

Electronic Supplementary Material (ESI) for New Journal of Chemistry

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Supporting information For

Nature of E-E bond in heavier ditetrel alkyne analogues ArEEAr (Ar = C₆H₃-2,6(C₆H₃-2,6-Prⁱ)₂; E = Si, Ge, Sn, and Pb)

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Fig. S1. Electron localization functions for ArEEAr (Ar = C₆H₃-2,6(C₆H₃-2,6-Prⁱ)₂, E = C, Si, Ge, Sn, Pb) on the line connecting two E-E atoms.

Table S1. Cartesian coordinates of the optimized structure of ArEEAr (Ar = C₆H₃-2,6(C₆H₃-2,6-Prⁱ)₂, E = C, Si, Ge, Sn, Pb).

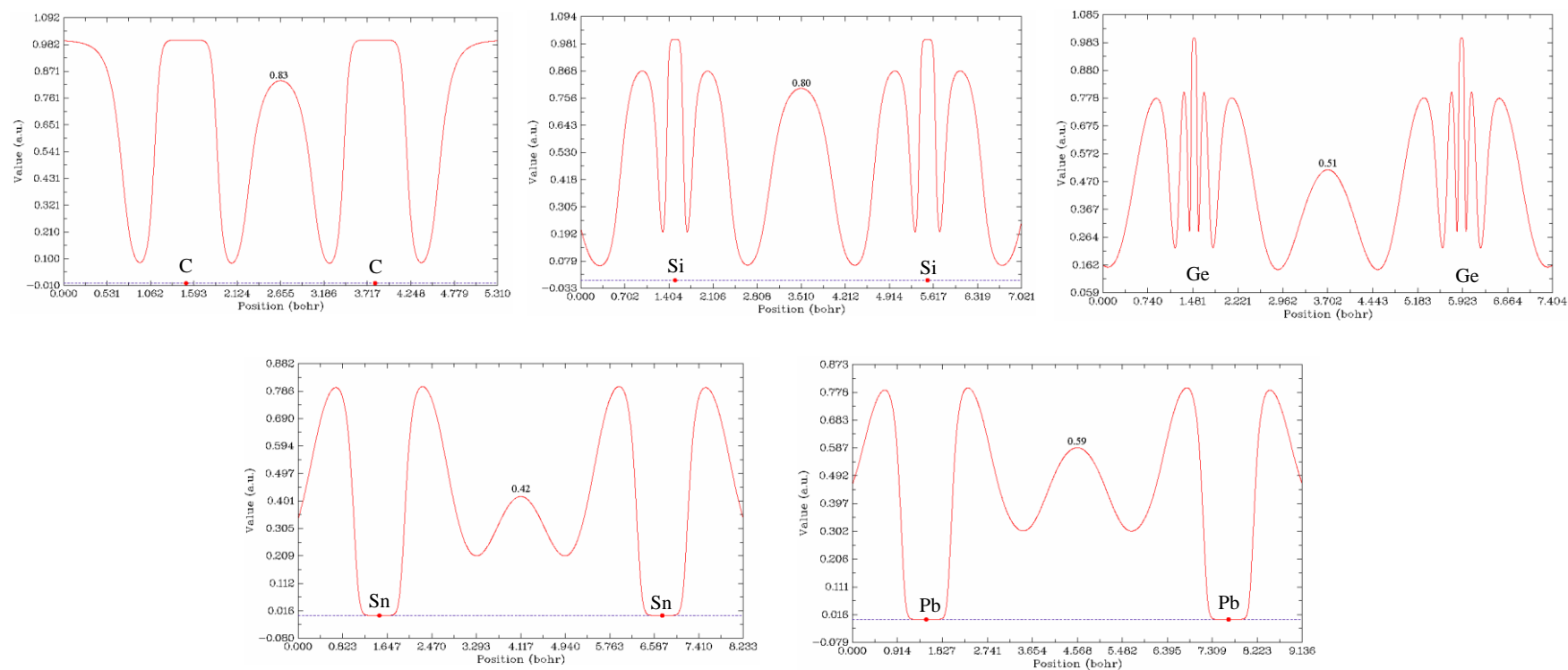


Fig. S1. Electron localization functions for ArEEAr ($\text{Ar} = \text{C}_6\text{H}_3\text{-}2,6(\text{C}_6\text{H}_3\text{-}2,6\text{-Pr}^1)_2$, $\text{E} = \text{C}, \text{Si}, \text{Ge}, \text{Sn}, \text{Pb}$) on the line connecting two E-E atoms.

Table S1. Cartesian coordinates of the optimized structure of ArEEAr (Ar = C₆H₃-2,6(C₆H₃-2,6-Prⁱ)₂, E = C, Si, Ge, Sn, Pb).

