

**Uncovering f-Element Bonding Differences and Electronic Structure in a Series of 1:3 and 1:4
Complexes with a Diselenophosphinate Ligand**

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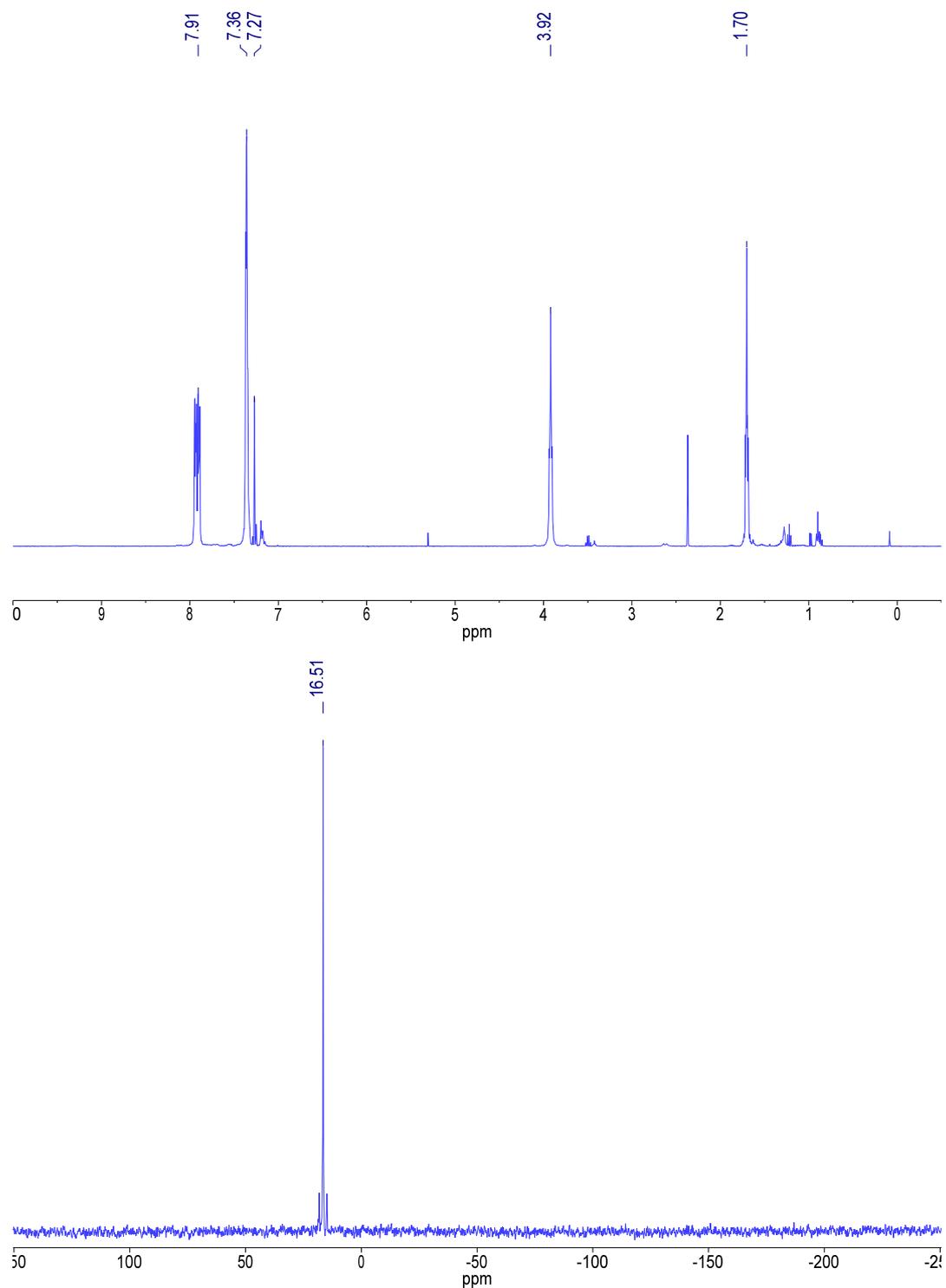
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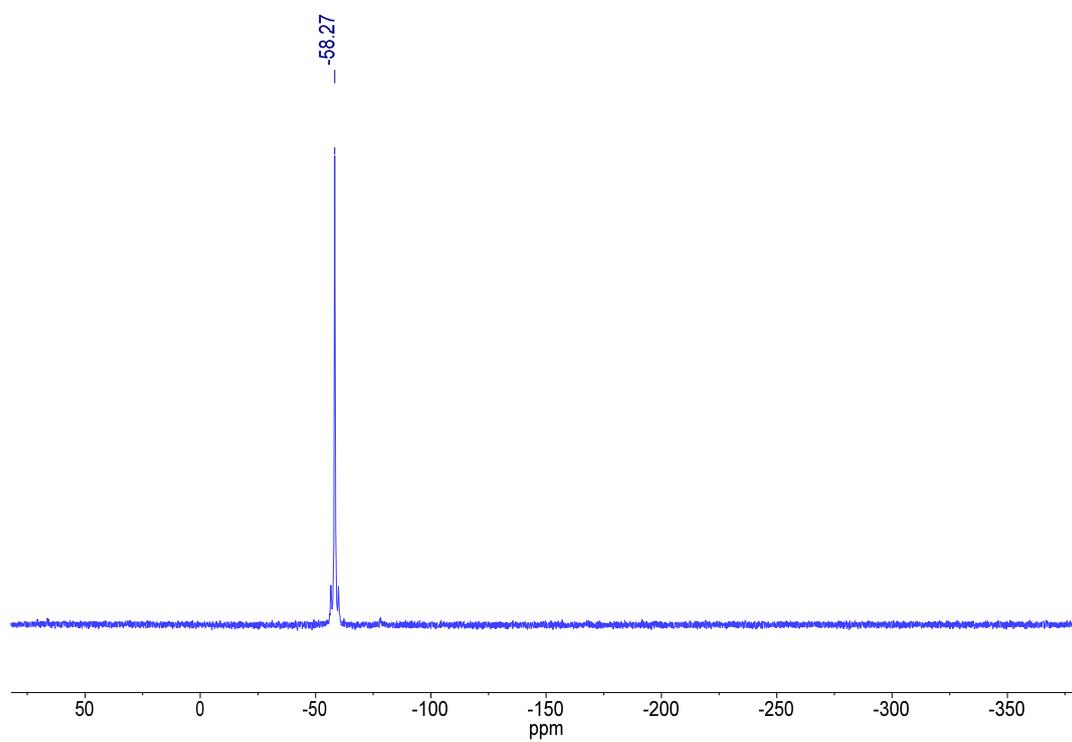
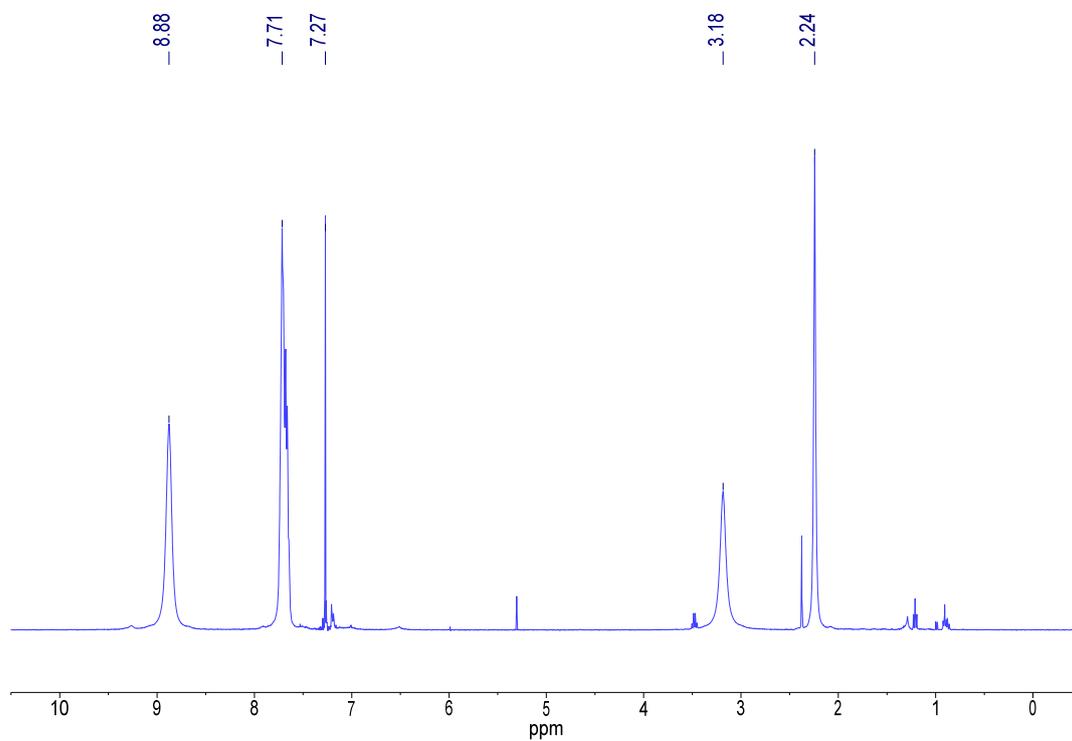
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Spectroscopic Data

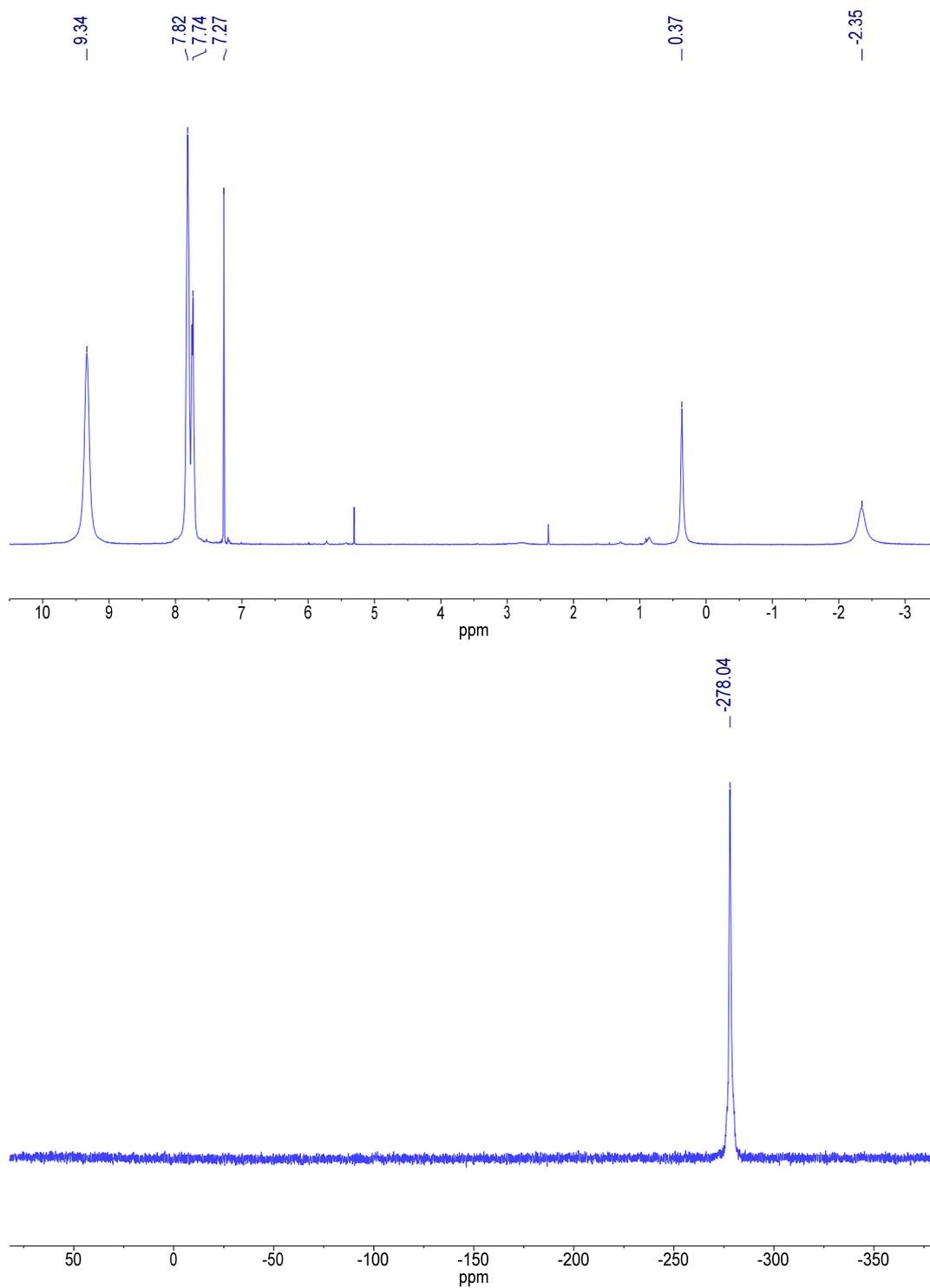
^1H and ^{31}P NMR spectra of $[\text{La}(\text{Se}_2\text{PPh}_2)_3(\text{THF})_2]$ (**1**).



