Electronic Supplementary Material (ESI) for RSC Advances.

– Electronic Supplementary Information –

Exploring the Potential Energy Surface of Small Lead Clusters using the Gradient Embedded Genetic Algorithm and an Adequate Treatment of Relativistic Effects

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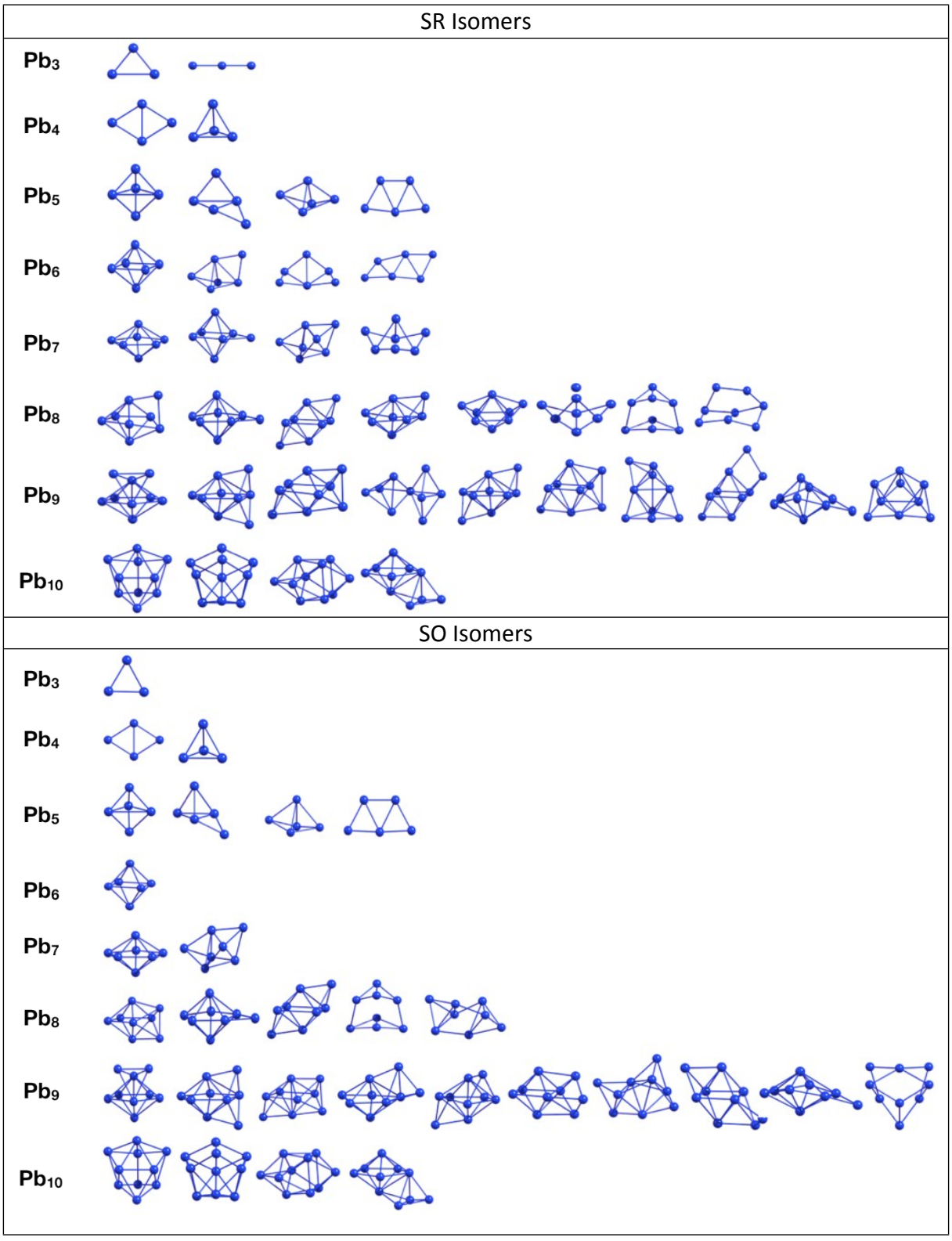

Figure ESI-1. The lowest energy isomers of Pb_x (x = 3 - 10) clusters at scalar (SR) and spin-orbit (SO) schemes.

