454275000	1.647392000	2.374007000
1	1.660919000	1.297886000	3.036669000

1	3.147815000	2.237881000	2.974303000
1	2.848587000	-0.819465000	3.428797000
1	4.300529000	0.176026000	3.575005000
1	4.311621000	-1.260396000	2.558491000
6	4.379622000	1.102148000	0.934940000
1	5.012926000	1.673852000	1.616581000
1	5.004321000	0.368995000	0.432271000
1	2.022619000	2.307034000	1.621502000
1	3.992346000	1.783125000	0.177254000

3e Sn^{II}(H-L2)$_2$

7	-2.296422000	-0.375505000	0.230182000
7	0.199380000	-1.441064000	0.389510000
6	-0.751052000	-1.913376000	1.209616000
6	-2.089338000	-1.384666000	1.135656000
7	2.311452000	0.698989000	-0.313018000
7	0.057738000	1.724013000	0.762071000
6	1.218673000	2.334058000	1.032754000
6	2.444781000	1.796592000	0.493146000
50	-0.113800000	0.286450000	-0.861009000
6	-3.457088000	-0.049598000	-0.310927000
6	-3.555228000	1.234448000	-0.974319000
6	-4.636784000	-0.893380000	-0.336684000
6	-4.717194000	1.693063000	-1.476702000
6	-5.796374000	-0.463831000	-0.871847000
6	-5.941888000	0.883592000	-1.439076000
1	-2.664409000	1.849855000	-1.008596000
1	-4.550147000	-1.907773000	0.025679000
1	-4.795254000	2.671768000	-1.932462000
1	-6.663630000	-1.108945000	-0.935334000
6	3.261160000	-0.171266000	-0.619655000
6	3.041821000	-1.043296000	-1.754452000
6	4.486412000	-0.367066000	0.130294000
6	3.966011000	-1.935819000	-2.162629000
6	5.398607000	-1.288189000	-0.241141000
6	5.229344000	-2.117848000	-1.441051000
1	2.127362000	-0.907453000	-2.319388000
1	4.618996000	0.183670000	1.050267000
1	3.816330000	-2.545797000	-3.044176000
1	6.282914000	-1.477951000	0.354305000
8	-7.007941000	1.290455000	-1.888467000
8	6.077772000	-2.930697000	-1.796276000
6	3.657497000	2.491352000	0.723244000
6	1.310147000	3.487577000	1.857235000
6	3.699005000	3.619316000	1.503246000
6	2.512981000	4.100470000	2.093743000

1	4.552660000	2.163007000	0.215741000
1	0.398261000	3.885498000	2.286426000
1	4.628215000	4.156823000	1.634430000
1	2.546732000	4.986746000	2.715409000
6	-0.501529000	-2.944563000	2.152983000
6	-1.480474000	-3.383178000	3.007360000
6	-3.057699000	-1.836199000	2.064477000
6	-2.766900000	-2.810451000	2.986614000
1	0.494651000	-3.368305000	2.197869000
1	-1.250691000	-4.158248000	3.728058000
1	-4.023289000	-1.351863000	2.087104000
1	-3.510146000	-3.113386000	3.711424000
1	1.121386000	-1.818021000	0.560409000
1	-0.752973000	2.188316000	1.148667000

4e $Sn^{IV}(H\text{-}L2)_2$

7	0.924781000	1.711532000	-1.797682000
7	1.872266000	-0.346431000	-0.341556000
6	2.798736000	0.638933000	-0.739243000
6	2.288744000	1.711861000	-1.515613000
6	2.044586000	-1.261295000	0.687692000
6	1.343871000	-2.493357000	0.631178000
6	2.838617000	-0.990979000	1.833159000
6	1.441051000	-3.418079000	1.629999000
6	2.945806000	-1.904172000	2.843107000
6	2.264877000	-3.183705000	2.800595000
1	0.744241000	-2.714209000	-0.247056000
1	3.335406000	-0.034548000	1.915914000
8	2.370443000	-4.023900000	3.714106000
7	-1.090798000	-1.129315000	-2.404031000
7	-1.749016000	0.139154000	-0.123306000
6	-2.672410000	-0.800271000	-0.620227000
6	-2.303847000	-1.483741000	-1.806612000
6	-2.032201000	1.155044000	0.780288000
6	-1.008857000	1.614781000	1.645619000
6	-3.294224000	1.804332000	0.819232000
6	-1.220348000	2.647084000	2.513772000
6	-3.521673000	2.840321000	1.678573000
6	-2.500281000	3.324529000	2.587263000
1	-0.049697000	1.106830000	1.638795000
1	-4.067870000	1.490739000	0.132155000
8	-2.705622000	4.269164000	3.373595000
50	0.016391000	0.036063000	-1.182899000
1	-0.442847000	2.983367000	3.187231000
1	-4.474956000	3.353158000	1.693983000
1	0.917650000	-4.363697000	1.574307000