ArCCAr

C	1.44403000	-0.43922200	1.44236100
C	1.08916700	-0.62515200	2.82604000
C	2.83888900	-0.56339000	1.11121800
C	2.08008900	-0.91448200	3.78805000
C	3.79012600	-0.85955400	2.11025200
C	3.42981100	-1.03633000	3.44821100
H	1.76873700	-1.04075000	4.82067400
H	4.83121500	-0.94821800	1.81400300
H	4.17796300	-1.26169000	4.20341200
C	-1.44751100	0.43084600	-1.44273200
C	-2.13540200	-0.60990000	-2.16240000
C	-1.81354700	1.78573500	-1.76313400
C	-3.11439100	-0.29011600	-3.12671200
C	-2.80072000	2.05276400	-2.73517400
C	-3.45977400	1.03075200	-3.42284500
H	-3.60527000	-1.10734300	-3.64717300
H	-3.04505300	3.09027100	-2.94319800
H	-4.21829400	1.25664000	-4.16757900
C	-0.30487900	-0.53459400	3.38885600
C	-0.74318900	0.70031900	3.94956000
C	-1.07435000	-1.72237500	3.55760400
C	-2.02848500	0.75961400	4.52909800
C	-2.35311500	-1.61827300	4.14569700
C	-2.84143600	-0.38257100	4.59966400
H	-2.38523700	1.69586700	4.95165300
H	-2.96127800	-2.51066000	4.27240400
H	-3.83426400	-0.31819900	5.03962200
C	3.42987000	-0.40398400	-0.26509700
C	3.66217600	-1.56406500	-1.06039700
C	3.95882500	0.86080200	-0.65571800
C	4.28649300	-1.40804000	-2.31639700

C	4.57804000	0.97159700	-1.91902600
C	4.71137300	-0.14551400	-2.75910000
H	4.46012500	-2.27991400	-2.94266400
H	4.98015700	1.92989700	-2.23920200
H	5.18464700	-0.04065200	-3.73298400
C	-1.22433600	3.02059900	-1.13461900
C	-1.90604800	3.64146100	-0.04768200
C	-0.13058900	3.67340200	-1.77428600
C	-1.37428700	4.83409700	0.48759000
C	0.36500100	4.86784100	-1.20990300
C	-0.22904000	5.42708100	-0.06737400
H	-1.87376400	5.31776700	1.32389500
H	1.20279400	5.37776100	-1.67960100
H	0.17115100	6.34350900	0.36076900
C	-1.90523300	-2.08834300	-1.99026100
C	-2.76618700	-2.83215000	-1.13228100
C	-0.98565900	-2.75680000	-2.85054800
C	-2.57995100	-4.22758900	-1.03428200
C	-0.83162300	-4.15358600	-2.71982000
C	-1.59756700	-4.88079900	-1.79516300
H	-3.22288500	-4.81097700	-0.37931600
H	-0.12859700	-4.67966500	-3.36152700
H	-1.46130400	-5.95597200	-1.70084300
C	-0.46783800	-3.11025000	3.29347300
C	-1.38367200	-4.09649100	2.53662700
C	-0.03075200	-3.74176600	4.64768100
H	0.43589100	-2.98257100	2.68635200
H	-1.63446500	-3.72591300	1.53988900
H	-0.86591100	-5.05821200	2.41570100
H	-2.31824400	-4.29161400	3.08053800
H	0.67350700	-3.09811100	5.18721900
H	-0.90166500	-3.90745400	5.29622000
H	0.45446200	-4.71228200	4.47637500
C	0.21419800	1.89567300	4.09696100
C	0.73810100	1.95431700	5.56181900

C	-0.38158800	3.26493000	3.70548900
H	1.08098300	1.72698400	3.44799900
H	1.22928100	1.01891400	5.85480400
H	1.46451400	2.77072000	5.67435800
H	-0.08783700	2.13531500	6.26273700
H	-0.68336900	3.28484400	2.65599300
H	-1.25245900	3.52675700	4.32124200
H	0.37324200	4.04965200	3.85211200
C	4.03754400	2.03263400	0.33741800
C	3.63476300	3.40862400	-0.23590700
C	5.47950300	2.11119700	0.91959100
H	3.36014800	1.82339900	1.17327300
H	2.58903800	3.42128400	-0.55119600
H	3.76088900	4.17904100	0.53724400
H	4.25854500	3.69755600	-1.09236500
H	5.77800800	1.16682200	1.38966900
H	6.20627100	2.33782700	0.12795500
H	5.54231900	2.90397000	1.67729300
C	3.42040100	-2.97798300	-0.50376700
C	4.78143600	-3.59375000	-0.06488500
C	2.69816900	-3.94692500	-1.46491700
H	2.79813600	-2.89355200	0.39428200
H	5.29635200	-2.95820400	0.66533100
H	4.62411000	-4.58021900	0.39217500
H	5.44740100	-3.72152700	-0.92882200
H	1.68904100	-3.60018700	-1.69772900
H	3.24537300	-4.07679900	-2.40810300
H	2.61246900	-4.93573800	-0.99369700
C	-3.99209200	-2.18064600	-0.47053400
C	-4.19800200	-2.53436800	1.01851700
C	-5.26898100	-2.55295900	-1.28026700
H	-3.87682300	-1.09195000	-0.52789200
H	-3.36107500	-2.18950200	1.63070300
H	-5.10894600	-2.04538800	1.39045000
H	-4.31761100	-3.61540700	1.17166200