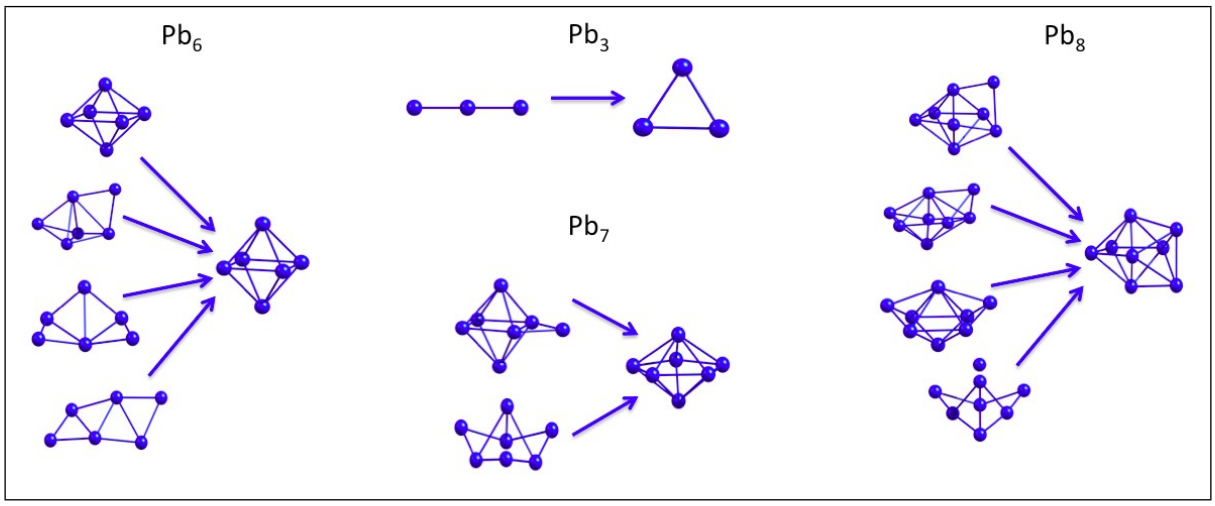

Figure ESI-2. Convergence of SR-isomers towards to SO-isomer.

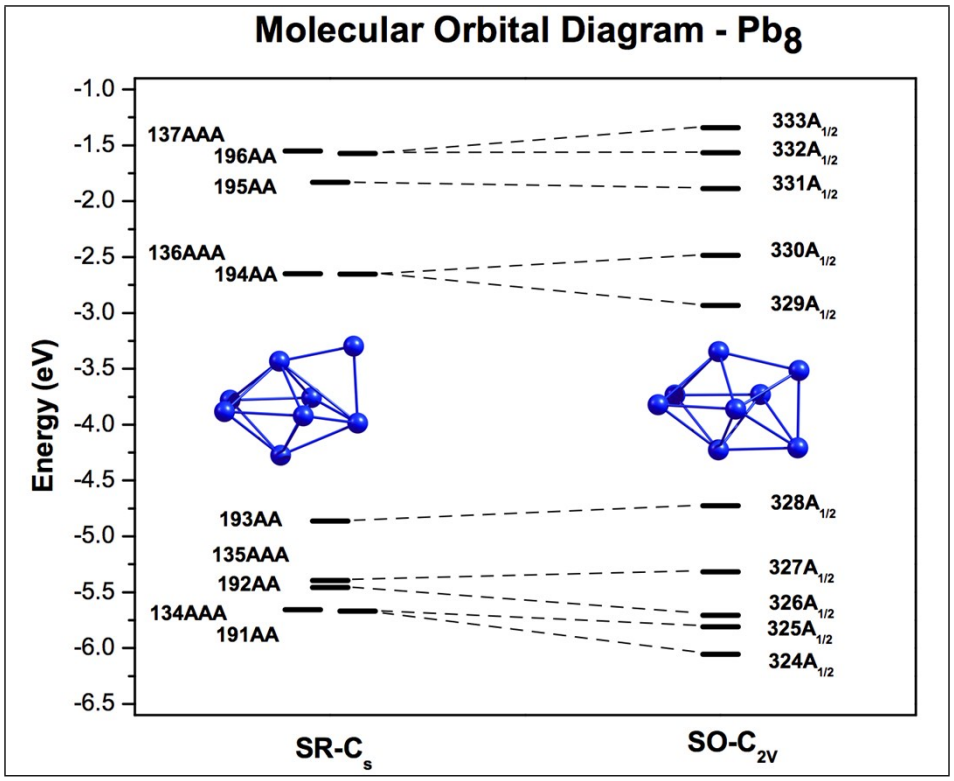

Figure ESI-3. Molecular orbital diagram for Pb_8 system calculated at PBE0/TZ2P-SR and PBE0/TZ2P-SO levels of theory.