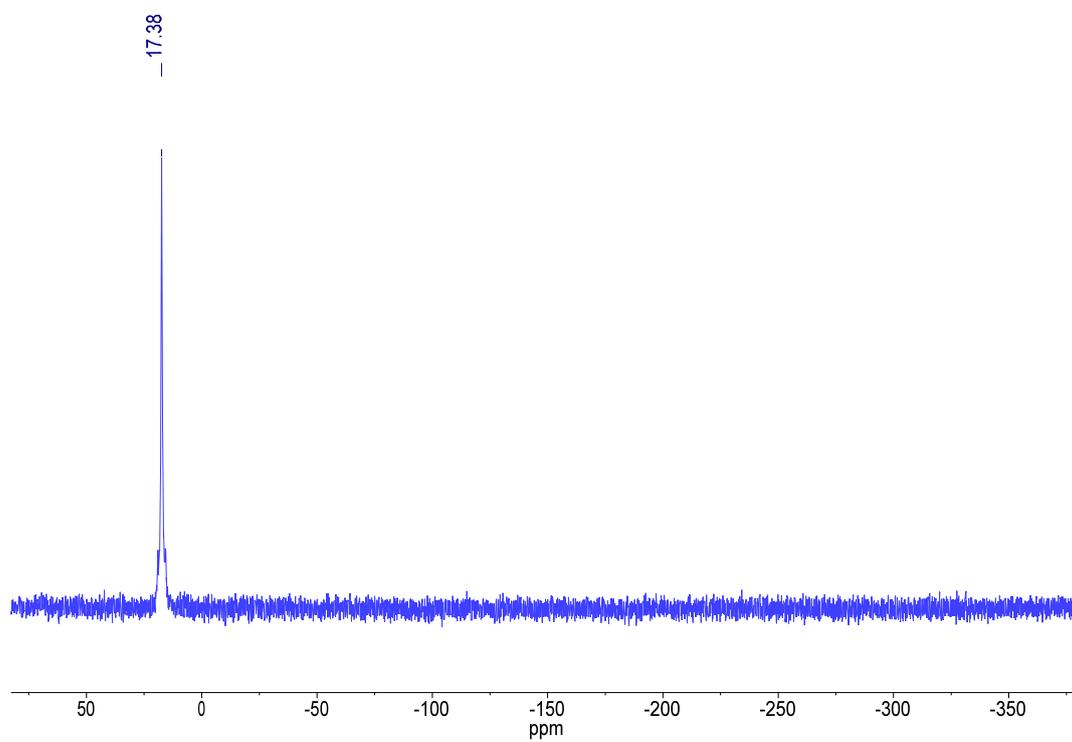
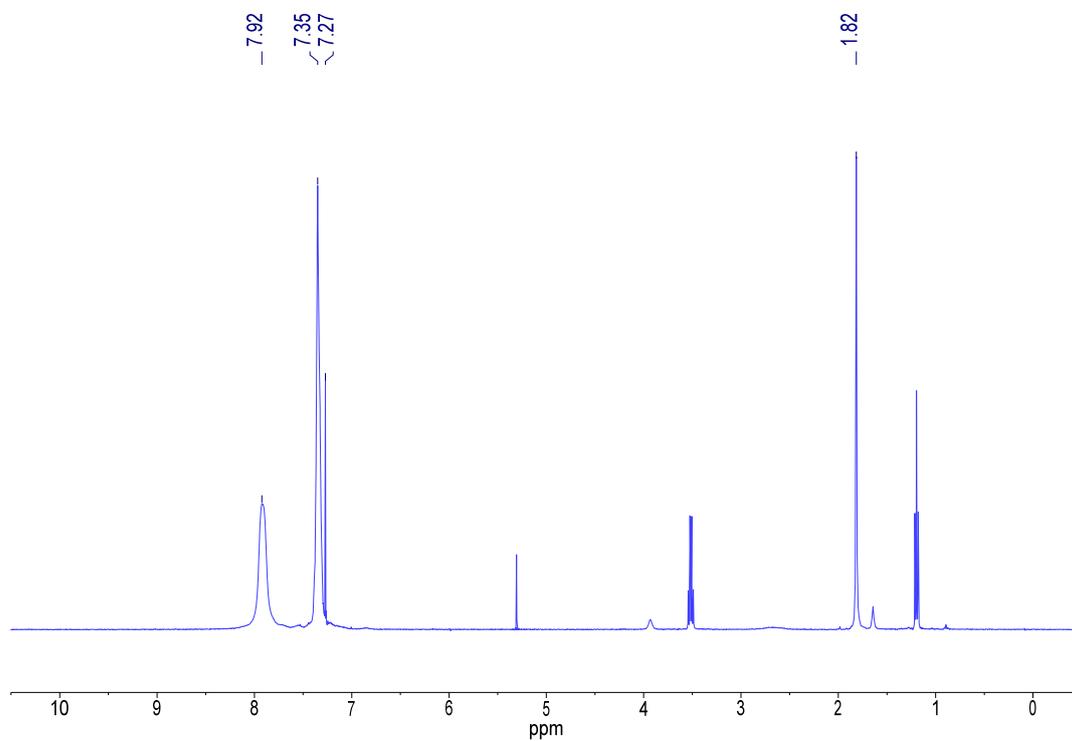
^1H and ^{31}P NMR spectra of $[\text{Ce}(\text{Se}_2\text{PPh}_2)_3(\text{THF})_2]$ (**2**).



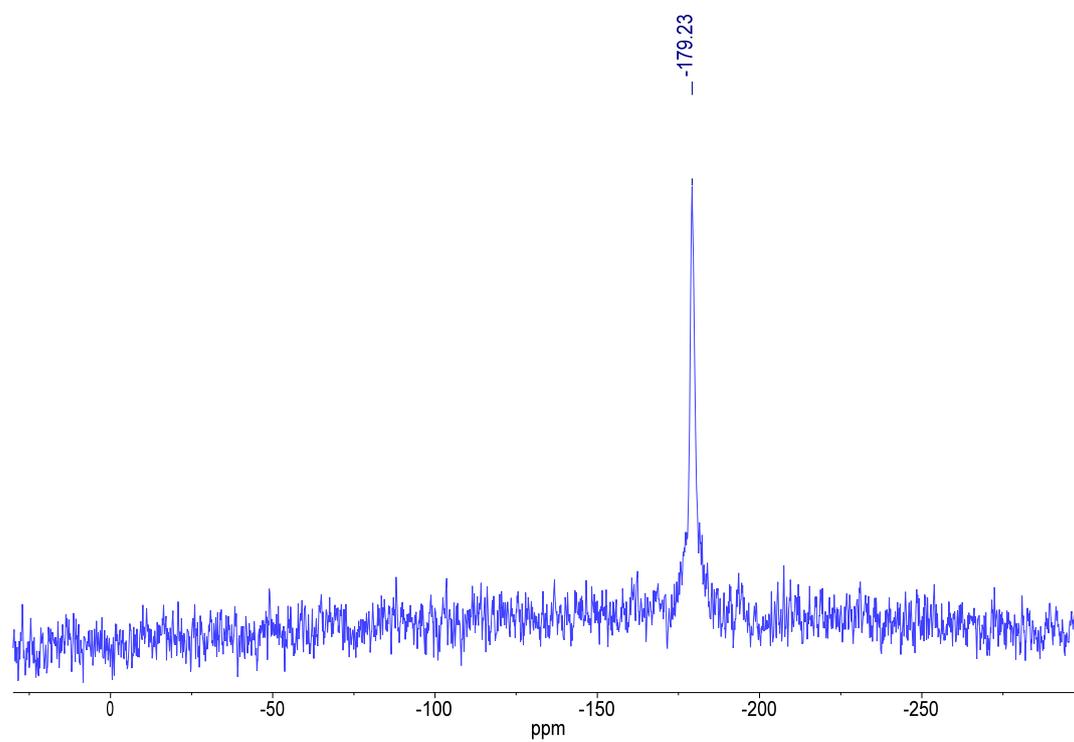
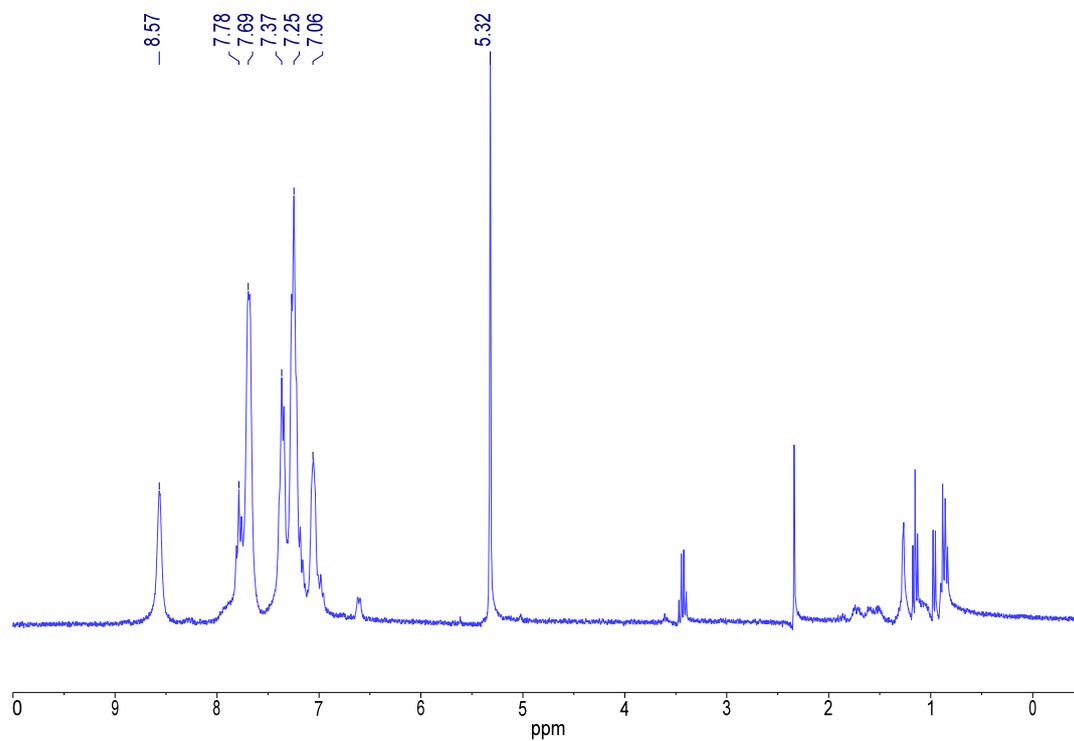
^1H and ^{31}P NMR spectra of $[\text{Nd}(\text{Se}_2\text{PPh}_2)_3(\text{THF})_2]$ (**3**).



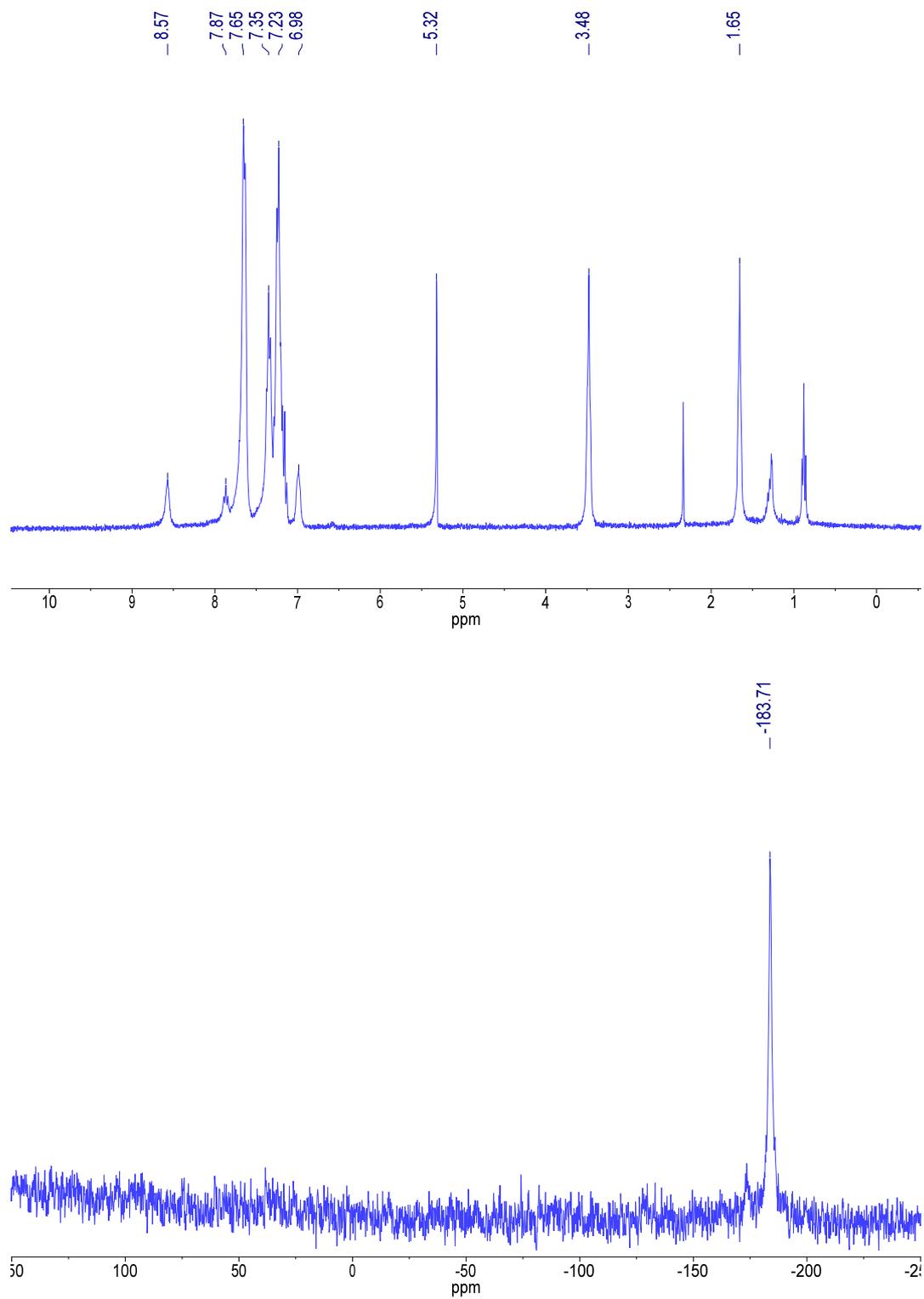
^1H and ^{31}P NMR spectra of $[\text{La}(\text{Se}_2\text{PPh}_2)_3(\text{MeCN})_2]$ (**4**).