H	-5.18140900	-2.25711800	-2.33276700
H	-5.44757100	-3.63650000	-1.24935300
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C	-0.31799300	-2.02597200	-4.02815400
C	-1.08599500	-2.36827900	-5.33823000
C	1.18742300	-2.31372400	-4.21558300
H	-0.41844600	-0.94692700	-3.86636600
H	-2.14961700	-2.11278600	-5.26114000
H	-0.66202200	-1.81284800	-6.18581300
H	-1.01316700	-3.44079700	-5.56332900
H	1.76950300	-1.98314600	-3.35218500
H	1.38623700	-3.38139500	-4.37860400
H	1.55788700	-1.77095800	-5.09619800
C	0.37748000	3.21327100	-3.15132500
C	1.91322600	3.17010200	-3.30509400
C	-0.23257300	4.13028300	-4.25125500
H	0.00845500	2.19784700	-3.33397100
H	2.36615400	2.45555000	-2.61358700
H	2.17127100	2.85686100	-4.32645400
H	2.37158300	4.15412200	-3.13707200
H	-1.32832800	4.13312600	-4.21273000
H	0.11164800	5.16588100	-4.12853700
H	0.07314000	3.78573900	-5.24848200
C	-3.28558400	3.14599000	0.41876800
C	-4.38913600	4.06931000	-0.17490500
C	-3.46262500	3.04375400	1.94949600
H	-3.44743400	2.14248900	0.00921700
H	-4.33076400	4.11850700	-1.26883400
H	-5.38566500	3.69582100	0.09746300
H	-4.29152900	5.09210900	0.21312700
H	-2.77208800	2.31741200	2.38421400
H	-3.30733100	4.01018300	2.44747400
H	-4.48499200	2.71387800	2.18036100
C	0.42833500	-0.13279800	0.42680700
C	-0.43008300	0.12530900	-0.42936200

ArSiSiAr

Si	1.01447900	0.04735900	-0.23353000
Si	-1.03697200	-0.04640700	0.32301100
C	2.69174200	-0.20645700	0.62675500
C	2.90971800	-0.45784400	2.01677400
C	3.82412700	-0.11335100	-0.24303600
C	4.23285100	-0.60448800	2.49129600
C	5.12861100	-0.26450800	0.26620000
C	5.33859200	-0.50944800	1.63232300
H	4.38562000	-0.79292800	3.55138300
H	5.97287000	-0.19131900	-0.41513100
H	6.34689200	-0.62481700	2.02223300
C	-2.70121400	0.20517100	-0.58143400
C	-3.45375000	-0.92872500	-1.02494000
C	-3.29308600	1.50467900	-0.68163900
C	-4.76021700	-0.75198000	-1.53026400
C	-4.60263200	1.64221600	-1.19088500
C	-5.33975100	0.52321500	-1.60691700
H	-5.31580800	-1.62541200	-1.86273100
H	-5.03667100	2.63684800	-1.25777600
H	-6.35010200	0.64426600	-1.99040400
C	1.80341000	-0.57507900	3.03216200
C	1.40428200	0.57606100	3.76991400
C	1.24411000	-1.85334700	3.32295900
C	0.42237700	0.43295500	4.77336600
C	0.26481900	-1.95099200	4.33363000
C	-0.14937100	-0.81762400	5.05049900
H	0.10702900	1.30218800	5.34557300
H	-0.17214500	-2.91820300	4.56850200
H	-0.90576800	-0.91098400	5.82689000
C	3.64306200	0.13981200	-1.71784600
C	3.54590800	-0.96648400	-2.61551100
C	3.63223300	1.47956200	-2.21253900
C	3.38133200	-0.70907500	-3.99254600
C	3.46724900	1.68879600	-3.59779900

C	3.32985100	0.60609300	-4.48033900
H	3.29900800	-1.54007400	-4.68866600
H	3.45072500	2.70228700	-3.99045200
H	3.19795900	0.78621900	-5.54503000
C	-2.56761700	2.76742600	-0.29296200
C	-2.68455300	3.28045800	1.03018000
C	-1.84516000	3.48610800	-1.28994700
C	-2.03228100	4.49044100	1.34849600
C	-1.20592800	4.69000400	-0.92730400
C	-1.28959200	5.18625800	0.38294900
H	-2.10716100	4.89324500	2.35573800
H	-0.64428400	5.24693100	-1.67351100
H	-0.78860800	6.11509600	0.64676800
C	-2.90445300	-2.33270800	-1.00675900
C	-3.13084400	-3.17408300	0.12026600
C	-2.24331900	-2.83406000	-2.16565300
C	-2.64691700	-4.49893200	0.08612200
C	-1.77178400	-4.16340500	-2.15502400
C	-1.96288300	-4.98922000	-1.03642400
H	-2.80727700	-5.15209100	0.94042800
H	-1.25849700	-4.55826700	-3.02852200
H	-1.59152100	-6.01163800	-1.04401900
C	1.74387500	-3.12646800	2.62662100
C	0.60725700	-4.08202700	2.19444400
C	2.75677100	-3.87377100	3.53940300
H	2.28069700	-2.83016600	1.71785100
H	-0.12187600	-3.57487600	1.55414800
H	1.02506100	-4.92629600	1.62922800
H	0.07396700	-4.50007300	3.05873600
H	3.61402900	-3.23760000	3.79112200
H	2.27809400	-4.18412000	4.47800300
H	3.13529400	-4.77399500	3.03624100
C	2.06038700	1.94572500	3.54992100
C	3.04629500	2.26624300	4.70734900
C	1.03172900	3.08905100	3.37881500