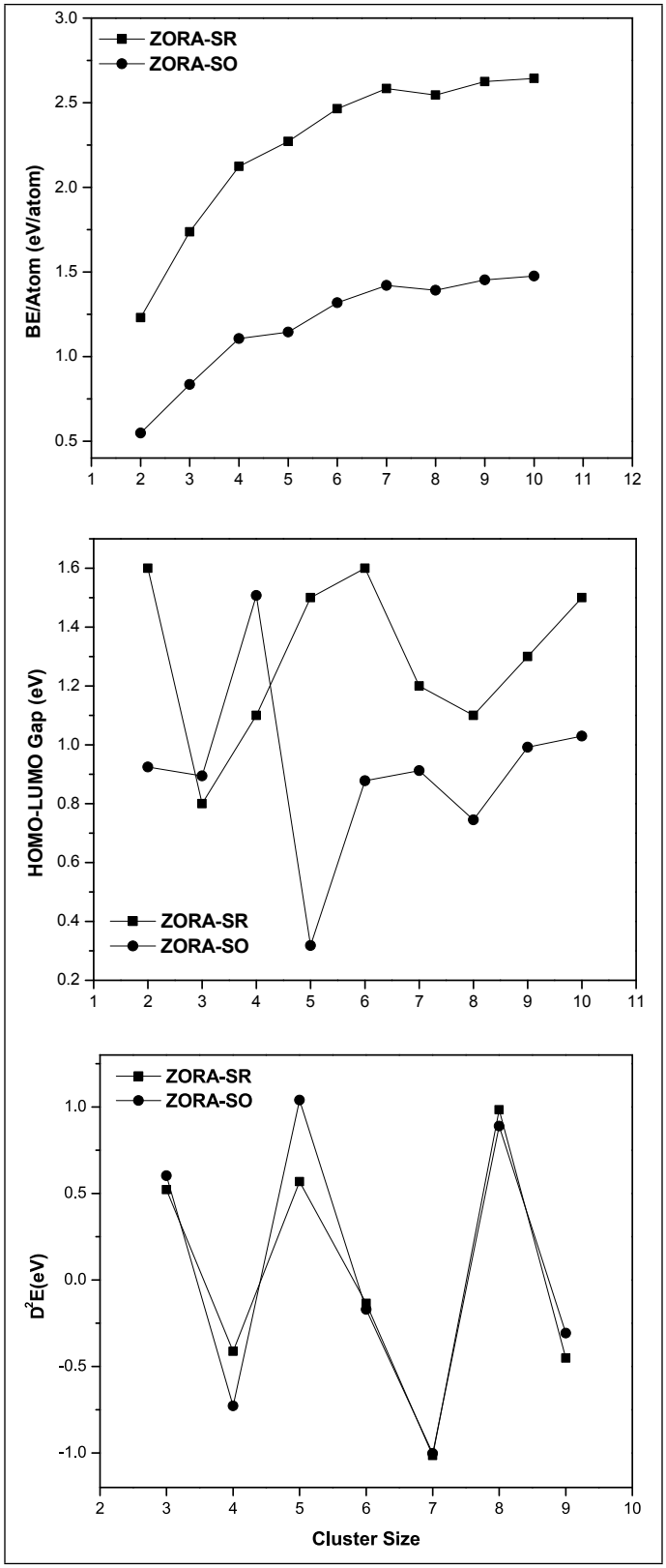

Figure ESI-4. Binding energy (BE), HOMO-LUMO gap and Second Order Difference in Total Energy behaviors calculated using the GGA-PBE/Def2-TZVP methodology.

Table ESI-1. Cartesians coordinates and relative energies for Pb_n (n = 3 - 10) isomers.

	GEGA				SR				SO			
					Pb_3							
0.0	82	1.812700000	-0.713700000	0.000000000	0.0	82	0.000000000	-1.749711000	-0.730828000	0.0	82	0.000000000	-1.498630000	-0.866094000
	82	0.000000000	1.427800000	0.000000000		82	0.000000000	0.000000000	1.461658000		82	0.000000000	0.000000000	1.732190000
	82	-1.812700000	-0.714100000	0.000000000		82	0.000000000	1.749711000	-0.730828000		82	0.000000000	1.498630000	-0.866094000
9.4	82	2.721000000	-0.035800000	0.000000000	12.1	82	0.000000000	0.000000000	-2.729530000					
	82	-2.721000000	0.035200000	0.000000000		82	0.000000000	0.000000000	2.729530000					
	82	0.000000000	0.000600000	0.000000000		82	0.000000000	0.000000000	0.000000000					
					Pb_4									
0.0	82	0.000000000	1.587800000	0.000000000	0.0	82	0.000000000	0.000000000	2.498375000	0.0	82	0.000000000	0.000000000	2.511409000
	82	2.504400000	0.000700000	0.000000000		82	0.000000000	1.565527000	0.000000000		82	0.000000000	1.585241000	0.000000000
	82	0.000000000	-1.588600000	0.000000000		82	0.000000000	-1.565527000	0.000000000		82	0.000000000	-1.585241000	0.000000000
	82	-2.504400000	0.000100000	0.000000000		82	0.000000000	0.000000000	-2.498375000		82	0.000000000	0.000000000	-2.511409000
27.7	82	-1.763100000	-0.170100000	0.823500000	21.8	82	-1.108528000	-1.108528000	1.108528000	8.7	82	-1.114344000	-1.114344000	1.114344000
	82	1.369500000	0.042300000	1.390800000		82	1.108528000	1.108528000	1.108528000		82	1.114344000	1.114344000	1.114344000
	82	0.317400000	-1.524600000	-1.177200000		82	1.108528000	-1.108528000	-1.108528000		82	1.114344000	-1.114344000	-1.114344000
	82	0.076300000	1.652400000	-1.037000000		82	-1.108528000	1.108528000	-1.108528000		82	-1.114344000	1.114344000	-1.114344000
					Pb_5									
0.0	82	-0.003900000	-0.014300000	1.880700000	0.0	82	-1.875667000	0.000000000	-0.001022000	11.2	82	-1.969251000	0.000000000	0.001342000
	82	-2.232800000	0.522900000	-0.000900000		82	1.875667000	0.000000000	-0.001022000		82	1.969251000	0.000000000	0.001342000
	82	0.664200000	-2.190400000	-0.015200000		82	0.000000000	-1.959106000	-1.127939000		82	0.000000000	-1.911972000	-1.107164000
	82	0.001100000	0.013000000	-1.875500000		82	0.000000000	0.000000000	2.257920000		82	0.000000000	0.000000000	2.211643000
	82	1.571300000	1.668800000	0.011000000		82	0.000000000	1.959106000	-1.127939000		82	0.000000000	1.911972000	-1.107164000
7.8	82	-0.490900000	-1.455200000	-0.739500000	9.5	82	-0.471553000	-1.407255000	-0.770496000	0.1	82	-0.432464000	-1.241745000	-0.997155000
	82	-2.931900000	-0.000800000	-0.000500000		82	-2.916898000	-0.000670000	-0.000364000		82	-2.933519000	-0.000871000	-0.000041000
	82	1.958400000	-1.237500000	0.869600000		82	1.931398000	-1.196852000	0.896691000		82	1.900313000	-1.031439000	1.097725000
	82	-0.491800000	1.455000000	0.741000000		82	-0.472399000	1.406950000	0.771748000		82	-0.433638000	1.241641000	0.996578000
	82	1.956200000	1.238400000	-0.870600000		82	1.929451000	1.197827000	-0.897578000		82	1.899306000	1.032414000	-1.097107000