1	3.532871000	-1.690270000	3.727152000
6	3.158117000	2.697136000	-1.979633000
6	4.516826000	2.626768000	-1.705656000
6	4.175106000	0.563338000	-0.512643000
6	5.026422000	1.554206000	-0.982220000
1	2.759449000	3.520230000	-2.560793000
1	5.176614000	3.403581000	-2.069186000
1	4.582425000	-0.284630000	0.018219000
1	6.088200000	1.479458000	-0.788963000
6	-3.140964000	-2.472537000	-2.319416000
6	-3.850408000	-1.167719000	0.034267000
6	-4.329249000	-2.793003000	-1.677572000
6	-4.679072000	-2.145875000	-0.497312000
1	-2.854592000	-2.986808000	-3.229319000
1	-4.108568000	-0.697464000	0.972051000
1	-4.972705000	-3.557260000	-2.093200000
1	-5.591031000	-2.410276000	0.021107000
1	-0.731633000	-1.763083000	-3.100649000
1	0.582945000	2.393421000	-2.453946000

3f $Sn^{II}(Me-L2)_2$

7	-2.454227000	-0.270220000	0.220261000
7	-0.114092000	-1.590863000	0.877111000
6	-1.294009000	-2.074585000	1.311529000
6	-2.535275000	-1.418425000	0.962715000
7	2.405073000	0.553579000	-0.248333000
7	0.321362000	1.552936000	1.208902000
6	1.496692000	2.200570000	1.233469000
6	2.619261000	1.697663000	0.463666000
50	-0.073661000	0.151139000	-0.450615000
6	-3.417377000	0.220299000	-0.545645000
6	-3.304988000	1.601151000	-0.961662000
6	-4.547627000	-0.530622000	-1.052649000
6	-4.267978000	2.210954000	-1.679669000
6	-5.500572000	0.055652000	-1.805090000
6	-5.460528000	1.485612000	-2.136299000
1	-2.436536000	2.155576000	-0.627563000
1	-4.580562000	-1.594987000	-0.867421000
1	-4.200922000	3.256164000	-1.953050000
1	-6.320600000	-0.513509000	-2.224454000
6	3.331256000	-0.264844000	-0.729307000
6	2.939082000	-1.203048000	-1.758885000
6	4.698420000	-0.348571000	-0.255527000
6	3.816442000	-2.054900000	-2.326485000
6	5.573059000	-1.231579000	-0.780336000
6	5.213264000	-2.125658000	-1.887298000

1	1.918780000	-1.152670000	-2.118985000
1	4.985005000	0.248706000	0.597890000
1	3.526543000	-2.712689000	-3.135834000
1	6.572380000	-1.341159000	-0.377975000
8	-6.345816000	2.030555000	-2.788051000
8	6.022054000	-2.900727000	-2.389965000
6	3.811762000	2.458293000	0.404210000
6	1.726682000	3.371800000	2.012005000
6	3.971654000	3.607550000	1.135950000
6	2.925401000	4.039540000	1.970483000
1	4.585622000	2.154558000	-0.285291000
1	0.931194000	3.759212000	2.629460000
1	4.877621000	4.191342000	1.046789000
1	3.049920000	4.938078000	2.562601000
6	-1.394780000	-3.242366000	2.121159000
6	-2.602118000	-3.691259000	2.598018000
6	-3.749878000	-1.894046000	1.511153000
6	-3.793953000	-3.002759000	2.318902000
1	-0.498307000	-3.783807000	2.379018000
1	-2.626883000	-4.575073000	3.223771000
1	-4.650314000	-1.321396000	1.342119000
1	-4.729314000	-3.322659000	2.757517000
6	1.101887000	-2.228254000	1.357920000
1	1.145852000	-2.242442000	2.452496000
1	1.193503000	-3.261037000	1.003587000
1	1.969711000	-1.683037000	1.001034000
6	-0.755694000	2.033155000	2.060837000
1	-1.076921000	3.051798000	1.808869000
1	-1.614999000	1.375590000	1.961996000
1	-0.454967000	2.031893000	3.113728000