H	2.64825100	1.89939800	2.62611000
H	3.82256400	1.49575100	4.79496300
H	3.54100600	3.23184100	4.53473800
H	2.51782300	2.32247400	5.66853500
H	0.34140100	2.88101700	2.55424000
H	0.43972600	3.24323500	4.29082000
H	1.55112900	4.03196100	3.15970900
C	3.89191200	2.67791000	-1.28879500
C	2.89897500	3.84675700	-1.49365700
C	5.35634800	3.16911300	-1.46154700
H	3.78384200	2.34004100	-0.25190400
H	1.86646700	3.52689000	-1.31698900
H	3.12813700	4.65810000	-0.78965800
H	2.96035000	4.26361000	-2.50769500
H	6.07254600	2.36363600	-1.25662400
H	5.53280500	3.52499200	-2.48546300
H	5.56687400	3.99758400	-0.77191000
C	3.70861200	-2.41379300	-2.13033200
C	5.11532000	-2.94735800	-2.51958600
C	2.60290100	-3.36638300	-2.64470500
H	3.65263000	-2.41732500	-1.03598400
H	5.90956800	-2.31223800	-2.10752500
H	5.25887400	-3.96643200	-2.13575800
H	5.23800100	-2.97449200	-3.61059000
H	1.61190100	-3.03492000	-2.31688700
H	2.59595500	-3.43342900	-3.74077000
H	2.77059200	-4.37859700	-2.25263200
C	-3.94701400	-2.70203300	1.33130700
C	-3.23800800	-2.96425600	2.68215400
C	-5.35711000	-3.35425700	1.31729100
H	-4.09304500	-1.61856400	1.24809400
H	-2.25597900	-2.47942800	2.71621600
H	-3.84424900	-2.56731500	3.50784700
H	-3.09463500	-4.03755600	2.86454800
H	-5.89375300	-3.12082800	0.38896100

H	-5.28531100	-4.44711200	1.39826300
H	-5.95838400	-2.98984600	2.16129500
C	-2.09959400	-1.99522600	-3.44349700
C	-3.08520800	-2.50047900	-4.53312800
C	-0.65281700	-1.96281400	-3.99062400
H	-2.37711200	-0.96104100	-3.21049700
H	-4.12280300	-2.46853500	-4.17746600
H	-3.01285000	-1.87731400	-5.43483100
H	-2.85903100	-3.53675100	-4.81786600
H	0.04360000	-1.57292300	-3.24017100
H	-0.30775500	-2.96026200	-4.29289000
H	-0.59982600	-1.31256800	-4.87440800
C	-1.80690200	3.02349200	-2.75349900
C	-0.37974900	2.99481800	-3.35022900
C	-2.74189000	3.91020200	-3.62189500
H	-2.19419500	1.99938800	-2.79989400
H	0.28223400	2.34692100	-2.76530100
H	-0.41106300	2.60880200	-4.37814000
H	0.06772800	3.99657300	-3.38796900
H	-3.77330000	3.88759400	-3.24843500
H	-2.40562000	4.95572300	-3.61774000
H	-2.74697300	3.55901800	-4.66274000
C	-3.55747900	2.59458600	2.09013800
C	-4.87059400	3.39631900	2.30563600
C	-2.82116700	2.37607200	3.43401500
H	-3.84335200	1.60498100	1.71438800
H	-5.43001200	3.50118300	1.36731900
H	-5.51669100	2.88843900	3.03453700
H	-4.65822900	4.40482400	2.68457600
H	-1.91223800	1.78011800	3.29567600
H	-2.53588100	3.32796700	3.90116300
H	-3.47495900	1.84465400	4.13905700

ArGeGeAr

Ge	1.16103800	0.10358300	-0.12018000
Ge	-1.16044300	-0.10290300	-0.11940700
C	2.56850100	-1.30586000	0.05296200
C	2.47491400	-2.65557000	-0.40277800
C	3.79814900	-0.84921600	0.61836500
C	3.59192200	-3.51051000	-0.26645000
C	4.89234500	-1.73051700	0.74333500
C	4.79282300	-3.06065400	0.30523700
H	3.51095300	-4.53578000	-0.62019700
H	5.81888100	-1.36457100	1.18017400
H	5.64009700	-3.73528700	0.40118300
C	-2.56834800	1.30625000	0.05519900
C	-2.47527300	2.65614700	-0.40024700
C	-3.79767800	0.84913500	0.62101500
C	-3.59231300	3.51081300	-0.26285700
C	-4.89189500	1.73024700	0.74703100
C	-4.79274400	3.06058100	0.30950900
H	-3.51185800	4.53614800	-0.61653200
H	-5.81827400	1.36393600	1.18390100
H	-5.64004500	3.73507800	0.40618600
C	1.23803200	-3.23370500	-1.04074900
C	0.29965700	-3.94651100	-0.23856000
C	1.06373800	-3.14606600	-2.45264900
C	-0.81952100	-4.53526000	-0.86343400
C	-0.06824000	-3.75271000	-3.03678100
C	-1.00752400	-4.43608900	-2.25053700
H	-1.54845700	-5.07443400	-0.26390600
H	-0.21392000	-3.69478700	-4.11266600
H	-1.87554000	-4.89734500	-2.71675200
C	3.98686100	0.57678800	1.07799100
C	4.49630000	1.54959200	0.16421100
C	3.77082000	0.91814400	2.44780200
C	4.77080400	2.85027400	0.63745700
C	4.06437500	2.22888300	2.87695500