15.4	82	2.524700000	-0.000400000	-0.073400000	13.9	82	2.503008000	0.000442000	0.067886000	0.0	82	2.592597190	0.207174940	0.078822910
	82	-2.494600000	0.012900000	-0.138200000		82	-2.479645000	-0.001332000	0.122150000		82	-2.588787120	0.205247550	0.166439000
	82	0.053200000	-0.009700000	-1.586200000		82	0.044093000	0.000093000	1.602427000		82	0.031957220	-0.201438460	1.890311140
	82	-0.050600000	-1.866900000	0.901900000		82	-0.034662000	1.816746000	-0.895971000		82	-0.018884970	1.569037750	-1.074910390
	82	-0.032600000	1.864200000	0.895900000		82	-0.032793000	-1.815949000	-0.896493000		82	-0.016882330	-1.780021790	-1.060662660
7.8	82	-0.490900000	-1.455200000	-0.739500000	31.2	82	1.473667000	-1.505163000	0.000000000	9.2	82	1.513774000	-1.587085000	0.000000000
	82	-2.931900000	-0.000800000	-0.000500000		82	-0.000877000	1.208835000	0.000000000		82	-0.000038000	1.142552000	0.000000000
	82	1.958400000	-1.237500000	0.869600000		82	-1.473770000	-1.504501000	0.000000000		82	-1.512693000	-1.586320000	0.000000000
	82	-0.491800000	1.455000000	0.741000000		82	3.022979000	0.900433000	0.000000000		82	3.048078000	1.015505000	0.000000000
	82	1.956200000	1.238400000	-0.870600000		82	-3.022000000	0.900395000	0.000000000		82	-3.049121000	1.015349000	0.000000000
					Pb_6									
0.0	82	-0.006200000	0.011000000	-1.795000000	0.0	82	0.000000000	1.726891000	1.725921000	0.0	82	0.000000000	1.564081000	1.563878000
	82	1.805100000	-1.670400000	0.007100000		82	0.000000000	-1.726891000	1.725921000		82	0.000000000	-1.564081000	1.563878000
	82	-1.655400000	-1.825100000	-0.006200000		82	-1.786605000	0.000000000	0.000678000		82	-2.222749000	0.000000000	0.000885000
	82	1.686900000	1.801200000	-0.005700000		82	1.786605000	0.000000000	0.000678000		82	2.222749000	0.000000000	0.000885000
	82	-0.008600000	0.012400000	1.794800000		82	0.000000000	-1.725497000	-1.726599000		82	0.000000000	-1.564112000	-1.564763000
	82	-1.822000000	1.670900000	0.005000000		82	0.000000000	1.725497000	-1.726599000		82	0.000000000	1.564112000	-1.564763000
11.7	82	1.380100000	1.605500000	0.001300000	14.8	82	-1.388183000	-1.586126000	0.005558000	0.0	82	0.000000000	1.564081000	1.563878000
	82	-2.723300000	-0.950800000	0.002900000		82	2.722574000	0.942882000	0.001155000		82	0.000000000	-1.564081000	1.563878000
	82	-1.009300000	0.912200000	-1.730200000		82	1.008208000	-0.906524000	-1.695877000		82	-2.222749000	0.000000000	0.000885000
	82	0.268800000	-1.606400000	-0.022400000		82	-0.262534000	1.566906000	-0.028189000		82	2.222749000	0.000000000	0.000885000
	82	-0.987400000	0.880500000	1.750300000		82	0.986225000	-0.862134000	1.721141000		82	0.000000000	-1.564112000	-1.564763000
	82	3.071200000	-0.841100000	-0.002000000		82	-3.066290000	0.844996000	-0.003788000		82	0.000000000	1.564112000	-1.564763000
32.3	82	2.238600000	1.201500000	-0.717100000	39.0	82	2.222198000	1.254288000	-0.683008000	0.0	82	0.000000000	1.564081000	1.563878000
	82	-2.231000000	1.228200000	-0.685500000		82	-2.225107000	1.246614000	-0.692595000		82	0.000000000	-1.564081000	1.563878000
	82	2.819700000	-1.537100000	0.266600000		82	2.790526000	-1.480563000	0.272859000		82	-2.222749000	0.000000000	0.000885000
	82	0.023100000	1.858900000	1.160400000		82	-0.006235000	1.636992000	1.247010000		82	2.222749000	0.000000000	0.000885000