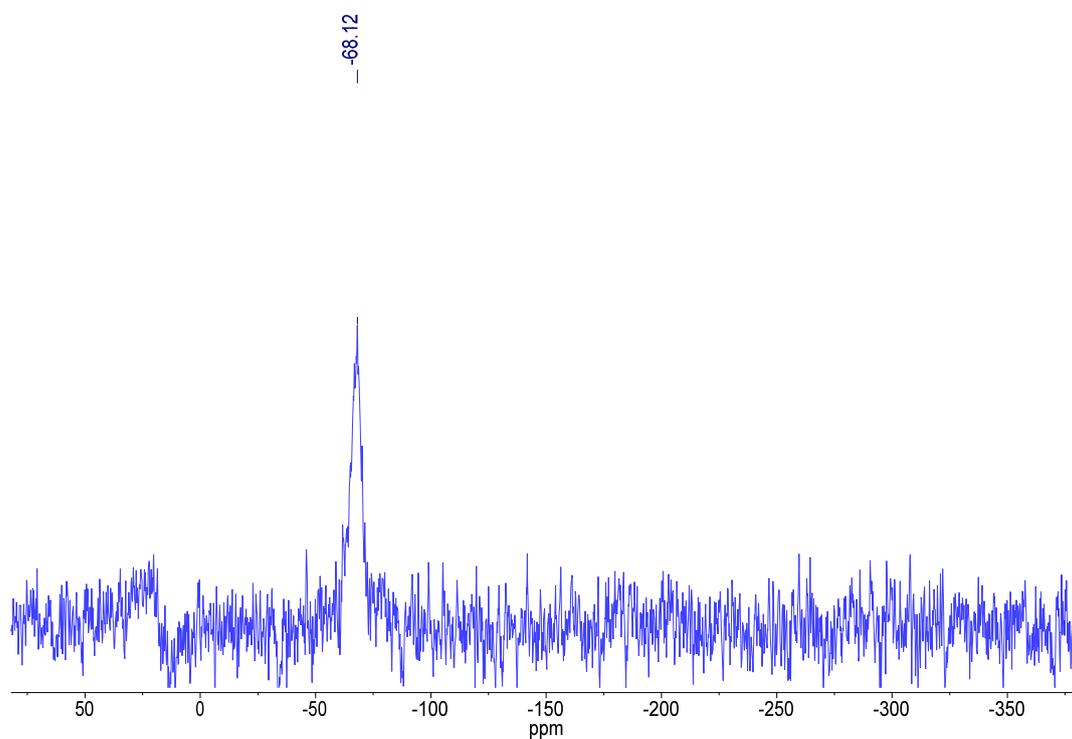
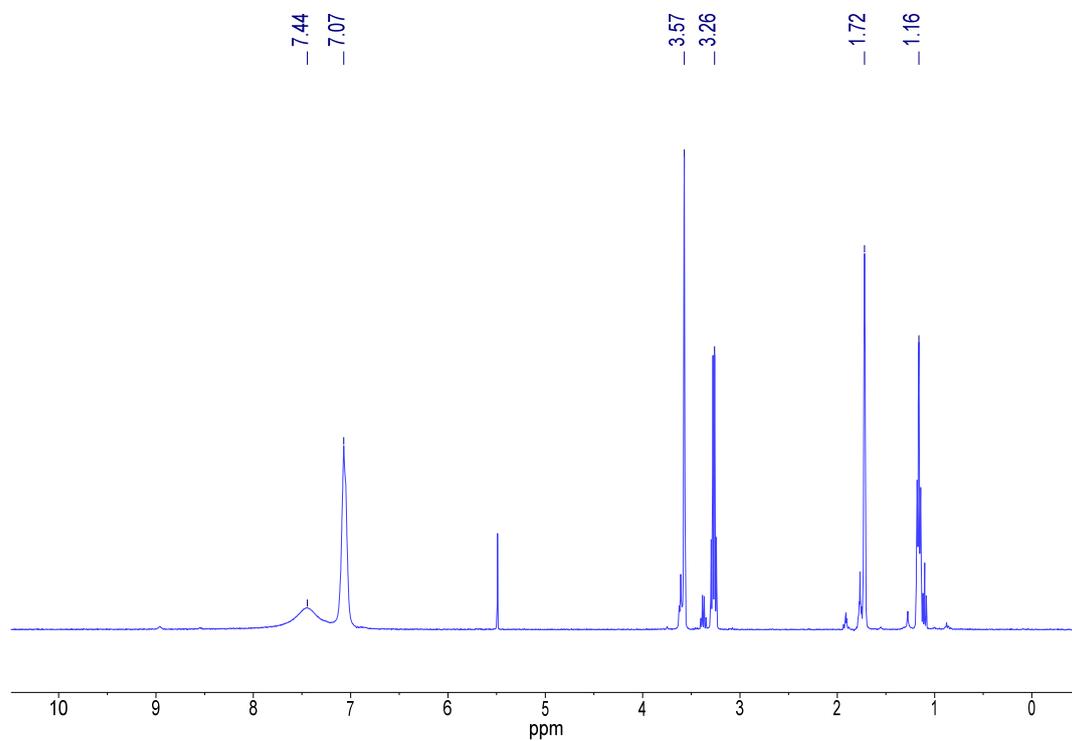
^1H and ^{31}P NMR spectra of $[\text{Pu}(\text{Se}_2\text{PPh}_2)_3(\text{py})_2]$.



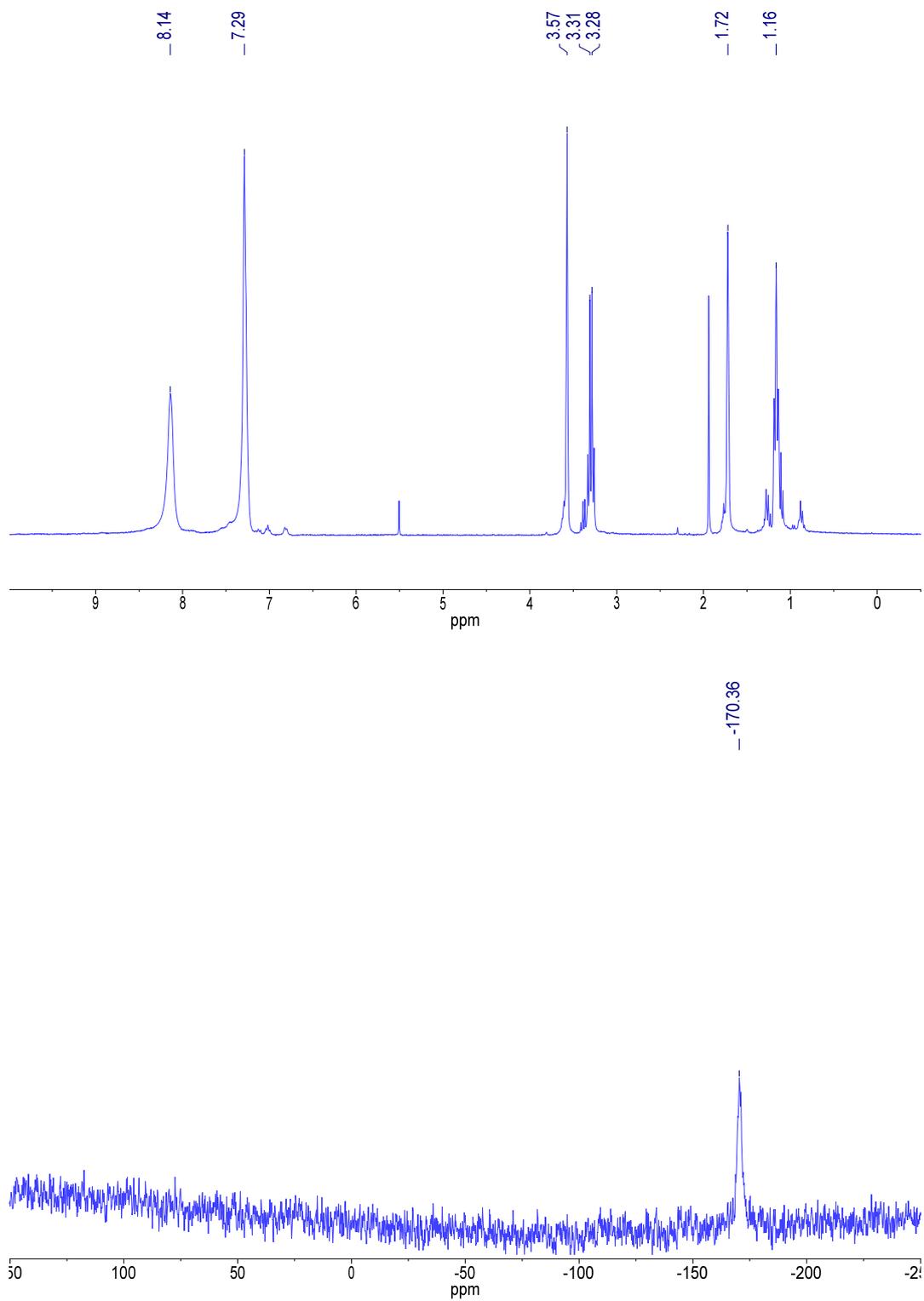
^1H and ^{31}P NMR spectra of $[\text{Pu}(\text{Se}_2\text{PPh}_2)_3(\text{THF})_2]$ (**5**).



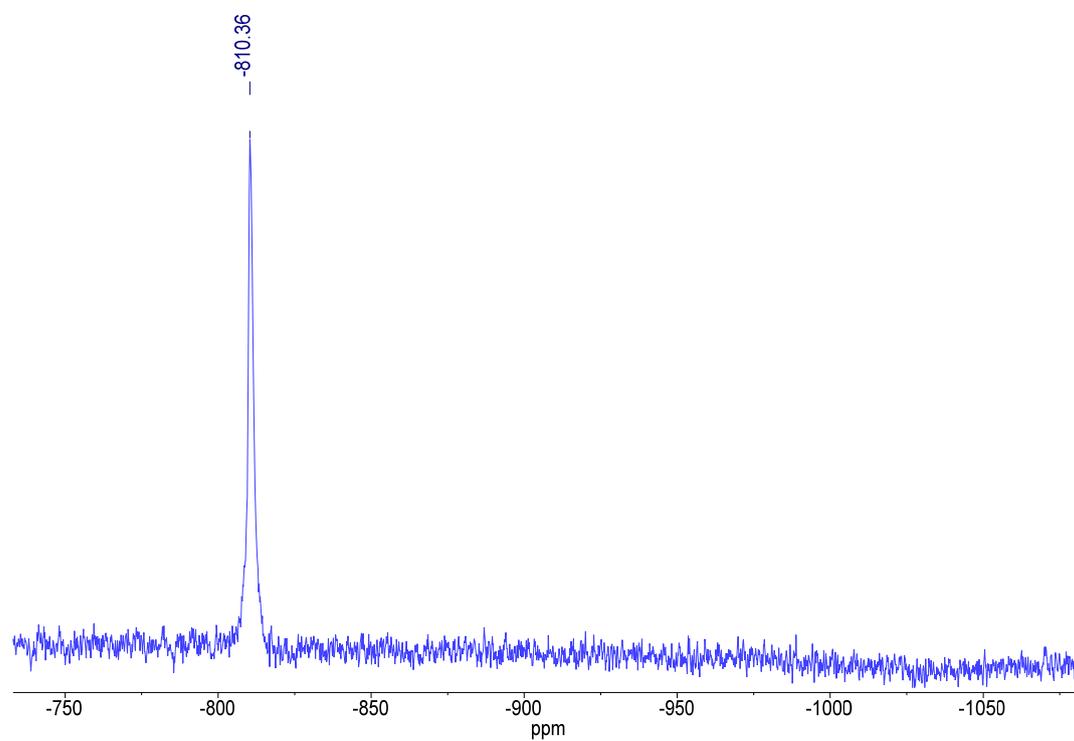
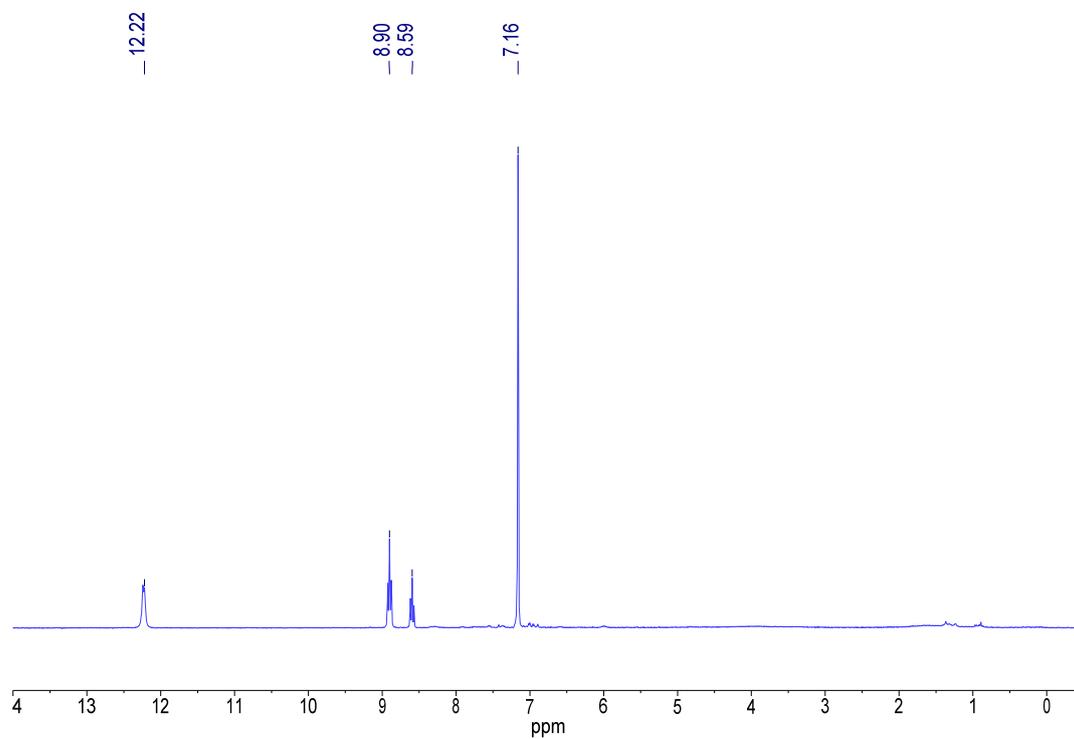
^1H and ^{31}P NMR spectra of $[\text{Et}_4\text{N}][\text{Ce}(\text{Se}_2\text{PPh}_2)_4]$ (**6**).