4f Sn^{IV}(Me-L2)$_2$

7	0.882047000	1.688755000	-1.633715000
7	1.884671000	-0.396820000	-0.212718000
6	2.786814000	0.607783000	-0.614922000
6	2.247477000	1.697055000	-1.358842000
6	2.089734000	-1.315587000	0.808751000
6	1.405776000	-2.557166000	0.755061000
6	2.900048000	-1.041781000	1.941832000
6	1.534147000	-3.487386000	1.745341000
6	3.037965000	-1.960248000	2.943204000
6	2.374683000	-3.249169000	2.903207000
1	0.793096000	-2.778807000	-0.113560000
1	3.385300000	-0.079235000	2.022227000
8	2.507910000	-4.093796000	3.808992000
7	-1.089090000	-1.202830000	-2.159787000

7	-1.739972000	0.095759000	0.126182000
6	-2.669090000	-0.835693000	-0.372177000
6	-2.310772000	-1.522300000	-1.567470000
6	-2.015880000	1.126263000	1.015114000
6	-0.984579000	1.592188000	1.868274000
6	-3.273054000	1.785356000	1.051355000
6	-1.183064000	2.640415000	2.720264000
6	-3.487496000	2.837174000	1.894736000
6	-2.457123000	3.329683000	2.788816000
1	-0.030361000	1.074648000	1.865739000
1	-4.053606000	1.465625000	0.375073000
8	-2.649996000	4.290429000	3.558486000
50	0.003035000	0.008489000	-0.964841000
1	-0.399463000	2.981155000	3.384396000
1	-4.437001000	3.357104000	1.907240000
1	1.023836000	-4.440276000	1.691899000
1	3.637100000	-1.744069000	3.818574000
6	3.109348000	2.702985000	-1.801052000
6	4.474418000	2.633201000	-1.548060000
6	4.165029000	0.536517000	-0.414287000
6	5.004927000	1.545397000	-0.869139000
1	2.712874000	3.544953000	-2.350078000
1	5.120796000	3.427521000	-1.897977000
1	4.584747000	-0.323343000	0.087087000
1	6.070229000	1.471240000	-0.696189000
6	-3.179129000	-2.491568000	-2.074188000
6	-3.845623000	-1.185068000	0.289452000
6	-4.370554000	-2.789139000	-1.422448000
6	-4.699308000	-2.145832000	-0.237340000
1	-2.924122000	-3.018064000	-2.982716000
1	-4.085789000	-0.713003000	1.231202000
1	-5.030938000	-3.538660000	-1.838756000
1	-5.610972000	-2.395713000	0.288662000
6	0.268114000	2.761041000	-2.396376000
1	0.710572000	2.853836000	-3.393650000
1	-0.796325000	2.564586000	-2.518465000
1	0.372939000	3.721556000	-1.882777000
6	-0.616580000	-1.937800000	-3.319917000
1	0.358081000	-1.558427000	-3.625443000
1	-0.517123000	-3.010274000	-3.119976000
1	-1.299884000	-1.811901000	-4.165166000

3g Sn^II(Ph-L2)₂

7	2.141847000	1.224990000	-0.607548000
7	-0.378012000	1.525745000	0.461762000
6	0.587234000	2.423665000	0.764509000