	82	-2.840800000	-1.524300000	0.248300000		82	-2.784108000	-1.483969000	0.278657000		82	0.000000000	-1.564112000	-1.564763000
	82	-0.009500000	-1.227200000	-0.272700000		82	0.002726000	-1.173362000	-0.422924000		82	0.000000000	1.564112000	-1.564763000
33.7	82	2.348500000	2.994900000	0.000000000	41.1	82	-3.751208000	0.543109000	-0.186488000	0.0	82	0.000000000	1.564081000	1.563878000
	82	-2.422500000	-2.863600000	0.000000000		82	3.751176000	-0.543396000	-0.186363000		82	0.000000000	-1.564081000	1.563878000
	82	2.832700000	-0.078300000	0.000000000		82	-1.902295000	-1.695390000	0.497193000		82	-2.222749000	0.000000000	0.000885000
	82	0.000000000	1.412900000	0.000000000		82	0.978571000	-1.213279000	-0.310648000		82	2.222749000	0.000000000	0.000885000
	82	0.091000000	-1.532200000	0.000000000		82	1.902417000	1.695448000	0.497003000		82	0.000000000	-1.564112000	-1.564763000
	82	-2.849700000	0.066300000	0.000000000		82	-0.978661000	1.213507000	-0.310697000		82	0.000000000	1.564112000	-1.564763000
					Pb_7									
0.0	82	2.629600000	-0.576400000	0.002400000	0.0	82	0.000000000	-1.574316000	2.166780000	0.0	82	0.000000000	-1.590019000	2.188789000
	82	-1.788600000	2.011200000	0.001200000		82	0.000000000	1.574316000	2.166780000		82	0.000000000	1.590019000	2.188789000
	82	0.000500000	0.000400000	1.692500000		82	-1.671623000	0.000000000	-0.000285000		82	-1.691763000	0.000000000	-0.000076000
	82	0.000100000	-0.000000000	-1.694000000		82	0.000000000	0.000000000	-2.677674000		82	0.000000000	0.000000000	-2.705493000
	82	1.360600000	2.322000000	-0.001800000		82	0.000000000	2.546781000	-0.827658000		82	0.000000000	2.572409000	-0.835966000
	82	-2.466500000	-1.079100000	0.000900000		82	1.671623000	0.000000000	-0.000285000		82	1.691763000	0.000000000	-0.000076000
	82	0.264300000	-2.678100000	-0.001300000		82	0.000000000	-2.546781000	-0.827658000		82	0.000000000	-2.572409000	-0.835966000
24.4	82	-0.493400000	0.698900000	2.231400000	25.4	82	0.390016000	0.008899000	-2.273655000	0.0	82	0.000000000	-1.590019000	2.188789000
	82	-2.274600000	-1.485600000	0.291900000		82	2.138983000	-1.519868000	-0.006120000		82	0.000000000	1.590019000	2.188789000
	82	-2.044100000	1.455300000	-0.515900000		82	2.133239000	1.522684000	0.006467000		82	-1.691763000	0.000000000	-0.000076000
	82	-0.188900000	-0.462100000	-2.286000000		82	0.390551000	-0.008645000	2.272980000		82	0.000000000	0.000000000	-2.705493000
	82	1.123700000	1.841900000	-0.298200000		82	-0.925750000	1.794724000	0.005659000		82	0.000000000	2.572409000	-0.835966000
	82	0.706800000	-1.736300000	0.493200000		82	-0.918386000	-1.792107000	-0.005905000		82	1.691763000	0.000000000	-0.000076000
	82	3.170500000	-0.312000000	0.083600000		82	-3.208653000	-0.005686000	0.000574000		82	0.000000000	-2.572409000	-0.835966000
22.3	82	1.869800000	-1.910200000	-0.194000000	26.2	82	-2.952078000	0.793756000	-0.786388000	21.5	82	-2.956637000	0.805869000	-0.911534000
	82	0.897200000	1.277200000	-1.383000000		82	2.951556000	-0.792704000	-0.789122000		82	2.957781000	-0.802874000	-0.913113000
	82	-0.002500000	-0.022400000	1.587000000		82	-0.913849000	1.248649000	1.374834000		82	-0.971947000	1.252025000	1.404575000

	82	-1.851600000	1.905300000	-0.205000000		82	1.838853000	1.889461000	0.192945000		82	1.853291000	1.879162000	0.305359000