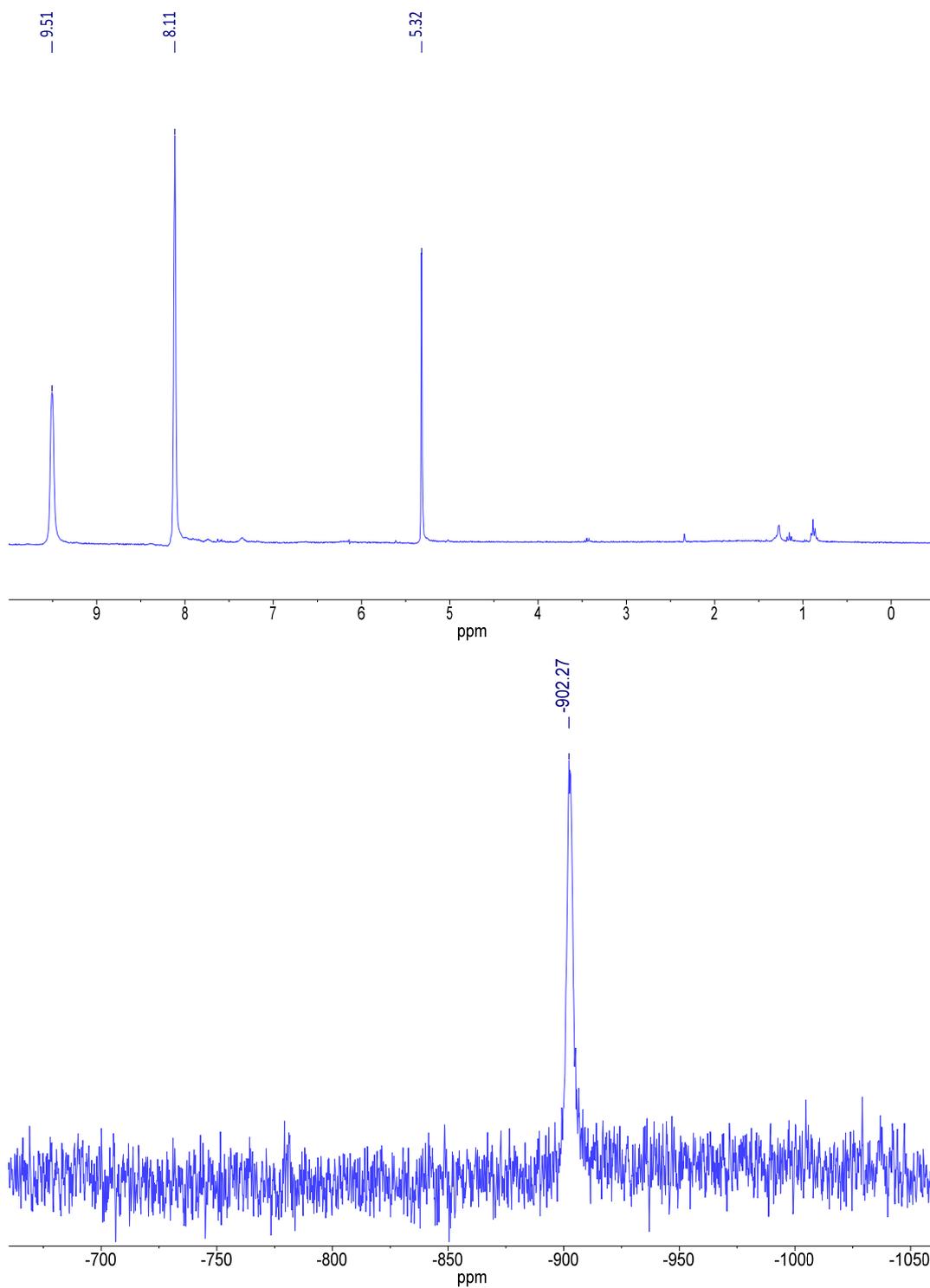
^1H and ^{31}P NMR spectra of $[\text{Et}_4\text{N}][\text{Pu}(\text{Se}_2\text{PPh}_2)_4]$ (**7**).



^1H and ^{31}P NMR spectra of $[\text{U}(\text{Se}_2\text{PPh}_2)_4]$ (**8**).

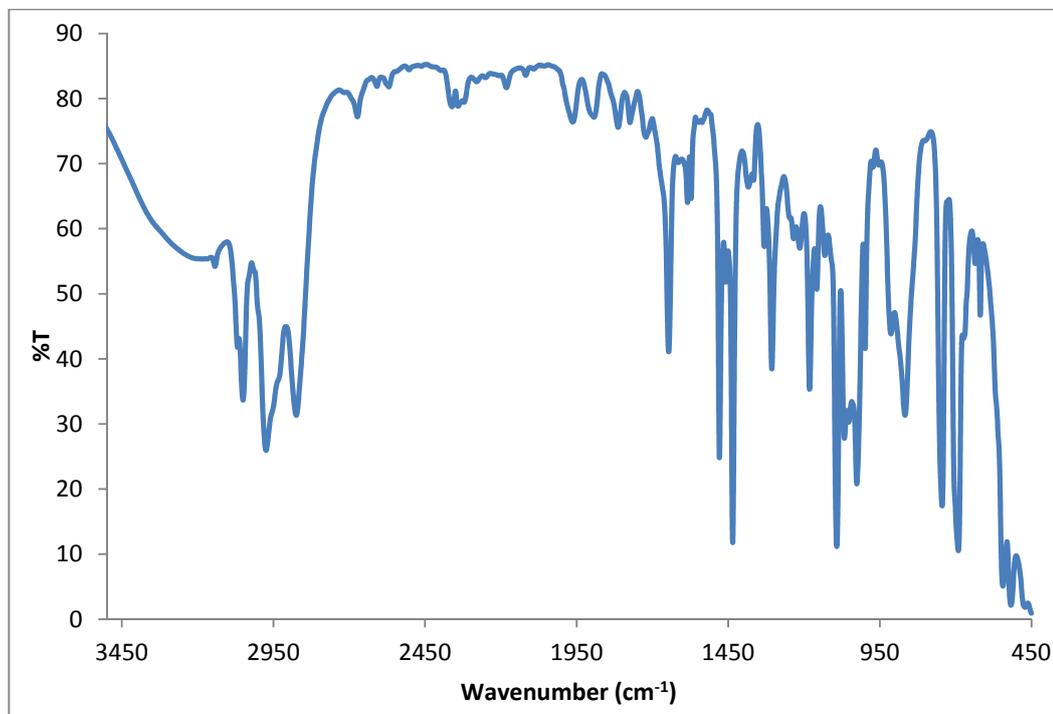


^1H and ^{31}P NMR spectra of $[\text{Np}(\text{Se}_2\text{PPh}_2)_4]$ (**9**).

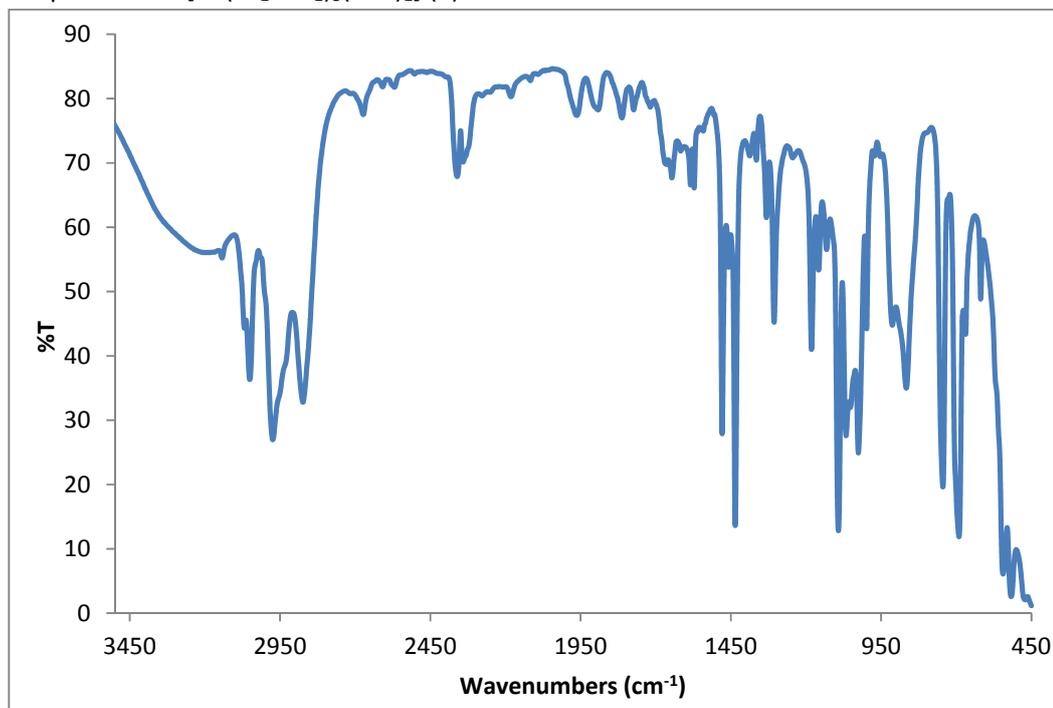


FT-IR Spectra

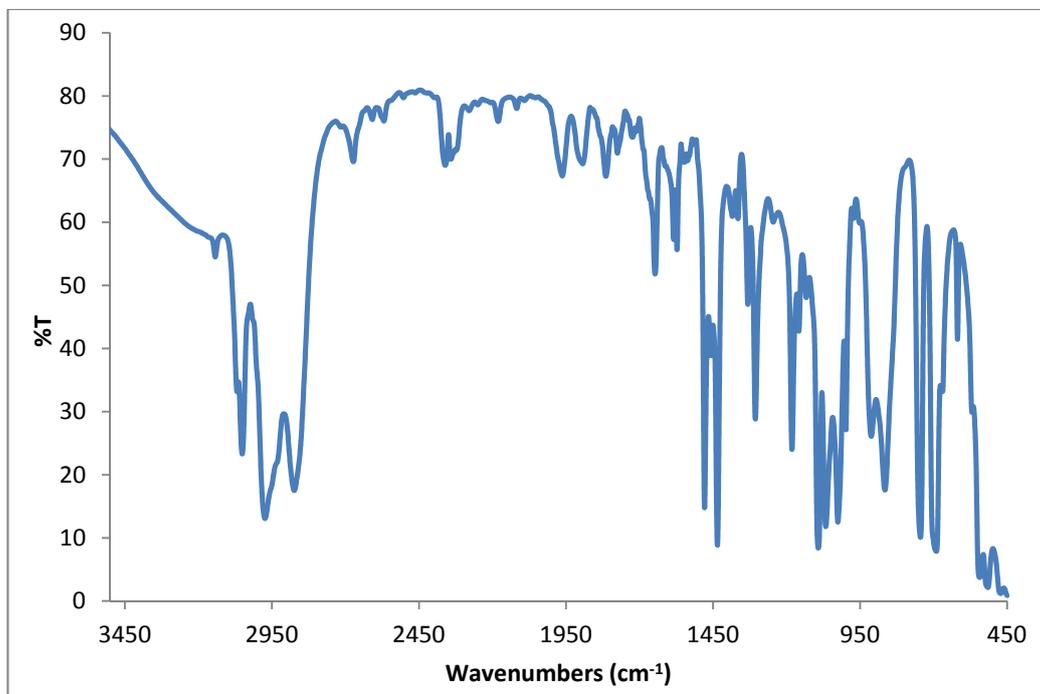
FT-IR spectrum of $[\text{La}(\text{Se}_2\text{PPh}_2)_3(\text{THF})_2]$ (**1**).