6	1.919702000	2.289584000	0.217472000
7	-2.141803000	-1.225093000	-0.607479000
7	0.378010000	-1.525671000	0.461999000
6	-0.587157000	-2.423715000	0.764607000
6	-1.919604000	-2.289719000	0.217489000
50	-0.000010000	-0.000070000	-1.108413000
6	3.316992000	0.751088000	-0.992074000
6	3.355824000	-0.075888000	-2.180799000
6	4.574605000	0.963693000	-0.303444000
6	4.512416000	-0.537500000	-2.695872000
6	5.731584000	0.462873000	-0.780092000
6	5.798187000	-0.294376000	-2.035832000
1	2.421696000	-0.247110000	-2.700686000
1	4.556063000	1.456341000	0.657432000
1	4.538172000	-1.100127000	-3.620366000
1	6.658776000	0.564705000	-0.230124000
6	-3.316986000	-0.751221000	-0.991941000
6	-3.355908000	0.075856000	-2.180592000
6	-4.574553000	-0.963911000	-0.303256000
6	-4.512544000	0.537474000	-2.695564000
6	-5.731577000	-0.463089000	-0.779798000
6	-5.798266000	0.294297000	-2.035449000
1	-2.421819000	0.247146000	-2.700528000
1	-4.555941000	-1.456621000	0.657588000
1	-4.538370000	1.100158000	-3.620022000
1	-6.658735000	-0.565000000	-0.229786000
8	6.858360000	-0.722612000	-2.483834000
8	-6.858491000	0.722437000	-2.483424000
6	-2.863908000	-3.322123000	0.447481000
6	-0.359146000	-3.523238000	1.640184000
6	-2.585757000	-4.389731000	1.260824000
6	-1.328717000	-4.461695000	1.887411000
1	-3.800919000	-3.294961000	-0.087894000
1	0.611102000	-3.626181000	2.101479000
1	-3.311121000	-5.181050000	1.392748000
1	-1.104330000	-5.290754000	2.547513000
6	0.359262000	3.523176000	1.640110000
6	1.328892000	4.461557000	1.887416000
6	2.864062000	3.321922000	0.447517000
6	2.585950000	4.389529000	1.260878000
1	-0.611002000	3.626187000	2.101354000
1	1.104532000	5.290614000	2.547531000
1	3.801090000	3.294710000	-0.087828000
1	3.311359000	5.180799000	1.392850000
6	1.677834000	-1.711050000	1.015033000
6	2.048101000	-1.030084000	2.176154000

6	2.601584000	-2.562804000	0.406172000
6	3.312536000	-1.210794000	2.724499000
6	3.866654000	-2.738829000	0.954876000
6	4.224939000	-2.067562000	2.118175000
1	1.335895000	-0.364303000	2.645650000
1	2.318064000	-3.091751000	-0.495148000
1	3.583570000	-0.680762000	3.629221000
1	4.573060000	-3.400801000	0.470126000
1	5.209739000	-2.206507000	2.545279000
6	-1.677867000	1.711274000	1.014678000
6	-2.601438000	2.563182000	0.405762000
6	-2.048355000	1.030282000	2.175714000
6	-3.866537000	2.739359000	0.954350000
6	-3.312820000	1.211138000	2.723941000
6	-4.225034000	2.068082000	2.117579000
1	-2.317756000	3.092127000	-0.495508000
1	-1.336292000	0.364362000	2.645229000
1	-4.572801000	3.401455000	0.469563000
1	-3.584025000	0.681087000	3.628601000
1	-5.209861000	2.207140000	2.544586000

4g Sn^{IV}(Ph-L2)$_2$

7	-0.886859000	-1.410744000	1.133393000
7	1.051072000	-1.618372000	-0.760146000
6	0.497326000	-2.815223000	-0.266784000
6	-0.522565000	-2.698968000	0.717219000
6	2.283272000	-1.489825000	-1.384690000
6	3.381340000	-2.344867000	-1.101520000
6	2.482767000	-0.415845000	-2.289390000
6	4.593959000	-2.148856000	-1.697477000
6	3.688049000	-0.207010000	-2.895837000
6	4.824470000	-1.071638000	-2.640790000
1	3.256851000	-3.137762000	-0.377457000
1	1.643941000	0.232159000	-2.525688000
8	5.929838000	-0.891373000	-3.186613000
7	0.960105000	1.627094000	0.768014000
7	-1.028456000	1.408458000	-1.064530000
6	-0.481092000	2.688950000	-0.857131000
6	0.564418000	2.795356000	0.100655000
6	-2.259392000	1.129434000	-1.640571000
6	-2.442073000	-0.117817000	-2.291208000
6	-3.370291000	2.008553000	-1.544792000
6	-3.645360000	-0.473608000	-2.829081000
6	-4.581290000	1.667114000	-2.074592000
6	-4.796663000	0.405327000	-2.756480000
1	-1.591774000	-0.785623000	-2.392636000