	82	-2.957300000	-0.793100000	0.787000000		82	-1.838237000	-1.890225000	0.187526000		82	-1.854156000	-1.879693000	0.301198000
	82	-0.893000000	-1.292300000	-1.381000000		82	0.913747000	-1.251536000	1.371878000		82	0.971533000	-1.256188000	1.400192000
	82	2.937300000	0.835500000	0.790000000		82	0.000008000	0.002599000	-1.551673000		82	0.000135000	0.001699000	-1.586677000
	82	-3.186500000	-0.276900000	0.064900000		82	-3.160341000	0.166252000	0.103568000		82	0.000000000	-1.590019000	2.188789000
	82	2.106000000	0.181000000	-0.739700000		82	2.053421000	-0.108116000	-0.721748000		82	0.000000000	1.590019000	2.188789000
	82	0.059500000	0.008100000	1.834600000		82	0.015852000	-0.001425000	1.777992000		82	-1.691763000	0.000000000	-0.000076000
22.1	82	-0.907600000	-1.913100000	-0.660100000	26.9	82	-1.128697000	-1.732044000	-0.691959000	0.0	82	0.000000000	0.000000000	-2.705493000
	82	1.343500000	2.854300000	0.076400000		82	1.724097000	2.643527000	0.110961000		82	0.000000000	2.572409000	-0.835966000
	82	-1.232000000	1.733200000	-0.656000000		82	-0.939956000	1.841759000	-0.690281000		82	1.691763000	0.000000000	-0.000076000
	82	1.817100000	-2.586600000	0.080000000		82	1.435624000	-2.809953000	0.111468000		82	0.000000000	-2.572409000	-0.835966000
							Pb_8							
	82	-0.062200000	0.003700000	-1.667600000		82	0.498658000	-0.342273000	-2.450240000		82	0.574120000	-0.152421000	-2.306013000
	82	2.218100000	-0.007700000	1.464700000		82	-0.087312000	1.623492000	0.000000000		82	-0.261459000	1.876217000	0.000000000
	82	-2.476600000	1.567700000	-0.489600000		82	-0.986643000	-1.894178000	0.000000000		82	-0.855880000	-1.831441000	0.000000000
0.0	82	-1.019200000	-0.003900000	1.927300000	0.0	82	0.498658000	-0.342273000	2.450240000	0.0	82	0.574120000	-0.152421000	2.306013000
	82	0.480900000	2.482100000	0.369400000		82	2.827602000	1.465441000	0.000000000		82	2.749739000	1.226942000	0.000000000
	82	0.480600000	-2.484300000	0.359600000		82	-2.478744000	0.464526000	1.554367000		82	-2.549928000	0.365330000	1.533052000
	82	2.855300000	0.007100000	-1.465700000		82	-2.478744000	0.464526000	-1.554367000		82	-2.549928000	0.365330000	-1.533052000
	82	-2.477000000	-1.564700000	-0.498100000		82	2.206527000	-1.439259000	0.000000000		82	2.319219000	-1.697533000	0.000000000
	82	-1.519500000	-1.655800000	0.000700000		82	0.000000000	1.646705000	1.529908000		82	0.000000000	1.678231000	1.548687000
	82	0.544000000	-0.000300000	-1.910900000		82	1.831982000	0.000000000	-0.549038000		82	1.827698000	0.000000000	-0.527083000
	82	3.131200000	0.000600000	0.000400000		82	0.000000000	0.000000000	-3.138532000		82	0.000000000	0.000000000	-3.154231000
9.9	82	-3.953900000	0.001100000	-0.000200000	9.3	82	0.000000000	0.000000000	3.955200000	10.5	82	0.000000000	0.000000000	3.970253000
	82	-1.519000000	1.654700000	-0.000300000		82	0.000000000	-1.646705000	1.529908000		82	0.000000000	-1.678231000	1.548687000
	82	1.386800000	2.571000000	0.000200000		82	0.000000000	-2.548038000	-1.389204000		82	0.000000000	-2.530362000	-1.429615000
	82	1.386700000	-2.570700000	-0.000600000		82	0.000000000	2.548038000	-1.389204000		82	0.000000000	2.530362000	-1.429615000
	82	0.543700000	-0.000500000	1.910800000		82	-1.831982000	0.000000000	-0.549038000		82	-1.827698000	0.000000000	-0.527083000