C	4.56025800	3.18927300	1.98198200
H	5.16001900	3.59897100	-0.04778300
H	3.90652400	2.50118700	3.91763800
H	4.78409600	4.19459900	2.33217200
C	-3.98592800	-0.57741600	1.07907000
C	-4.49425400	-1.54956200	0.16407000
C	-3.76989600	-0.92017600	2.44858600
C	-4.76741500	-2.85115600	0.63566700
C	-4.06229300	-2.23167400	2.87611700
C	-4.55688800	-3.19152800	1.97986800
H	-5.15561300	-3.59947500	-0.05054000
H	-3.90432800	-2.50508400	3.91649400
H	-4.77970100	-4.19752300	2.32878000
C	-1.23910700	3.23437500	-1.03940400
C	-1.06627800	3.14596700	-2.45147900
C	-0.30011300	3.94784800	-0.23867800
C	0.06476500	3.75285800	-3.03715000
C	0.81810700	4.53679100	-0.86506400
C	1.00462400	4.43706400	-2.25231700
H	0.20930300	3.69462900	-4.11315700
H	1.54736000	5.07668900	-0.26659800
H	1.87193200	4.89843300	-2.71973400
C	2.10591400	-2.47854700	-3.35986600
C	1.48442000	-1.45039400	-4.33653000
C	2.91359700	-3.55390800	-4.13753300
H	2.81621600	-1.93538600	-2.72627300
H	0.93113000	-0.67741000	-3.79130000
H	2.27437600	-0.95946400	-4.92125900
H	0.79568700	-1.92684100	-5.04669300
H	3.41060700	-4.25044800	-3.45051700
H	2.25642600	-4.13960400	-4.79403600
H	3.68381200	-3.08076700	-4.76171300
C	0.51602000	-4.14851100	1.26722300
C	1.05649100	-5.57822300	1.54864400
C	-0.75505200	-3.88151000	2.10724000

H	1.28248000	-3.43894100	1.60021500
H	1.99972000	-5.76071700	1.01951000
H	1.23561800	-5.71674100	2.62367000
H	0.33432900	-6.33910800	1.22331800
H	-1.16248500	-2.88359400	1.91162300
H	-1.54682800	-4.61166900	1.89621500
H	-0.51901400	-3.95261900	3.17798600
C	3.28104100	-0.11370400	3.47168200
C	2.06232400	0.38899900	4.28548700
C	4.43715400	-0.53562900	4.41864700
H	2.96162800	-1.01010700	2.92839100
H	1.24320300	0.69142000	3.62214200
H	1.69281600	-0.40920300	4.94327000
H	2.32227800	1.24644300	4.92036300
H	5.28082400	-0.95128100	3.85353900
H	4.80745700	0.32253000	4.99523300
H	4.09278700	-1.29898900	5.12935700
C	4.81821700	1.20173800	-1.29555000
C	6.35284600	1.06895300	-1.49557000
C	4.22144400	2.21780000	-2.30063800
H	4.37753500	0.22410500	-1.52170100
H	6.77434600	0.30113800	-0.83493600
H	6.58145800	0.79015500	-2.53309600
H	6.86144200	2.01795100	-1.27899600
H	3.13895900	2.32461800	-2.16461400
H	4.67644200	3.21161800	-2.19289300
H	4.40757000	1.88085400	-3.32942100
C	-2.10925900	2.47771700	-3.35730700
C	-1.48832400	1.45125400	-4.33612000
C	-2.91996200	3.55256800	-4.13250300
H	-2.81750700	1.93301000	-2.72270800
H	-0.93289100	0.67857500	-3.79269300
H	-2.27877800	0.95979800	-4.91971200
H	-0.80165100	1.92924600	-5.04722800
H	-3.41683800	4.24774200	-3.44400900