1	-3.257206000	2.941793000	-1.011241000
8	-5.901998000	0.089894000	-3.237561000
50	0.029178000	0.001314000	0.015552000
1	-3.774629000	-1.418058000	-3.341712000
1	-5.435882000	2.324960000	-1.979737000
1	5.437920000	-2.785950000	-1.465054000
1	3.830235000	0.603781000	-3.598480000
6	-1.115259000	-3.857639000	1.219840000
6	-0.738263000	-5.108001000	0.748452000
6	0.824651000	-4.079684000	-0.760472000
6	0.219445000	-5.220144000	-0.252044000
1	-1.877665000	-3.772267000	1.981122000
1	-1.209331000	-5.993151000	1.155589000
1	1.547101000	-4.165905000	-1.559164000
1	0.492086000	-6.190194000	-0.645722000
6	1.179161000	4.031518000	0.300244000
6	-0.829221000	3.811406000	-1.611038000
6	0.783516000	5.145283000	-0.428535000
6	-0.212123000	5.034858000	-1.391217000
1	1.976928000	4.113482000	1.024782000
1	-1.575249000	3.718925000	-2.386974000
1	1.271886000	6.095102000	-0.253899000
1	-0.502310000	5.893019000	-1.982595000
6	-1.985414000	-1.173918000	2.014074000
6	-1.739506000	-0.785211000	3.330059000
6	-3.301954000	-1.298825000	1.567405000
6	-2.800074000	-0.520783000	4.189858000
6	-4.357895000	-1.038232000	2.431099000
6	-4.110032000	-0.647518000	3.743215000
1	-0.715932000	-0.695863000	3.671779000
1	-3.491374000	-1.593849000	0.543182000
1	-2.600165000	-0.217351000	5.209679000
1	-5.375543000	-1.131696000	2.074170000
1	-4.934916000	-0.439830000	4.412524000
6	1.967680000	1.623526000	1.776325000
6	3.236989000	1.113913000	1.507886000
6	1.678290000	2.110664000	3.052689000
6	4.203188000	1.081576000	2.508206000
6	2.650243000	2.088121000	4.044098000
6	3.913890000	1.570145000	3.776100000
1	3.466905000	0.751783000	0.513601000
1	0.690708000	2.504121000	3.257320000
1	5.184533000	0.680727000	2.289371000
1	2.417443000	2.468233000	5.030803000
1	4.667662000	1.547715000	4.552474000

3h Sn^{II}(Bu^t-L2)$_2$

7	-2.718929000	0.188367000	0.395995000
7	-1.033491000	2.335941000	0.162185000
6	-2.354548000	2.544888000	0.039398000
6	-3.265418000	1.412466000	0.141800000
7	2.957159000	-0.413325000	0.585176000
7	0.325283000	-0.877360000	-0.518146000
6	1.099034000	-1.910138000	0.080860000
6	2.414121000	-1.694713000	0.583490000
50	-0.460387000	0.329866000	1.054030000
6	-3.320830000	-0.984751000	0.198249000
6	-2.862283000	-2.131141000	0.942951000
6	-4.380767000	-1.204008000	-0.759672000
6	-3.456044000	-3.338479000	0.832771000
6	-4.944698000	-2.420014000	-0.922125000
6	-4.554840000	-3.574629000	-0.107020000
1	-2.069293000	-1.982046000	1.665431000
1	-4.656774000	-0.389288000	-1.414301000
1	-3.149219000	-4.177432000	1.444156000
1	-5.686643000	-2.598340000	-1.690235000
6	4.180242000	-0.154474000	0.256094000
6	4.680299000	1.188447000	0.545288000
6	5.101479000	-1.075403000	-0.416281000
6	5.945328000	1.548386000	0.284915000
6	6.358775000	-0.711441000	-0.710540000
6	6.890293000	0.618622000	-0.357246000
1	3.982181000	1.863982000	1.021333000
1	4.725764000	-2.046258000	-0.708432000
1	6.328066000	2.530991000	0.530315000
1	7.036661000	-1.370492000	-1.238812000
8	-5.094721000	-4.672523000	-0.224663000
8	8.044724000	0.935900000	-0.604904000
6	3.097244000	-2.744648000	1.225494000
6	0.563669000	-3.195404000	0.239019000
6	2.529297000	-3.998156000	1.362445000
6	1.255458000	-4.228089000	0.856703000
1	4.064860000	-2.539950000	1.664948000
1	-0.437139000	-3.371125000	-0.128110000
1	3.069313000	-4.782533000	1.877246000
1	0.790446000	-5.200095000	0.962744000
6	-2.984097000	3.807651000	-0.208157000
6	-4.344098000	3.951466000	-0.284884000
6	-4.667405000	1.622851000	0.120557000
6	-5.210369000	2.860721000	-0.087142000
1	-2.380933000	4.686878000	-0.333603000