	82	-3.583400000	-0.107200000	-0.507600000		82	3.603494000	-0.001137000	-0.405968000		82	3.590944000	-0.001478000	-0.377210000
	82	3.584400000	-0.138300000	0.473200000		82	-3.602985000	-0.001176000	0.405674000		82	-3.593109000	-0.001271000	0.378435000
	82	-0.885200000	0.164000000	-1.597000000		82	0.943910000	0.002210000	-1.606320000		82	0.930230000	0.002307000	-1.645661000
9.0	82	-1.613300000	1.780000000	1.118200000	11.3	82	1.471318000	-1.803204000	1.020636000	11.1	82	1.477345000	-1.804584000	1.013416000
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	82	0.916600000	0.125700000	1.640500000		82	-0.944001000	0.001792000	1.606542000		82	-0.929876000	0.001672000	1.645038000
	82	1.401700000	-1.828400000	-1.025000000		82	-1.474510000	1.802049000	-1.024144000		82	-1.478933000	1.805231000	-1.014793000
	82	-1.438800000	-1.821900000	0.989900000		82	1.474285000	1.802076000	1.024561000		82	1.479583000	1.803614000	1.014761000
	82	-1.453500000	2.556900000	0.167000000		82	-1.414700000	2.536814000	0.099476000		82	0.574120000	-0.152421000	-2.306013000
	82	-1.472200000	-2.550900000	0.160100000		82	-1.416254000	-2.536185000	0.099770000		82	-0.261459000	1.876217000	0.000000000
	82	3.232700000	-0.012000000	-0.886600000		82	3.220301000	-0.000567000	-0.940405000		82	-0.855880000	-1.831441000	0.000000000
13.3	82	-2.846700000	0.009100000	-1.001200000	14.0	82	-2.870383000	0.000656000	-0.919471000	0.0	82	0.574120000	-0.152421000	2.306013000
	82	1.643600000	-2.016300000	0.702600000		82	1.643733000	-1.911263000	0.737103000		82	2.749739000	1.226942000	0.000000000
	82	-0.927900000	-0.001300000	1.692400000		82	-0.935320000	0.000284000	1.671690000		82	-2.549928000	0.365330000	1.533052000
	82	1.660500000	2.010300000	0.699100000		82	1.644895000	1.910491000	0.737367000		82	-2.549928000	0.365330000	-1.533052000
	82	0.163500000	0.004200000	-1.533500000		82	0.127728000	-0.000231000	-1.485529000		82	2.319219000	-1.697533000	0.000000000
	82	-1.584190000	2.494385000	-0.402036000		82	-1.517245000	2.510945000	-0.352108000		82	0.574120000	-0.152421000	-2.306013000
	82	-0.002949000	-0.001686000	-1.572531000		82	-0.087963000	0.001049000	-1.560933000		82	-0.261459000	1.876217000	0.000000000
	82	0.001579000	0.005808000	1.735753000		82	0.034519000	0.000979000	1.664882000		82	-0.855880000	-1.831441000	0.000000000
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	82	-1.564811000	-2.507937000	-0.396249000		82	-1.598481000	-2.463317000	-0.362405000		82	2.749739000	1.226942000	0.000000000
	82	1.583559000	-2.494069000	-0.401178000		82	1.517461000	-2.466777000	-0.395213000		82	-2.549928000	0.365330000	1.533052000
	82	1.564120000	2.504717000	-0.400582000		82	1.596904000	2.418403000	-0.406889000		82	-2.549928000	0.365330000	-1.533052000
	82	2.896498000	0.009571000	0.717648000		82	2.922014000	-0.043215000	0.689486000		82	2.319219000	-1.697533000	0.000000000
	82	-3.182100000	0.005100000	-1.306400000		82	3.194048000	-0.030768000	-1.260953000		82	0.574120000	-0.152421000	-2.306013000
	82	1.909700000	-2.736000000	-0.064300000		82	-1.924260000	-2.696546000	-0.001699000		82	-0.261459000	1.876217000	0.000000000
	82	-0.732500000	1.680300000	-0.655600000		82	-1.900417000	2.703337000	-0.028122000		82	-0.855880000	-1.831441000	0.000000000
18.4	82	-0.736000000	-1.677700000	-0.661200000	21.5	82	0.734524000	1.634753000	-0.653296000	0.0	82	0.574120000	-0.152421000	2.306013000