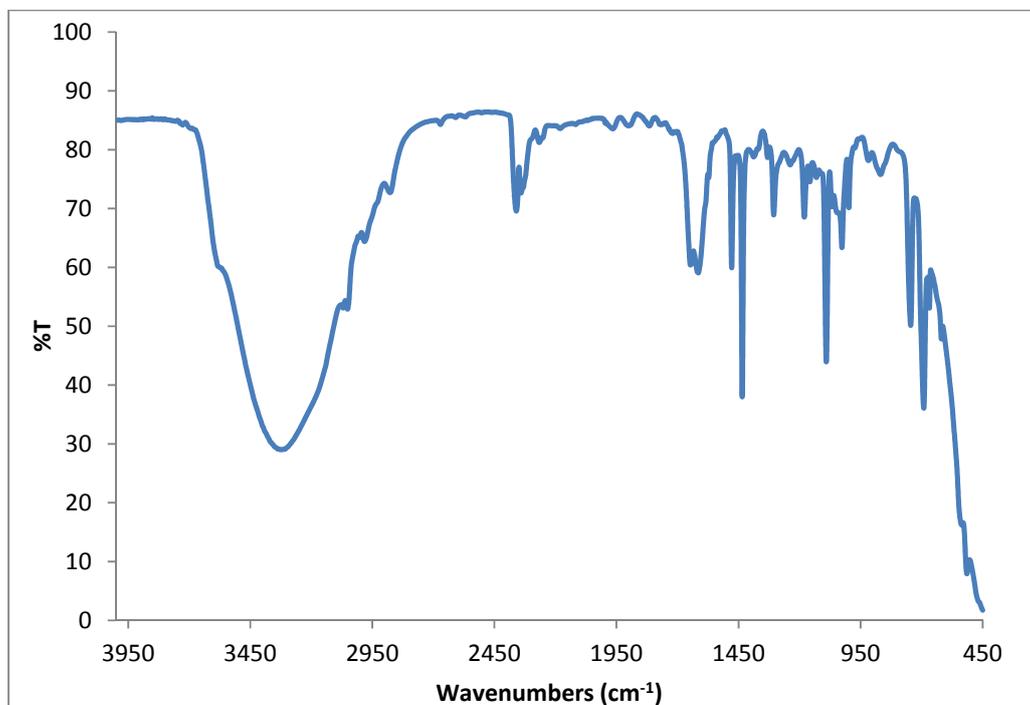
FT-IR spectrum of $[\text{Ce}(\text{Se}_2\text{PPh}_2)_3(\text{THF})_2]$ (**2**).



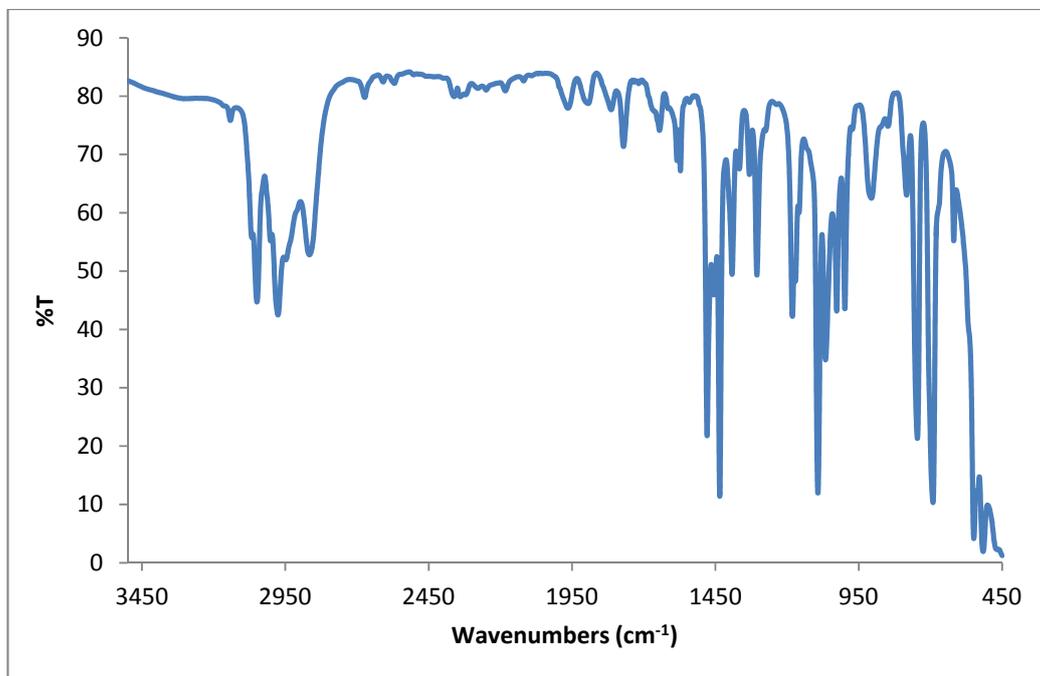
FT-IR spectrum of $[\text{Nd}(\text{Se}_2\text{PPh}_2)_3(\text{THF})_2]$ (**3**).



FT-IR spectrum of $[\text{La}(\text{Se}_2\text{PPh}_2)_3(\text{MeCN})_2]$ (**4**).

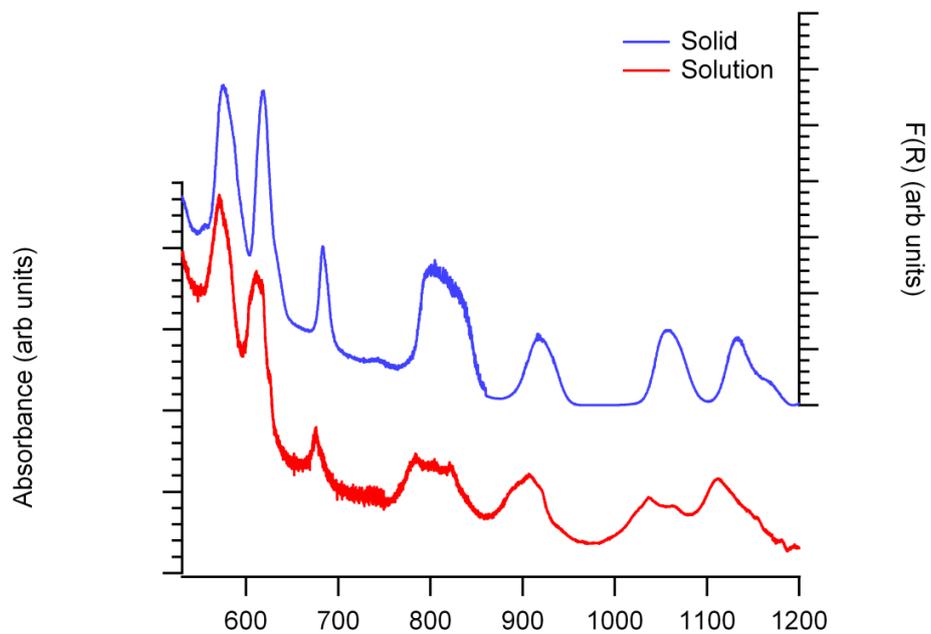


FT-IR spectrum of $[\text{Et}_4\text{N}][\text{Ce}(\text{Se}_2\text{PPh}_2)_4]$ (**6**).

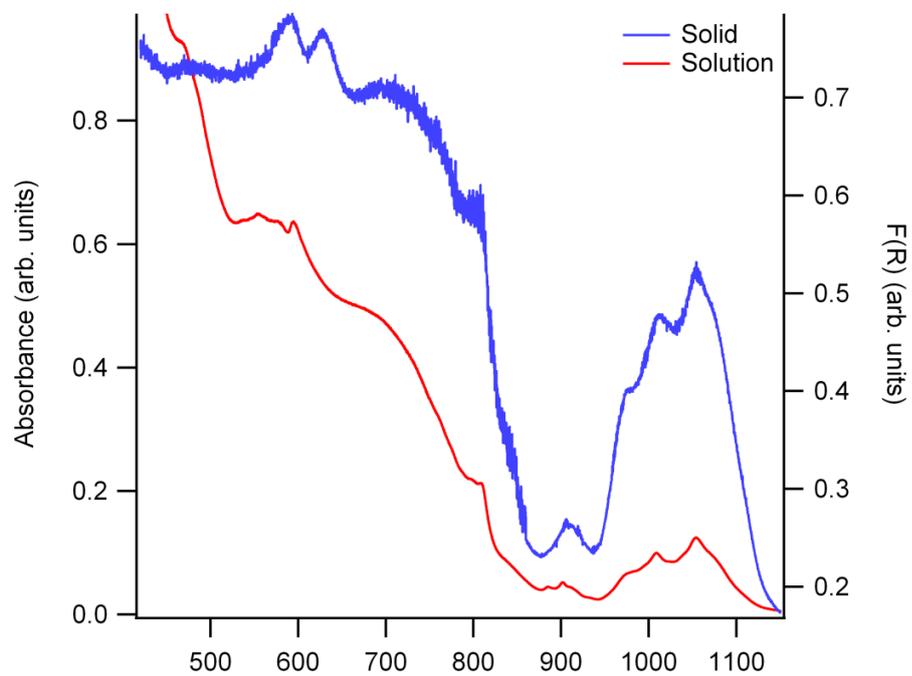


Electronic Absorption Spectra

Visible/near-IR spectrum of $[\text{NEt}_4][\text{Pu}(\text{Se}_2\text{PPh}_2)_4]$ (**7**) in the solid state (top, blue) and in THF solution (bottom, red).



Visible/near-IR spectrum of $\text{Np}(\text{Se}_2\text{PPh}_2)_4$ (**9**) in the solid state (top, blue) and in THF solution (bottom, red).



DFT converged Cartesian atomic coordinates (Bohr)

1a

Atom	Charge	X	Y	Z
La1	57.0	-4.8925009600E-03	-1.1076251800E-01	3.5521182100E-02
Se2	34.0	2.8191671400E+00	-5.2369564600E+00	1.3412123400E+00
Se3	34.0	5.7537209700E+00	4.8458625200E-01	-9.3017233500E-01
Se4	34.0	3.7945133800E-01	4.9308567300E+00	3.1032288900E+00
Se5	34.0	8.4246258700E-01	4.4299961600E+00	-3.7312302300E+00
P6	15.0	6.3862671100E+00	-3.2937189500E+00	6.0262043600E-01
P7	15.0	1.0268941900E+00	6.9127542500E+00	-4.5100770800E-01
O8	8.0	-5.5407148200E-01	-6.7471726700E-01	4.9243522900E+00
O9	8.0	2.0163377800E-03	-1.6893660300E+00	-4.6092007800E+00
C10	6.0	8.2968501500E+00	-3.1544593600E+00	3.4850102600E+00
C11	6.0	8.3300526300E+00	-5.1636520900E+00	-1.5644437900E+00
C12	6.0	-1.2623672900E+00	9.4810319100E+00	-7.8170789200E-01
C13	6.0	1.9836852100E+00	-3.1277178500E+00	-5.8267343100E+00
H14	1.0	3.6507713600E+00	-1.8906936700E+00	-5.9606970000E+00
H15	1.0	2.4398991100E+00	-4.7503122900E+00	-4.6099472200E+00
C16	6.0	9.4023701700E-01	-3.8701213300E+00	-8.4032606200E+00
H17	1.0	-8.5717977400E-03	-5.7202312400E+00	-8.3039290600E+00
H18	1.0	2.4332699500E+00	-3.9887829000E+00	-9.8419677100E+00
C19	6.0	1.4685099600E+00	-8.8467339900E-01	6.7433233000E+00
H20	1.0	2.6399039400E+00	8.3419125500E-01	6.5941880000E+00
H21	1.0	2.6039141100E+00	-2.5465854900E+00	6.2283275700E+00
C22	6.0	1.8449585200E-01	-1.0930043700E+00	9.3054139900E+00
H23	1.0	-2.3798266100E-01	-3.0833073900E+00	9.7464911900E+00
H24	1.0	1.3619275100E+00	-3.2715694700E-01	1.0835005600E+01
Se25	34.0	-3.8235943800E+00	-4.7264223800E+00	1.8661234500E-01
Se26	34.0	-5.5610501600E+00	1.8454555200E+00	-5.4918842900E-01
P27	15.0	-6.9189072000E+00	-2.0356866900E+00	-2.2065954100E-01
C28	6.0	-9.1315894200E+00	-2.3210655700E+00	2.4265028400E+00
C29	6.0	-8.8844982800E+00	-2.8545409300E+00	-2.9501100500E+00
C30	6.0	4.1024726000E+00	8.4850989900E+00	-3.5666124100E-01
C31	6.0	-2.1046994900E+00	-1.4071562200E+00	-6.3057855600E+00
H32	1.0	-2.9367137800E+00	4.6587229400E-01	-5.9730652600E+00
H33	1.0	-3.5128062400E+00	-2.8775218900E+00	-5.8484264800E+00
C34	6.0	-9.9070593300E-01	-1.7902660700E+00	-8.9154387700E+00
H35	1.0	-2.4256184500E+00	-2.3182309800E+00	-1.0321092700E+01