H	-2.26481700	4.13982900	-4.78964300
H	-3.69055600	3.07880100	-4.75574100
C	-0.51486500	4.15036400	1.26727600
C	-1.05495700	5.58015200	1.54898900
C	0.75705900	3.88368000	2.10615000
H	-1.28091300	3.44081700	1.60127800
H	-1.99865400	5.76280300	1.02073000
H	-1.23308000	5.71888000	2.62414700
H	-0.33293900	6.34085100	1.22288500
H	1.16384900	2.88536000	1.91122200
H	1.54892500	4.61323100	1.89355300
H	0.52220000	3.95601200	3.17708400
C	-3.28060800	0.11075500	3.47368200
C	-2.06141700	-0.39218600	4.28665100
C	-4.43676200	0.53090000	4.42135500
H	-2.96166100	1.00788600	2.93134400
H	-1.24208300	-0.69281000	3.62277200
H	-1.69260500	0.40534100	4.94565400
H	-2.32051200	-1.25086900	4.92018300
H	-5.28067000	0.94700500	3.85693600
H	-4.80670600	-0.32821100	4.99676000
H	-4.09263600	1.29340000	5.13309300
C	-4.81683900	-1.20004400	-1.29517800
C	-6.35159700	-1.06766800	-1.49428800
C	-4.22009200	-2.21447600	-2.30194200
H	-4.37669200	-0.22192200	-1.52031300
H	-6.77314500	-0.30090700	-0.83246700
H	-6.58082500	-0.78760700	-2.53133800
H	-6.85965500	-2.01718200	-1.27869400
H	-3.13752500	-2.32121300	-2.16641400
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Sn	-1.34616100	0.31743600	-0.35600200
Sn	1.34867300	-0.32041200	-0.35603000
C	-2.98930800	-1.06104400	0.06511900
C	-3.04161600	-2.42422700	-0.34704400
C	-4.13675200	-0.47788300	0.67800600
C	-4.22301600	-3.17124600	-0.14141800
C	-5.30471100	-1.24536600	0.87371800
C	-5.35043100	-2.58940300	0.46401200
H	-4.25327100	-4.21172600	-0.45842700
H	-6.17293000	-0.78771100	1.34374000
H	-6.25360400	-3.17617900	0.61398700
C	2.98849500	1.06098600	0.06652600
C	4.13524600	0.47640400	0.67971700
C	3.04174800	2.42487100	-0.34295600
C	5.30356300	1.24273900	0.87745700
C	4.22352300	3.17080200	-0.13525600
C	5.35027800	2.58741100	0.46993300
H	6.17111400	0.78370300	1.34737400
H	4.25438300	4.21190300	-0.45022100
H	6.25356400	3.17359300	0.62146600
C	-1.85620500	-3.09697400	-0.99265800
C	-1.66939600	-3.01918500	-2.40581100
C	-0.94862100	-3.84618500	-0.18556600
C	-0.55869000	-3.67160200	-2.98263800
C	0.15182500	-4.47635200	-0.80401900
C	0.35208200	-4.38494700	-2.19004000
H	-0.40203600	-3.61890800	-4.05678000
H	0.85633800	-5.04340100	-0.20073000
H	1.20772300	-4.87477000	-2.65003000
C	-4.11801900	0.96431500	1.12661500
C	-3.73318900	1.28489900	2.46604300
C	-4.55027500	1.99619300	0.23607100
C	-3.78031300	2.63094400	2.88509100
C	-4.58122900	3.32911200	0.70043300

C	-4.19934500	3.64662200	2.01205300
H	-3.48930700	2.88748200	3.90027400
H	-4.91060000	4.12171600	0.03353000
H	-4.23318300	4.67858900	2.35467600
C	1.85696400	3.10025400	-0.98697200
C	1.67139300	3.02943200	-2.40059900
C	0.94933400	3.84645400	-0.17719400
C	0.56189900	3.68572000	-2.97534400
C	-0.15085000	4.47930800	-0.79338700
C	-0.34982100	4.39486200	-2.17998600
H	0.40683200	3.63898700	-4.05002100
H	-0.85603500	5.04323500	-0.18788700
H	-1.20484500	4.88741800	-2.63823800
C	4.11583600	-0.96671900	1.12567100
C	4.54775100	-1.99686000	0.23285100
C	3.73155900	-1.28993800	2.46471000
C	4.57953900	-3.33060000	0.69477900
C	3.78033100	-2.63667600	2.88147500
C	4.19949200	-3.65048300	2.00636000
H	4.90790400	-4.12191400	0.02587700
H	3.49114600	-2.89523700	3.89667300
H	4.23437600	-4.68298400	2.34728700
C	-1.17599100	-4.04030200	1.31987300
C	0.08315700	-3.74373300	2.16922700
C	-1.69789300	-5.47577800	1.60474500
H	-1.95567900	-3.34059300	1.64098500
H	0.44470500	-2.72348200	1.99476700
H	-0.15115300	-3.84516200	3.23790200
H	0.90596400	-4.43399500	1.94412600
H	-2.62789400	-5.67659100	1.05844400
H	-0.95945500	-6.22958200	1.30015900
H	-1.89574300	-5.60760200	2.67730100
C	-2.68519100	-2.31618400	-3.31673100
C	-3.63526700	-3.36130500	-3.96474100
C	-2.02508800	-1.43530000	-4.40594900