1	-4.756301000	4.936856000	-0.465971000
1	-5.314747000	0.787668000	0.342880000
1	-6.281775000	3.004479000	-0.060032000
6	-0.032778000	3.444185000	0.159506000
6	0.045660000	4.130309000	-1.221941000
6	1.351622000	2.830273000	0.410014000
1	1.434133000	2.411882000	1.415561000
1	1.581596000	2.044770000	-0.309448000
1	2.116197000	3.603073000	0.318006000
1	0.351584000	3.409948000	-1.981442000
1	0.795271000	4.923451000	-1.191939000
1	-0.891634000	4.571704000	-1.548334000
6	-0.271350000	4.461367000	1.296245000
1	-0.290431000	3.947164000	2.258826000
1	0.548453000	5.182112000	1.317916000
1	-1.197915000	5.020557000	1.202942000
6	0.308758000	-0.815368000	-2.012750000
6	-0.704864000	0.235244000	-2.467707000
6	-0.102842000	-2.160669000	-2.642021000
1	0.612638000	-2.952179000	-2.421177000
1	-1.085372000	-2.475152000	-2.287101000
1	-0.153878000	-2.057105000	-3.728165000
1	-1.717050000	-0.043487000	-2.174910000
1	-0.685337000	0.321018000	-3.555521000
1	-0.485526000	1.214690000	-2.047397000
6	1.697409000	-0.431921000	-2.557979000
1	2.449425000	-1.170414000	-2.276309000
1	1.680580000	-0.380582000	-3.649254000
1	2.013231000	0.539022000	-2.175232000

4h $Sn^{IV}(Bu^t\text{-}L2)_2$

7	1.457985000	1.625114000	-1.070647000
7	-0.501024000	1.492436000	0.824167000
6	-0.064210000	2.769204000	0.430373000
6	0.966783000	2.836896000	-0.559268000
6	-1.699103000	1.202108000	1.463475000
6	-1.769707000	0.062438000	2.304211000
6	-2.882013000	1.961142000	1.259849000
6	-2.925498000	-0.284371000	2.942565000
6	-4.047421000	1.625471000	1.886243000
6	-4.140043000	0.491317000	2.785223000
1	-0.873642000	-0.529246000	2.459604000
1	-2.860138000	2.794025000	0.571305000
8	-5.195996000	0.194621000	3.376487000
7	1.686864000	-1.381718000	1.086531000
7	-0.242427000	-1.539298000	-0.835167000