H36	1.0	-4.9161225300E-02	-4.8683124600E-02	-9.5597938000E+00
C37	6.0	-2.9391912100E+00	-3.9451623500E-01	6.2079657800E+00
H38	1.0	-4.0568319400E+00	1.0144408900E+00	5.1660936200E+00
H39	1.0	-3.9219773000E+00	-2.2333312600E+00	6.1538704800E+00
C40	6.0	-2.2581849300E+00	3.7938708800E-01	8.8823383200E+00
H41	1.0	-3.7547989000E+00	-8.5289009600E-02	1.0245439400E+01
H42	1.0	-1.9039822300E+00	2.4292599500E+00	8.9708531000E+00
H43	1.0	4.1607763200E+00	9.7897205600E+00	1.2610123600E+00
H44	1.0	5.5572177900E+00	7.0224264000E+00	-1.2840500100E-01
H45	1.0	4.4105565400E+00	9.5107270700E+00	-2.1384443300E+00
H46	1.0	-3.1609543500E+00	8.6463909000E+00	-8.4219424600E-01
H47	1.0	-8.9290882600E-01	1.0507929900E+01	-2.5512361000E+00
H48	1.0	-1.1104408700E+00	1.0757969000E+01	8.5188287200E-01
H49	1.0	7.2860129600E+00	-2.0058876000E+00	4.8854825200E+00
H50	1.0	1.0121076500E+01	-2.2560665500E+00	3.0505754500E+00
H51	1.0	8.5878188400E+00	-5.0752771600E+00	4.2252311000E+00
H52	1.0	7.3170762800E+00	-5.3422406600E+00	-3.3655909000E+00
H53	1.0	8.6488003000E+00	-7.0519968300E+00	-7.5496070800E-01
H54	1.0	1.0139926500E+01	-4.1896626800E+00	-1.8795934200E+00
H55	1.0	-9.8372396200E+00	-4.2744320100E+00	2.5237216900E+00
H56	1.0	-8.1308395900E+00	-1.8574288200E+00	4.1816256700E+00
H57	1.0	-1.0705090700E+01	-9.8999728500E-01	2.1522506700E+00
H58	1.0	-1.0478752500E+01	-1.5248256900E+00	-3.0670066200E+00
H59	1.0	-7.7334963300E+00	-2.7019474300E+00	-4.6677690600E+00
H60	1.0	-9.5750344500E+00	-4.8046343600E+00	-2.7423384400E+00

2a

Atom	Charge	X	Y	Z
Ce1	58.0	2.7212056300E-04	-1.1398072100E-01	3.2669585400E-02
Se2	34.0	2.8131975000E+00	-5.1796259500E+00	1.4328508300E+00
Se3	34.0	5.6657504400E+00	4.7569698000E-01	-1.0218713000E+00
Se4	34.0	4.1598541400E-01	4.9258451800E+00	3.0088843100E+00
Se5	34.0	8.1821173100E-01	4.3351205700E+00	-3.7919924900E+00
P6	15.0	6.3676892100E+00	-3.2581543000E+00	5.9785454600E-01
P7	15.0	9.9371059700E-01	6.8857727400E+00	-5.6675343400E-01
O8	8.0	-4.9778976800E-01	-5.8702641600E-01	4.9394493100E+00
O9	8.0	-6.9271690900E-02	-1.7378564000E+00	-4.5825499700E+00
C10	6.0	8.3193284400E+00	-3.0300643600E+00	3.4464541800E+00
C11	6.0	8.2912697800E+00	-5.1685351400E+00	-1.5513650000E+00
C12	6.0	-1.3418926400E+00	9.4108852700E+00	-9.1065713400E-01
C13	6.0	1.8574949600E+00	-3.2884012600E+00	-5.7464228400E+00
H14	1.0	3.5590100400E+00	-2.1089494800E+00	-5.9544722400E+00
H15	1.0	2.2804232300E+00	-4.8654400800E+00	-4.4597442200E+00
C16	6.0	7.7018812100E-01	-4.1170027100E+00	-8.2770666000E+00
H17	1.0	-2.5258268500E-01	-5.9193063300E+00	-8.0795259700E+00
H18	1.0	2.2479539600E+00	-4.3687350100E+00	-9.7145340300E+00
C19	6.0	1.5381142400E+00	-7.5226973800E-01	6.7452186900E+00
H20	1.0	2.7216969600E+00	9.5167741900E-01	6.5305344700E+00
H21	1.0	2.6584157000E+00	-2.4378166300E+00	6.2759959200E+00
C22	6.0	2.7757809200E-01	-8.6688540700E-01	9.3253260300E+00
H23	1.0	-1.5375756700E-01	-2.8385614000E+00	9.8363986900E+00
H24	1.0	1.4743435400E+00	-5.8923550500E-02	1.0817894100E+01
Se25	34.0	-3.7699734000E+00	-4.7070980400E+00	3.0726757900E-01
Se26	34.0	-5.4858655200E+00	1.8220172500E+00	-5.7461658400E-01
P27	15.0	-6.8766415900E+00	-2.0366315500E+00	-1.2048704900E-01
C28	6.0	-9.0491009900E+00	-2.2379686400E+00	2.5670172100E+00
C29	6.0	-8.8913428700E+00	-2.9169718100E+00	-2.7939959900E+00
C30	6.0	4.0414325600E+00	8.5144936800E+00	-5.2828994800E-01
C31	6.0	-2.1627518700E+00	-1.4358592700E+00	-6.2900365800E+00
H32	1.0	-2.9095338500E+00	4.8505868300E-01	-6.0415886200E+00
H33	1.0	-3.6353625400E+00	-2.8189233700E+00	-5.7681074500E+00
C34	6.0	-1.0771420100E+00	-1.9871679700E+00	-8.8820019500E+00
H35	1.0	-2.5391097300E+00	-2.5211630000E+00	-1.0257278500E+01
H36	1.0	-6.8003684600E-02	-3.1835838200E-01	-9.6112075800E+00
C37	6.0	-2.8669375300E+00	-2.4761648400E-01	6.2330500000E+00

H38	1.0	-3.9836711900E+00	1.1367968800E+00	5.1574896900E+00
H39	1.0	-3.8652760700E+00	-2.0792883400E+00	6.2481432400E+00
C40	6.0	-2.1592199800E+00	6.0725404400E-01	8.8760927800E+00
H41	1.0	-3.6469503400E+00	1.9744047600E-01	1.0266381300E+01
H42	1.0	-1.7907025900E+00	2.6564957400E+00	8.8942549400E+00
H43	1.0	4.0944204800E+00	9.8430448500E+00	1.0700196300E+00
H44	1.0	5.5245878900E+00	7.0812875900E+00	-2.9627504300E-01
H45	1.0	4.3120300000E+00	9.5204402600E+00	-2.3273489100E+00
H46	1.0	-3.2270645300E+00	8.5445365500E+00	-9.3777848300E-01
H47	1.0	-1.0091062000E+00	1.0417429000E+01	-2.6990712700E+00
H48	1.0	-1.1943900600E+00	1.0715110000E+01	7.0168176900E-01
H49	1.0	7.3198031500E+00	-1.8532298500E+00	4.8315138300E+00
H50	1.0	1.0130279400E+01	-2.1302051200E+00	2.9621854000E+00
H51	1.0	8.6364074800E+00	-4.9287912600E+00	4.2317260900E+00
H52	1.0	7.2524703200E+00	-5.3987056800E+00	-3.3318479500E+00
H53	1.0	8.6352131700E+00	-7.0339348300E+00	-6.9996022900E-01
H54	1.0	1.0090090600E+01	-4.1920135000E+00	-1.9180077700E+00
H55	1.0	-9.7631226700E+00	-4.1841824700E+00	2.7269031600E+00
H56	1.0	-8.0196915700E+00	-1.7331339800E+00	4.2937298900E+00
H57	1.0	-1.0620623700E+01	-9.0704019800E-01	2.2807671600E+00
H58	1.0	-1.0481575800E+01	-1.5831615300E+00	-2.9193623100E+00
H59	1.0	-7.7698414300E+00	-2.8171697000E+00	-4.5347134400E+00
H60	1.0	-9.5879148200E+00	-4.8569514300E+00	-2.5216524400E+00

3a

Atom	Charge	X	Y	Z
Nd1	60.0	1.0777108100E-02	-1.0638591200E-01	1.9277096300E-02
Se2	34.0	2.6995040200E+00	-5.2197372700E+00	1.2206308000E+00
Se3	34.0	5.6550602500E+00	4.8909135900E-01	-8.7629246400E-01
Se4	34.0	4.2272984600E-01	4.8147141600E+00	3.1064792200E+00
Se5	34.0	8.6041309500E-01	4.3670796100E+00	-3.6729473000E+00
P6	15.0	6.3037125300E+00	-3.3267192400E+00	5.5399967200E-01
P7	15.0	1.0645526500E+00	6.8612044200E+00	-4.0568073700E-01
O8	8.0	-5.2735453400E-01	-7.1364184600E-01	4.8144496000E+00
O9	8.0	-5.2398326200E-02	-1.5947833500E+00	-4.5349780000E+00
C10	6.0	8.2189575200E+00	-3.2832366400E+00	3.4365180000E+00
C11	6.0	8.2367436300E+00	-5.1476328800E+00	-1.6639492100E+00
C12	6.0	-1.2255233000E+00	9.4314171500E+00	-7.1300311900E-01
C13	6.0	1.9209538600E+00	-3.0081699900E+00	-5.7965383800E+00
H14	1.0	3.5801995400E+00	-1.7611605100E+00	-5.9327498400E+00
H15	1.0	2.3960877000E+00	-4.6447673100E+00	-4.6065740600E+00
C16	6.0	8.4938276400E-01	-3.7191832300E+00	-8.3702716700E+00
H17	1.0	-8.5313576000E-02	-5.5771638500E+00	-8.2863224800E+00
H18	1.0	2.3251927300E+00	-3.8061578800E+00	-9.8289399400E+00
C19	6.0	1.5143225900E+00	-9.6461448400E-01	6.6077316700E+00
H20	1.0	2.7027562400E+00	7.4253197900E-01	6.4606920800E+00
H21	1.0	2.6233612800E+00	-2.6340325600E+00	6.0620222300E+00
C22	6.0	2.6034945900E-01	-1.1886660800E+00	9.1834756300E+00
H23	1.0	-1.6706501800E-01	-3.1806547500E+00	9.6120957500E+00
H24	1.0	1.4613554500E+00	-4.4305952000E-01	1.0704820400E+01
Se25	34.0	-3.7694726200E+00	-4.6584980600E+00	1.1589501400E-01
Se26	34.0	-5.4476061200E+00	1.8935093600E+00	-4.2909633400E-01
P27	15.0	-6.8729528400E+00	-1.9683765300E+00	-1.8749295800E-01
C28	6.0	-9.0642887100E+00	-2.3018546200E+00	2.4725781400E+00
C29	6.0	-8.8818753400E+00	-2.7000747100E+00	-2.9111117700E+00
C30	6.0	4.1391918700E+00	8.4356032900E+00	-3.1347910900E-01
C31	6.0	-2.1854550400E+00	-1.3101244500E+00	-6.1994147600E+00
H32	1.0	-3.0302419900E+00	5.4918465000E-01	-5.8263658200E+00
H33	1.0	-3.5691257500E+00	-2.8025602300E+00	-5.7406421700E+00
C34	6.0	-1.1023585100E+00	-1.6463388600E+00	-8.8277290200E+00
H35	1.0	-2.5516764100E+00	-2.1651763900E+00	-1.0222061600E+01
H36	1.0	-1.8231699800E-01	1.1144848800E-01	-9.4591602200E+00
C37	6.0	-2.8952777500E+00	-4.4247937400E-01	6.1311257300E+00

H38	1.0	-4.0209536000E+00	9.7878365100E-01	5.1162010700E+00
H39	1.0	-3.8806565500E+00	-2.2797278100E+00	6.0687685500E+00
C40	6.0	-2.1796535900E+00	2.9939309100E-01	8.8049880500E+00
H41	1.0	-3.6623988500E+00	-1.7311025200E-01	1.0180653900E+01
H42	1.0	-1.8150479400E+00	2.3466581300E+00	8.9109809000E+00
H43	1.0	4.2030362700E+00	9.7299353000E+00	1.3123373200E+00
H44	1.0	5.5964088200E+00	6.9731385600E+00	-1.0030477300E-01
H45	1.0	4.4401666600E+00	9.4743460600E+00	-2.0889788600E+00
H46	1.0	-3.1242105200E+00	8.5971975500E+00	-7.7509385000E-01
H47	1.0	-8.6052081000E-01	1.0472554200E+01	-2.4751595100E+00
H48	1.0	-1.0701594700E+00	1.0697017800E+01	9.2911219900E-01
H49	1.0	7.2237464800E+00	-2.1618712600E+00	4.8695483400E+00
H50	1.0	1.0052007000E+01	-2.3930320100E+00	3.0225073500E+00
H51	1.0	8.4928846700E+00	-5.2257995200E+00	4.1249338900E+00
H52	1.0	7.2250806300E+00	-5.2690572400E+00	-3.4704215700E+00
H53	1.0	8.5429019400E+00	-7.0600640800E+00	-9.0766569700E-01
H54	1.0	1.0054170700E+01	-4.1786625800E+00	-1.9501973700E+00
H55	1.0	-9.7871637600E+00	-4.2506989400E+00	2.5255774000E+00
H56	1.0	-8.0459814400E+00	-1.8929670100E+00	4.2309229600E+00
H57	1.0	-1.0629127500E+01	-9.5154891800E-01	2.2462947800E+00
H58	1.0	-1.0466577000E+01	-1.3550451300E+00	-2.9704548400E+00
H59	1.0	-7.7556155700E+00	-2.5125118400E+00	-4.6414338300E+00
H60	1.0	-9.5877787600E+00	-4.6486677100E+00	-2.7440921000E+00