H	-3.30458400	-1.65824900	-2.69561800
H	-4.16756100	-3.94093700	-3.20040700
H	-4.38198800	-2.86268300	-4.59760000
H	-3.07201500	-4.06518700	-4.59208300
H	-1.32911800	-0.71183400	-3.96358700
H	-1.47180900	-2.03695500	-5.13875200
H	-2.79571600	-0.87798800	-4.95555400
C	-5.04564500	1.68559800	-1.18297000
C	-4.43020400	2.61802300	-2.25642500
C	-6.59716400	1.74134000	-1.23625500
H	-4.74935300	0.66009600	-1.43196300
H	-3.33365100	2.59803600	-2.22042100
H	-4.74544300	2.29518000	-3.25769500
H	-4.75774100	3.65849600	-2.12957800
H	-7.04430800	1.03043000	-0.53052600
H	-6.96263700	2.74551900	-0.98272100
H	-6.95553400	1.49321400	-2.24441800
C	-3.34573800	0.19572700	3.47563000
C	-4.53126100	-0.08965700	4.43881100
C	-2.06581400	0.53525900	4.27847000
H	-3.14781100	-0.72829600	2.92089600
H	-5.42708900	-0.39671500	3.88542100
H	-4.27037300	-0.89394400	5.13985500
H	-4.78494400	0.80395400	5.02491000
H	-1.21652600	0.72966400	3.61222300
H	-2.20524200	1.41620000	4.91883900
H	-1.79982900	-0.30651700	4.93186300
C	5.04165500	-1.68326000	-1.18605700
C	4.43321100	-2.61968100	-2.25985500
C	6.59366900	-1.72813100	-1.23847300
H	4.73846100	-0.65981800	-1.43529900
H	3.33651700	-2.60663400	-2.22459300
H	4.74689300	-2.29451500	-3.26088400
H	4.76769400	-3.65787700	-2.13313400
H	7.03547700	-1.01574900	-0.53098200

H	6.96571500	-2.73040400	-0.98691900
H	6.95089200	-1.47530900	-2.24588600
C	3.34217800	-0.20302000	3.47611100
C	4.52875000	0.08852200	4.43566300
C	2.06634800	-0.54982700	4.28271000
H	3.13752600	0.72016600	2.92230900
H	5.42055000	0.40251900	3.87974500
H	4.26479800	0.88999700	5.13877000
H	4.79058600	-0.80412400	5.01967500
H	1.21679100	-0.75110300	3.61883800
H	2.21352100	-1.42879600	4.92406900
H	1.79617100	0.29111500	4.93538000
C	1.17682600	4.03511300	1.32883500
C	-0.08173200	3.73389900	2.17724600
C	1.69769400	5.46990600	1.61884800
H	1.95739400	3.33512800	1.64722000
H	-0.44072100	2.71333400	1.99962500
H	0.15223700	3.83253300	3.24627400
H	-0.90583300	4.42312800	1.95387300
H	2.62792900	5.67286400	1.07370900
H	0.95916000	6.22448900	1.31648700
H	1.89499500	5.59826100	2.69193500
C	2.68628400	2.32910700	-3.31459800
C	3.62836700	3.37656400	-3.97047100
C	2.02393300	1.44239400	-4.39786400
H	3.31190100	1.67586100	-2.69490300
H	4.16186700	3.96082700	-3.21046500
H	4.37409300	2.87941800	-4.60564900
H	3.05879100	4.07604200	-4.59704600
H	1.33292100	0.71772800	-3.94973600
H	1.46449000	2.03986000	-5.12939000
H	2.79361200	0.88612000	-4.94993700

ArPbPbAr

Pb	-1.29069700	0.24351700	0.95838100
Pb	1.27580500	-0.43377500	-0.91196800
C	3.01917800	-0.69537300	0.55681200
C	3.12384200	-1.93850000	1.25006100
C	4.13093900	0.19451000	0.60285100
C	4.30598300	-2.28616300	1.93775000
C	5.30466900	-0.16431700	1.30507300
C	5.39929900	-1.40286600	1.96313500
H	4.37184700	-3.24445500	2.44906500
H	6.14333200	0.52933300	1.33125600
H	6.31042300	-1.67429100	2.49108800
C	-2.92308700	0.72990400	-0.57790000
C	-3.84326100	-0.19977000	-1.14761600
C	-3.17286300	2.12096700	-0.77320200
C	-4.96498200	0.26295400	-1.87643900
C	-4.29317100	2.56331700	-1.51113600
C	-5.19356600	1.63620400	-2.06154400
H	-5.66168600	-0.46203100	-2.29350900
H	-4.46033700	3.63105000	-1.64275000
H	-6.06045000	1.97766600	-2.62236000
C	1.93095300	-2.86258500	1.22890200
C	1.03738100	-2.90509100	2.34526400
C	1.67502600	-3.66507200	0.06956300
C	-0.14030400	-3.67609200	2.24295900
C	0.47458300	-4.41008100	0.00977000
C	-0.43506300	-4.39959500	1.07640300
H	-0.83369700	-3.71382500	3.07898800
H	0.25390200	-5.00790500	-0.86945200
H	-1.36216000	-4.96034900	1.00401800
C	4.08541100	1.54478200	-0.07166600
C	4.54813800	1.69811800	-1.41422500
C	3.64632500	2.68316800	0.67039600
C	4.55356200	2.98641000	-1.99183200
C	3.66662300	3.95214500	0.05271700