6	0.400828000	-2.732208000	-0.462486000
6	1.419433000	-2.646561000	0.538074000
6	-1.471643000	-1.444728000	-1.474053000
6	-2.507616000	-2.397929000	-1.286738000
6	-1.734062000	-0.321232000	-2.298325000
6	-3.712974000	-2.256334000	-1.911374000
6	-2.932340000	-0.166549000	-2.934023000
6	-3.997199000	-1.140278000	-2.792489000
1	-2.343813000	-3.226167000	-0.611733000
1	-0.950763000	0.415309000	-2.443838000
8	-5.087907000	-1.018574000	-3.382626000
50	0.722304000	0.060371000	0.013454000
1	-4.511454000	-2.968978000	-1.748819000
1	-3.121354000	0.682717000	-3.577906000
1	-2.969401000	-1.144017000	3.598786000
1	-4.955443000	2.188283000	1.711292000
6	1.420805000	4.110984000	-0.923398000
6	0.911100000	5.265066000	-0.341634000
6	-0.521475000	3.938375000	1.040196000
6	-0.051136000	5.183734000	0.653056000
1	2.185887000	4.219144000	-1.671858000
1	1.288817000	6.227239000	-0.662718000
1	-1.247416000	3.864454000	1.836613000
1	-0.428942000	6.075889000	1.134207000
6	2.089025000	-3.830256000	0.872950000
6	0.156342000	-3.947092000	-1.104540000
6	1.791973000	-5.039649000	0.256875000
6	0.834301000	-5.101328000	-0.743630000
1	2.859298000	-3.822263000	1.623990000
1	-0.567796000	-3.979476000	-1.905399000
1	2.330889000	-5.929248000	0.556439000
1	0.619494000	-6.033047000	-1.249563000
6	2.513088000	1.488051000	-2.111801000
6	2.058502000	2.131343000	-3.436573000
6	2.708637000	-0.009906000	-2.386624000
1	3.049523000	-0.545135000	-1.495187000
1	1.792651000	-0.476507000	-2.754195000
1	3.474652000	-0.152782000	-3.148662000
1	1.132447000	1.669215000	-3.781377000
1	2.820737000	1.972730000	-4.201444000
1	1.885423000	3.200947000	-3.357774000
6	3.867348000	2.051995000	-1.640807000
1	4.205617000	1.525771000	-0.746185000
1	4.620060000	1.908697000	-2.418217000
1	3.830472000	3.112290000	-1.405718000
6	2.673178000	-1.092957000	2.163266000

6	2.585068000	0.404838000	2.489529000
6	4.118874000	-1.385826000	1.718106000
1	4.275985000	-2.423236000	1.434936000
1	4.385471000	-0.764606000	0.860975000
1	4.811985000	-1.152290000	2.528425000
1	2.843050000	1.026326000	1.626249000
1	3.294287000	0.657770000	3.277598000
1	1.590676000	0.682689000	2.843943000
6	2.311160000	-1.854947000	3.452892000
1	2.350416000	-2.934543000	3.338789000
1	3.005173000	-1.578562000	4.248506000
1	1.303385000	-1.590923000	3.776456000

3′h Sn^{II}(Bu^t-L2)$_2$

7	-1.145809000	1.326668000	0.051000000
7	-2.079069000	-0.907839000	-1.278513000
6	-2.937378000	0.091079000	-1.050796000
6	-2.474866000	1.240832000	-0.270610000
7	0.841051000	-1.367316000	0.602700000
7	2.498116000	0.291987000	-0.746361000
6	2.984644000	-0.910013000	-0.438476000
6	2.128619000	-1.787250000	0.348883000
50	0.098514000	-0.103415000	-1.223647000
6	-2.412583000	-2.165822000	-1.995977000
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1	-3.290925000	-3.137488000	-0.257753000
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1	-1.878435000	-1.432369000	-3.971981000
6	-1.171480000	-3.072844000	-1.927758000
1	-0.875226000	-3.260438000	-0.895512000
1	-1.385181000	-4.034746000	-2.394899000
1	-0.322806000	-2.641107000	-2.465039000
6	3.220621000	1.279973000	-1.584444000
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6	3.544902000	0.759931000	-3.001040000
1	4.206694000	-0.102475000	-3.007067000
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1	4.023198000	1.549094000	-3.584879000
1	1.385909000	2.245614000	-2.287466000
1	2.806199000	3.277349000	-2.327311000
1	2.033376000	2.921084000	-0.780828000
6	4.488234000	1.781440000	-0.859728000

1	5.238432000	1.008072000	-0.714205000
1	4.945728000	2.586832000	-1.437798000
1	4.221666000	2.178142000	0.120527000
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6	1.176078000	3.262373000	2.077630000
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1	0.941234000	1.218911000	1.582472000
1	-1.760183000	3.948011000	-0.383443000
1	2.001360000	3.103008000	2.759729000
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6	-1.872683000	-1.905432000	2.974187000
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1	-1.759486000	-1.284225000	0.955656000
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6	4.681764000	-2.681482000	-0.323214000
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