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Atom	Charge	X	Y	Z
Pu1	94.0	7.6760675500E-03	-8.8958857700E-02	2.2831671100E-02
Se2	34.0	3.0772697200E+00	-5.0546167800E+00	1.0804868200E+00
Se3	34.0	5.6095896600E+00	9.3977781300E-01	-6.8581751800E-01
Se4	34.0	-2.2087119000E-01	4.8661525100E+00	3.1146390500E+00
Se5	34.0	5.8331688300E-01	4.4854407200E+00	-3.6017254100E+00
P6	15.0	6.5428214700E+00	-2.9023226500E+00	4.9759323700E-01
P7	15.0	3.1389862800E-01	7.0007172300E+00	-3.5977928900E-01
O8	8.0	-3.3043562200E-01	-7.5790490100E-01	4.7855708000E+00
O9	8.0	1.0597206200E-01	-1.3601606200E+00	-4.5958612000E+00
C10	6.0	8.5129611200E+00	-2.9089707100E+00	3.3443579400E+00
C11	6.0	8.5640725400E+00	-4.4389175500E+00	-1.8542767600E+00
C12	6.0	-2.2681381200E+00	9.2575906900E+00	-7.8941797400E-01
C13	6.0	2.2169794600E+00	-2.4624397600E+00	-5.9396832500E+00
H14	1.0	3.7257972700E+00	-1.0319227500E+00	-6.0018684600E+00
H15	1.0	2.8787993400E+00	-4.1048782200E+00	-4.8512784700E+00
C16	6.0	1.2104489600E+00	-3.1362764200E+00	-8.5494970800E+00
H17	1.0	4.8983591100E-01	-5.0888302800E+00	-8.5729561400E+00
H18	1.0	2.6748393100E+00	-2.9720894500E+00	-1.0012878300E+01
C19	6.0	1.8044541300E+00	-7.6306574300E-01	6.4895274100E+00
H20	1.0	2.7761267400E+00	1.0686023300E+00	6.2834168700E+00
H21	1.0	3.0702834000E+00	-2.2987460200E+00	5.8941710800E+00
C22	6.0	7.0002070000E-01	-1.1295308800E+00	9.1189717200E+00
H23	1.0	5.8075063500E-01	-3.1559692500E+00	9.5804844200E+00
H24	1.0	1.8447997800E+00	-2.0077962200E-01	1.0581582000E+01
Se25	34.0	-3.2710875900E+00	-5.0039324400E+00	-1.8487001800E-01
Se26	34.0	-5.6034782900E+00	1.3401786600E+00	-6.1858295200E-02
P27	15.0	-6.6465126300E+00	-2.6489916400E+00	-2.0799459700E-01
C28	6.0	-8.7280573000E+00	-3.4480339900E+00	2.4398291900E+00
C29	6.0	-8.6259251600E+00	-3.3177751600E+00	-2.9685254300E+00
C30	6.0	3.1521331100E+00	8.9587116100E+00	-1.3165910900E-01
C31	6.0	-2.0587564700E+00	-1.2064691900E+00	-6.2380067500E+00
H32	1.0	-3.0841407600E+00	5.3456761800E-01	-5.7586739400E+00
H33	1.0	-3.2749048400E+00	-2.8588759600E+00	-5.8614315800E+00
C34	6.0	-9.6423464900E-01	-1.2714058500E+00	-8.8826633600E+00
H35	1.0	-2.3573520900E+00	-1.8697385000E+00	-1.0302133000E+01
H36	1.0	-2.5127499400E-01	6.1118656400E-01	-9.4141299300E+00
C37	6.0	-2.6552201700E+00	-8.6265998000E-01	6.2024043100E+00

H38	1.0	-4.0291663500E+00	3.5913300300E-01	5.2368185100E+00
H39	1.0	-3.3416046100E+00	-2.8326144400E+00	6.1770706400E+00
C40	6.0	-1.9433868000E+00	-1.1385600000E-02	8.8432058800E+00
H41	1.0	-3.2824939800E+00	-6.8703072300E-01	1.0279993000E+01
H42	1.0	-1.8767626100E+00	2.0676268400E+00	8.9340393400E+00
H43	1.0	2.9746689300E+00	1.0244942400E+01	1.4920767300E+00
H44	1.0	4.7768232600E+00	7.6983171900E+00	1.4843231900E-01
H45	1.0	3.3943090700E+00	1.0035282900E+01	-1.8936057400E+00
H46	1.0	-4.0391705600E+00	8.1878431800E+00	-9.4579848100E-01
H47	1.0	-1.9503882300E+00	1.0343767500E+01	-2.5334802400E+00
H48	1.0	-2.3590698500E+00	1.0526849800E+01	8.5470234300E-01
H49	1.0	7.4827315600E+00	-1.9497211600E+00	4.8670822500E+00
H50	1.0	1.0274926600E+01	-1.8758498700E+00	2.9541332700E+00
H51	1.0	8.9282870100E+00	-4.8688567000E+00	3.9003286000E+00
H52	1.0	7.5397257000E+00	-4.5151491100E+00	-3.6557942600E+00
H53	1.0	9.0105373400E+00	-6.3697905800E+00	-1.2254193700E+00
H54	1.0	1.0307329800E+01	-3.3309900200E+00	-2.0938883600E+00
H55	1.0	-9.2581330400E+00	-5.4546585800E+00	2.3141850800E+00
H56	1.0	-7.7027996200E+00	-3.1132916800E+00	4.2104742300E+00
H57	1.0	-1.0421206600E+01	-2.2429216200E+00	2.3758014900E+00
H58	1.0	-1.0337686300E+01	-2.1403756300E+00	-2.8822197500E+00
H59	1.0	-7.5572264500E+00	-2.8530083600E+00	-4.6832496900E+00
H60	1.0	-9.1313210800E+00	-5.3345967200E+00	-2.9837282800E+00

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Atom	Charge	X	Y	Z
Th1	90.0	-8.5404865500E-05	9.7565810100E-06	-9.2259949100E-05
Se2	34.0	-3.0017231400E+00	8.8015486500E-01	-4.9157933900E+00
Se3	34.0	-5.5507835500E+00	2.2626783100E-01	1.3249648100E+00
Se4	34.0	8.7884311900E-01	3.0003922700E+00	4.9164819200E+00
Se5	34.0	2.2739169100E-01	5.5508311800E+00	-1.3242951700E+00
Se6	34.0	5.5503368600E+00	-2.2782402400E-01	1.3257528200E+00
Se7	34.0	3.0019753000E+00	-8.7722567400E-01	-4.9161448700E+00
Se8	34.0	-2.2632782400E-01	-5.5502348700E+00	-1.3263341900E+00
Se9	34.0	-8.8022626200E-01	-3.0028222900E+00	4.9154066700E+00
P10	15.0	-6.3511494200E+00	1.4153953400E+00	-2.5637514200E+00
P11	15.0	1.4145604900E+00	6.3503962400E+00	2.5652298600E+00
P12	15.0	6.3511640300E+00	-1.4135959200E+00	-2.5639592900E+00
P13	15.0	-1.4141454100E+00	-6.3519062100E+00	2.5626825100E+00
C14	6.0	-7.3678780200E+00	4.7105672200E+00	-2.6526214600E+00
C15	6.0	-8.9980277600E+00	-3.9428408500E-01	-3.8400592300E+00
C16	6.0	-3.9579027400E-01	8.9968653100E+00	3.8413808200E+00
C17	6.0	4.7096023600E+00	7.3674462400E+00	2.6555285400E+00
C18	6.0	8.9979853300E+00	3.9738559200E-01	-3.8384435100E+00
C19	6.0	7.3682670000E+00	-4.7085925100E+00	-2.6553974700E+00
C20	6.0	3.9679118900E-01	-8.9983589700E+00	3.8380549000E+00
C21	6.0	-4.7089371100E+00	-7.3699372800E+00	2.6520155400E+00
H22	1.0	1.0814262800E-01	-1.0671802800E+01	2.6381166000E+00
H23	1.0	2.4018752400E+00	-8.4665621500E+00	3.8397877800E+00
H24	1.0	-2.2770287400E-01	-9.3833016300E+00	5.7834391400E+00
H25	1.0	-5.8658162800E+00	-5.8075981700E+00	1.9218272500E+00
H26	1.0	-5.2496458900E+00	-7.7879438000E+00	4.6153181600E+00
H27	1.0	-4.9425173300E+00	-9.0531086200E+00	1.4541861700E+00
H28	1.0	5.8058259400E+00	-5.8653940700E+00	-1.9253698100E+00
H29	1.0	9.0517166800E+00	-4.9432936600E+00	-1.4581841600E+00
H30	1.0	7.7855604100E+00	-5.2482780900E+00	-4.6191101600E+00
H31	1.0	8.4666062700E+00	2.4025749700E+00	-3.8391049100E+00
H32	1.0	9.3827817200E+00	-2.2616532300E-01	-5.7841471100E+00
H33	1.0	1.0671380700E+01	1.0775254100E-01	-2.6386677300E+00
H34	1.0	5.2502062000E+00	7.7846044000E+00	4.6190276900E+00
H35	1.0	5.8661546300E+00	5.8051245300E+00	1.9247714400E+00
H36	1.0	4.9437008400E+00	9.0510157000E+00	1.4583549100E+00
H37	1.0	-1.0615468900E-01	1.0670803000E+01	2.6423609200E+00

H38	1.0	2.2829038000E-01	9.3805877000E+00	5.7871297700E+00
H39	1.0	-2.4010699900E+00	8.4658019400E+00	3.8422066300E+00
H40	1.0	-9.0512700100E+00	4.9445162000E+00	-1.4551776000E+00
H41	1.0	-5.8053281200E+00	5.8667261500E+00	-1.9217472100E+00
H42	1.0	-7.7851921600E+00	5.2518950100E+00	-4.6158806200E+00
H43	1.0	-9.3822479600E+00	2.3070233900E-01	-5.7854132300E+00
H44	1.0	-8.4669908000E+00	-2.3995203000E+00	-3.8420188700E+00
H45	1.0	-1.0671671400E+01	-1.0524033500E-01	-2.6404875300E+00

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Atom	Charge	X	Y	Z
Pa1	91.0	1.0411137600E-04	1.0208651300E-04	-8.6877772900E-05
Se2	34.0	2.3767268000E+00	1.9112688100E+00	-4.9040603600E+00
Se3	34.0	3.0192727300E+00	4.5845220300E+00	1.2239397600E+00
Se4	34.0	1.9111082600E+00	-2.3756418900E+00	4.9045045500E+00
Se5	34.0	4.5840233500E+00	-3.0200756800E+00	-1.2234861300E+00
Se6	34.0	-3.0201020000E+00	-4.5837472300E+00	1.2238282700E+00
Se7	34.0	-2.3751844000E+00	-1.9115124100E+00	-4.9044931100E+00
Se8	34.0	-4.5841949000E+00	3.0193557500E+00	-1.2243100500E+00
Se9	34.0	-1.9116710700E+00	2.3762334000E+00	4.9040982600E+00
P10	15.0	4.5198698500E+00	4.6187448900E+00	-2.6415819700E+00
P11	15.0	4.6184426500E+00	-4.5194501300E+00	2.6425023700E+00
P12	15.0	-4.5190814700E+00	-4.6186578400E+00	-2.6422981800E+00
P13	15.0	-4.6193890100E+00	4.5190098300E+00	2.6415669500E+00
C14	6.0	7.8793582200E+00	3.8344774700E+00	-2.6779610900E+00
C15	6.0	4.3074935800E+00	7.7834248500E+00	-4.0036852300E+00
C16	6.0	7.7832378600E+00	-4.3066770100E+00	4.0042787000E+00
C17	6.0	3.8341922400E+00	-7.8789422800E+00	2.6799605200E+00
C18	6.0	-4.3058756000E+00	-7.7835569600E+00	-4.0037551500E+00
C19	6.0	-7.8786114000E+00	-3.8346323100E+00	-2.6802457700E+00
C20	6.0	-7.7842332900E+00	4.3052540500E+00	4.0030692800E+00
C21	6.0	-3.8362516600E+00	7.8787626900E+00	2.6788191200E+00
H22	1.0	-9.1147842500E+00	5.3889705000E+00	2.8286082700E+00
H23	1.0	-8.3378804400E+00	2.3061892300E+00	4.0367952200E+00
H24	1.0	-7.7520673100E+00	5.0560368300E+00	5.9416826300E+00
H25	1.0	-1.9254555300E+00	8.0839556400E+00	1.8923510100E+00
H26	1.0	-3.8703567200E+00	8.5764397500E+00	4.6368513000E+00
H27	1.0	-5.2050383200E+00	8.9187086400E+00	1.5092657300E+00
H28	1.0	-8.0834301900E+00	-1.9237265500E+00	-1.8939534000E+00
H29	1.0	-8.9191734300E+00	-5.2030637300E+00	-1.5108246600E+00
H30	1.0	-8.5759029600E+00	-3.8686806500E+00	-4.6384140000E+00
H31	1.0	-2.3069600300E+00	-8.3377710400E+00	-4.0369840900E+00
H32	1.0	-5.0561859600E+00	-7.7512019700E+00	-5.9425461300E+00
H33	1.0	-5.3902421400E+00	-9.1138056100E+00	-2.8295530300E+00
H34	1.0	3.8679023400E+00	-8.5764927500E+00	4.6380456000E+00
H35	1.0	1.9233847300E+00	-8.0835248500E+00	1.8933601300E+00
H36	1.0	5.2027238200E+00	-8.9194362800E+00	1.5105998800E+00
H37	1.0	9.1135205200E+00	-5.3907997700E+00	2.8298895000E+00