C	4.11522300	4.10557700	-1.26796300
H	4.90991400	3.11662200	-3.01059900
H	3.33870000	4.82601500	0.61056900
H	4.13261500	5.09178700	-1.72725300
C	-2.25875600	3.16967200	-0.18042000
C	-2.55631900	3.73426800	1.10018500
C	-1.17000200	3.68338600	-0.95417100
C	-1.76278700	4.80042700	1.57812600
C	-0.40542900	4.74981900	-0.43608400
C	-0.70046700	5.30803100	0.81709400
H	-1.98416400	5.24171900	2.54641500
H	0.42269100	5.14849900	-1.01547400
H	-0.10546100	6.13512700	1.19796000
C	-3.69102400	-1.69692500	-1.00467800
C	-4.18092900	-2.36034200	0.16218800
C	-3.17340500	-2.46155600	-2.09455000
C	-4.13295600	-3.77025700	0.22062800
C	-3.14463000	-3.86905400	-1.99291200
C	-3.62044400	-4.52225100	-0.84661800
H	-4.51594700	-4.28421300	1.09882600
H	-2.75968800	-4.45912200	-2.82136300
H	-3.60367300	-5.60889700	-0.79069000
C	2.75602300	-3.86864400	-1.00738100
C	2.20769200	-4.11942200	-2.43110700
C	3.67948100	-5.04619400	-0.58107700
H	3.38203700	-2.96909600	-1.04484300
H	1.52774700	-3.32087600	-2.75263800
H	3.04009500	-4.15935800	-3.14577100
H	1.67199200	-5.07516200	-2.50233800
H	4.15269200	-4.84781200	0.38743600
H	3.10548100	-5.97882800	-0.49708800
H	4.47370500	-5.19820100	-1.32449900
C	1.38268000	-2.22099900	3.67648700
C	2.03862100	-3.25498200	4.63714000
C	0.17995100	-1.55363300	4.38470200

H	2.12508300	-1.43984200	3.47666700
H	2.92981600	-3.71151400	4.19167500
H	2.33583400	-2.76985800	5.57671400
H	1.33214000	-4.06099500	4.87742000
H	-0.32414500	-0.82780400	3.73581900
H	-0.56518600	-2.29135100	4.71080300
H	0.52635800	-1.02393800	5.28229100
C	3.23488900	2.56919800	2.14419700
C	1.91117700	3.30206500	2.46489200
C	4.37564000	3.08390300	3.06480400
H	3.08513400	1.50866800	2.37249800
H	1.09972100	2.97715900	1.80258800
H	1.61095300	3.10116700	3.50219500
H	2.00732900	4.38992100	2.35562800
H	5.30262800	2.52142400	2.89988200
H	4.58508400	4.14519800	2.87385700
H	4.09462300	2.97726200	4.12145100
C	5.11529300	0.51500600	-2.21070800
C	6.66819400	0.56319600	-2.21535400
C	4.57284400	0.43988700	-3.65953400
H	4.81992300	-0.40987400	-1.70164000
H	7.06770000	0.54586400	-1.19411900
H	7.07817900	-0.29965400	-2.75767500
H	7.03021300	1.47686300	-2.70587400
H	3.47629000	0.40302500	-3.67086800
H	4.89220800	1.30014000	-4.26237400
H	4.94839000	-0.46553900	-4.15498000
C	-4.86008800	-1.59083400	1.30427700
C	-4.40498800	-2.05568600	2.70977800
C	-6.40502900	-1.69281600	1.17298000
H	-4.59732200	-0.53125400	1.20783000
H	-3.31318500	-2.00525500	2.81277200
H	-4.84726600	-1.41082800	3.48074100
H	-4.72035400	-3.08546900	2.92277700
H	-6.74520900	-1.30128700	0.20661900

H	-6.73636700	-2.73706200	1.25224800
H	-6.89814600	-1.11724600	1.96817500
C	-2.71282900	-1.80402300	-3.40321700
C	-3.74600000	-2.05540800	-4.53588300
C	-1.30659300	-2.27306700	-3.84926000
H	-2.66150700	-0.72156200	-3.24223400
H	-4.73620000	-1.67101300	-4.26357800
H	-3.42941400	-1.55693400	-5.46210300
H	-3.84686500	-3.12878100	-4.74556200
H	-0.55778500	-2.07524000	-3.07271200
H	-1.28492100	-3.34708100	-4.07614200
H	-0.99987800	-1.73687300	-4.75746000
C	-0.87457400	3.15577800	-2.36422000
C	0.63641400	3.00520200	-2.65831400
C	-1.53012700	4.07324600	-3.43418800
H	-1.33377700	2.16446800	-2.45752900
H	1.15258100	2.43611100	-1.87252000
H	0.78460200	2.48383000	-3.61285100
H	1.14277800	3.97534400	-2.73207400
H	-2.61612300	4.12782100	-3.29908000
H	-1.12590800	5.09280200	-3.37240800
H	-1.33111400	3.68780300	-4.44338100
C	-3.76315300	3.27184000	1.92846100
C	-4.92978000	4.28966800	1.79950500
C	-3.41696300	3.03251700	3.41933400
H	-4.11608600	2.31952100	1.51584500
H	-5.23283300	4.41299800	0.75295200
H	-5.80328200	3.94557600	2.36966000
H	-4.63676400	5.27462300	2.18724000
H	-2.59144900	2.31712400	3.52558800
H	-3.12997200	3.96216800	3.92806800
H	-4.29009800	2.62575300	3.94689000