H38	1.0	7.7506977200E+00	-5.0574730500E+00	5.9428826000E+00
H39	1.0	8.3375332000E+00	-2.3077935600E+00	4.0380745600E+00
H40	1.0	8.9195063900E+00	5.2029882300E+00	-1.5082659700E+00
H41	1.0	8.0836970100E+00	1.9236623800E+00	-1.8913210100E+00
H42	1.0	8.5775209600E+00	3.8682008300E+00	-4.6358231900E+00
H43	1.0	5.0587488300E+00	7.7507071000E+00	-5.9421039400E+00
H44	1.0	2.3086290300E+00	8.3377598800E+00	-4.0379743100E+00
H45	1.0	5.3913706700E+00	9.1138019700E+00	-2.8291769700E+00

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Atom	Charge	X	Y	Z
U1	92.0	-2.2364986400E-05	6.4469333200E-04	-6.6266142400E-05
Se2	34.0	-1.2697474800E+00	-2.7504795900E+00	4.8884171300E+00
Se3	34.0	-3.7414030000E+00	-3.9378106600E+00	-1.2071326100E+00
Se4	34.0	2.7523495600E+00	-1.2713224500E+00	-4.8875821300E+00
Se5	34.0	3.9366839600E+00	-3.7423146100E+00	1.2087537500E+00
Se6	34.0	3.7431994800E+00	3.9371486400E+00	-1.2088295900E+00
Se7	34.0	1.2700235400E+00	2.7539495100E+00	4.8866559100E+00
Se8	34.0	-3.9383000900E+00	3.7420214300E+00	1.2072211800E+00
Se9	34.0	-2.7516233600E+00	1.2695972200E+00	-4.8875840200E+00
P10	15.0	-3.4229786900E+00	-5.4559855100E+00	2.6434980800E+00
P11	15.0	5.4563906400E+00	-3.4249986800E+00	-2.6413421500E+00
P12	15.0	3.4241098300E+00	5.4579752100E+00	2.6407126200E+00
P13	15.0	-5.4581184400E+00	3.4215591900E+00	-2.6425761400E+00
C14	6.0	-1.8967379800E+00	-8.5502652100E+00	2.6429160400E+00
C15	6.0	-6.5488419100E+00	-5.9846529100E+00	4.0095489700E+00
C16	6.0	5.9846194000E+00	-6.5512112200E+00	-4.0068450300E+00
C17	6.0	8.5511534700E+00	-1.8997485100E+00	-2.6401516200E+00
C18	6.0	6.5497182000E+00	5.9870377300E+00	4.0072019300E+00
C19	6.0	1.8980732700E+00	8.5523398200E+00	2.6380462200E+00
C20	6.0	-5.9897929500E+00	6.5465815600E+00	-4.0095133200E+00
C21	6.0	-8.5513111600E+00	1.8930198600E+00	-2.6407128700E+00
H22	1.0	-7.3397693100E+00	7.5981177300E+00	-2.8279318200E+00
H23	1.0	-4.1718290300E+00	7.5445517300E+00	-4.0642851400E+00
H24	1.0	-6.7304750500E+00	6.3359388300E+00	-5.9408361000E+00
H25	1.0	-8.3079250500E+00	-1.0353057900E-02	-1.8472830100E+00
H26	1.0	-9.2566916500E+00	1.7568432500E+00	-4.5915848700E+00
H27	1.0	-9.8660967700E+00	2.9940324800E+00	-1.4650386600E+00
H28	1.0	-5.3969693100E-03	8.3103956300E+00	1.8444784000E+00
H29	1.0	3.0003210300E+00	9.8660021100E+00	1.4623039700E+00
H30	1.0	1.7623258600E+00	9.2580752900E+00	4.5888161700E+00
H31	1.0	7.5457242400E+00	4.1680111900E+00	4.0626937400E+00
H32	1.0	6.3399454800E+00	6.7288304200E+00	5.9381902400E+00
H33	1.0	7.6025156400E+00	7.3353843300E+00	2.8248966700E+00
H34	1.0	9.2565083900E+00	-1.7650855600E+00	-4.5911275600E+00
H35	1.0	8.3099106500E+00	4.1483491400E-03	-1.8473831700E+00
H36	1.0	9.8647270500E+00	-3.0018412600E+00	-1.4641920600E+00
H37	1.0	7.3331097900E+00	-7.6037536400E+00	-2.8244811800E+00

H38	1.0	6.7259447600E+00	-6.3423017900E+00	-5.9381073400E+00
H39	1.0	4.1654512600E+00	-7.5470130800E+00	-4.0615166900E+00
H40	1.0	-2.9987443000E+00	-9.8646004000E+00	1.4677312600E+00
H41	1.0	6.8303377800E-03	-8.3085988800E+00	1.8494956300E+00
H42	1.0	-1.7612166400E+00	-9.2549177200E+00	4.5940922900E+00
H43	1.0	-6.3393839800E+00	-6.7252265200E+00	5.9410380500E+00
H44	1.0	-7.5451693000E+00	-4.1657622100E+00	4.0637255300E+00
H45	1.0	-7.6010994800E+00	-7.3338918100E+00	2.8278068500E+00

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Atom	Charge	X	Y	Z
Np1	93.0	5.0814735700E-02	-1.8632699700E-02	-7.1242675200E-04
Se2	34.0	-2.6534173800E+00	1.3460122400E+00	4.9103078500E+00
Se3	34.0	-3.7269254400E+00	3.9179918700E+00	-1.1365890100E+00
Se4	34.0	-1.2692950300E+00	-2.8337501600E+00	-4.8365594000E+00
Se5	34.0	-4.0415837400E+00	-3.6243907900E+00	1.1946073800E+00
Se6	34.0	3.6756817300E+00	-4.0568640600E+00	-1.1124798800E+00
Se7	34.0	2.8168560100E+00	-1.1816287400E+00	4.8559215300E+00
Se8	34.0	3.9831118300E+00	3.7396697500E+00	1.0500849100E+00
Se9	34.0	1.2240738800E+00	2.6448607000E+00	-4.9146693400E+00
P10	15.0	-5.2646258300E+00	3.6592089900E+00	2.7067454500E+00
P11	15.0	-3.7428596100E+00	-5.2694578600E+00	-2.6004389000E+00
P12	15.0	5.3378565000E+00	-3.6159115900E+00	2.6675959900E+00
P13	15.0	3.5651705500E+00	5.2921289000E+00	-2.7783471700E+00
C14	6.0	-8.4406129500E+00	2.3115300100E+00	2.7198147900E+00
C15	6.0	-5.6081459100E+00	6.7956970600E+00	4.1077128100E+00
C16	6.0	-6.8482049900E+00	-5.5432942900E+00	-4.0835356600E+00
C17	6.0	-2.5042159400E+00	-8.4879052400E+00	-2.4826655000E+00
C18	6.0	5.7147415900E+00	-6.6828482800E+00	4.2054664600E+00
C19	6.0	8.5118575200E+00	-2.2730136200E+00	2.5139329100E+00
C20	6.0	6.6471891500E+00	5.6965983200E+00	-4.2787387000E+00
C21	6.0	2.1542934600E+00	8.4394054200E+00	-2.7264571800E+00
H22	1.0	7.7985236900E+00	7.0095346900E+00	-3.1496159900E+00
H23	1.0	7.5719587600E+00	3.8415278800E+00	-4.3648251700E+00
H24	1.0	6.3844567500E+00	6.4377753700E+00	-6.2035060200E+00
H25	1.0	2.7671070800E-01	8.2685212600E+00	-1.8557639700E+00
H26	1.0	1.9666417700E+00	9.1467790400E+00	-4.6723025100E+00
H27	1.0	3.3512724500E+00	9.7130600400E+00	-1.6003788300E+00
H28	1.0	8.3592734700E+00	-4.0413305100E-01	1.6218517800E+00
H29	1.0	9.7291246000E+00	-3.5116213800E+00	1.3705994700E+00
H30	1.0	9.2751103400E+00	-2.0744638700E+00	4.4374662400E+00
H31	1.0	3.8423650300E+00	-7.5634890100E+00	4.3558338500E+00
H32	1.0	6.5150595000E+00	-6.4083693400E+00	6.1046506700E+00
H33	1.0	6.9696633600E+00	-7.8802524600E+00	3.0584197000E+00
H34	1.0	-2.3684013200E+00	-9.2510616900E+00	-4.4117489600E+00
H35	1.0	-6.1464287300E-01	-8.4004770600E+00	-1.6264683900E+00
H36	1.0	-3.7595477800E+00	-9.6676064600E+00	-1.3181822400E+00
H37	1.0	-8.0638658100E+00	-6.7638362800E+00	-2.9187254800E+00

H38	1.0	-6.6354426100E+00	-6.3433778800E+00	-5.9908135700E+00
H39	1.0	-7.6706572700E+00	-3.6428269600E+00	-4.2103154900E+00
H40	1.0	-9.6983390800E+00	3.5017796900E+00	1.5686730000E+00
H41	1.0	-8.3155811100E+00	4.0701488400E-01	1.9018600600E+00
H42	1.0	-9.1362608200E+00	2.1950510700E+00	4.6755490600E+00
H43	1.0	-6.3448254100E+00	6.6097139900E+00	6.0432024400E+00
H44	1.0	-3.7364704400E+00	7.6891614600E+00	4.1561143700E+00
H45	1.0	-6.9056545500E+00	7.9331062100E+00	2.9469617600E+00

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Atom	Charge	X	Y	Z
Pu1	94.0	-4.1655881800E-05	-3.0322223300E-05	-5.8756063100E-04
Se2	34.0	3.0025948400E+00	-4.2150183700E-01	4.9007913300E+00
Se3	34.0	4.3785748500E+00	-3.2682163400E+00	-9.6394915600E-01
Se4	34.0	4.2163600900E-01	3.0034659600E+00	-4.9005359300E+00
Se5	34.0	3.2683275100E+00	4.3778056900E+00	9.6476769600E-01
Se6	34.0	-4.3784333200E+00	3.2679742400E+00	-9.6448016900E-01
Se7	34.0	-3.0035796300E+00	4.2106342600E-01	4.9007251900E+00
Se8	34.0	-3.2682142600E+00	-4.3777076400E+00	9.6435195600E-01
Se9	34.0	-4.2163608200E-01	-3.0030674200E+00	-4.9010404900E+00
P10	15.0	5.9444847200E+00	-2.4125754200E+00	2.7913108400E+00
P11	15.0	2.4132782200E+00	5.9444486600E+00	-2.7904658400E+00
P12	15.0	-5.9447078400E+00	2.4126924400E+00	2.7908270700E+00
P13	15.0	-2.4125206000E+00	-5.9444849000E+00	-2.7907965400E+00
C14	6.0	8.8223699300E+00	-5.2367132400E-01	2.5612801400E+00
C15	6.0	6.8815182200E+00	-5.3020354000E+00	4.4317726400E+00
C16	6.0	5.3027306100E+00	6.8812931900E+00	-4.4310315800E+00
C17	6.0	5.2461981200E-01	8.8224490900E+00	-2.5601403500E+00
C18	6.0	-6.8811668200E+00	5.3023620700E+00	4.4312737600E+00
C19	6.0	-8.8229519800E+00	5.2439123600E-01	2.5607453500E+00
C20	6.0	-5.3018616200E+00	-6.8819662900E+00	-4.4311922100E+00
C21	6.0	-5.2304762300E-01	-8.8220036200E+00	-2.5604351500E+00
H22	1.0	-6.2873305200E+00	-8.3367126100E+00	-3.3190600300E+00
H23	1.0	-6.5077979300E+00	-5.2048994000E+00	-4.6242126200E+00
H24	1.0	-4.8187233300E+00	-7.6178855700E+00	-6.3148693300E+00
H25	1.0	1.2518256800E+00	-8.3314368800E+00	-1.6007226100E+00
H26	1.0	-1.1663985500E-01	-9.5392863200E+00	-4.4690490900E+00
H27	1.0	-1.5620212600E+00	-1.0243295000E+01	-1.4539797100E+00
H28	1.0	-8.3332696900E+00	-1.2507729100E+00	1.6011178500E+00
H29	1.0	-1.0243668700E+01	1.5640620700E+00	1.4542294400E+00
H30	1.0	-9.5404027600E+00	1.1849372700E-01	4.4693800800E+00
H31	1.0	-5.2037655400E+00	6.5078466700E+00	4.6240957400E+00
H32	1.0	-7.6170501400E+00	4.8195034500E+00	6.3150340200E+00
H33	1.0	-8.3357637800E+00	6.2881786400E+00	3.3192757500E+00
H34	1.0	1.1827631000E-01	9.5398111500E+00	-4.4687278400E+00
H35	1.0	-1.2503025100E+00	8.3324833000E+00	-1.6002369500E+00
H36	1.0	1.5642037600E+00	1.0243379400E+01	-1.4538247500E+00
H37	1.0	6.2884130200E+00	8.3359374100E+00	-3.3189693300E+00
H38	1.0	4.8196849200E+00	7.6172502400E+00	-6.3147238200E+00

H39	1.0	6.5084363400E+00	5.2040543800E+00	-4.6239669500E+00
H40	1.0	1.0243493000E+01	-1.5631683800E+00	1.4551006000E+00
H41	1.0	8.3324173600E+00	1.2512623300E+00	1.6013521800E+00
H42	1.0	9.5394749800E+00	-1.1736556600E-01	4.4699659000E+00
H43	1.0	7.6170935400E+00	-4.8190444400E+00	6.3156255100E+00
H44	1.0	5.2044059800E+00	-6.5079679300E+00	4.6243319600E+00
H45	1.0	8.3364686400E+00	-6.2874495400E+00	3.3198615700E+00