	82	1.915400000	2.735100000	-0.060600000		82	-0.805472000	0.020533000	1.860076000		82	2.749739000	1.226942000	0.000000000
	82	2.507000000	-0.000600000	-0.887600000		82	-2.420718000	-0.000795000	-0.977681000		82	-2.549928000	0.365330000	1.533052000
	82	0.756500000	-0.004900000	1.942100000		82	2.399144000	0.023774000	1.679299000		82	-2.549928000	0.365330000	-1.533052000
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	82	-2.143502000	0.007353000	-2.055624000		82	-2.131138000	-0.000269000	-2.005011000		82	-2.142445000	-0.002308000	-2.089490000
	82	1.876258000	2.557542000	-0.000136000		82	1.902085000	2.527562000	-0.000490000		82	2.062118000	2.424324000	0.001220000
	82	-1.072366000	1.942111000	-0.000049000		82	-1.046537000	1.946269000	-0.001175000		82	-1.067179000	1.976183000	-0.000621000
17.5	82	1.356122000	-0.004632000	-1.648486000	22.2	82	1.272881000	0.000347000	-1.624704000	18.4	82	1.144338000	0.001747000	-1.703801000
	82	-1.087483000	-1.934790000	0.000582000		82	-1.044479000	-1.947473000	0.001016000		82	-1.065198000	-1.977864000	-0.000207000
	82	1.856802000	-2.570960000	-0.000051000		82	1.904963000	-2.525476000	-0.000294000		82	2.064275000	-2.421228000	-0.000391000
	82	-2.143326000	0.008222000	2.055974000		82	-2.130972000	-0.001838000	2.005114000		82	-2.140727000	-0.001551000	2.089671000
	82	1.357495000	-0.004846000	1.647789000		82	1.273197000	0.000878000	1.624637000		82	1.144819000	0.000696000	1.703618000
	82	3.516312000	-0.593180000	0.750116000		82	3.524964000	-0.697367000	0.654308000		82	3.453254000	-1.133365000	-0.182681000
	82	-0.602038000	1.356242000	-0.679427000		82	-0.608033000	1.434255000	-0.439209000		82	-0.666710000	1.701533000	-0.001884000
	82	-2.379183000	-0.927290000	1.521610000		82	-2.371394000	-1.092919000	1.426883000		82	-2.259270000	-0.358483000	1.957434000
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	82	2.228622000	2.038346000	-0.140468000		82	2.243823000	1.990043000	0.130941000		82	2.372661000	1.719788000	0.677578000
	82	-1.489308000	-1.781846000	-1.263169000		82	-1.492085000	-1.504142000	-1.451052000		82	-1.373989000	-1.568918000	-1.032467000
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							Pb_9							
	82	1.651800000	-0.000500000	1.808200000		82	0.000000000	2.566365000	0.708426000		82	0.000000000	2.525494000	0.698189000
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	82	-1.427600000	-0.870800000	-2.383200000		82	1.402129000	0.157454000	-2.521414000		82	1.478708000	0.162488000	-2.538022000
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	82	-1.000100000	-1.722300000	0.656200000		82	0.817378000	1.820594000	0.120763000		82	0.805912000	1.846778000	0.123998000
12.0	82	1.718700000	0.373600000	1.637100000	16.1	82	-1.702342000	-0.084769000	1.646497000	15.3	82	-1.646030000	-0.083087000	1.686902000
	82	-3.231400000	0.282500000	-0.066500000		82	3.256871000	0.001135000	-0.004867000		82	3.324295000	0.000515000	-0.003722000
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	82	2.366100000	2.311500000	-0.601700000		82	-2.145936000	-2.509698000	-0.124864000		82	-2.300826000	-2.483913000	-0.119198000
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	82	1.988500000	-1.828200000	-0.959700000		82	-1.997196000	1.783205000	-0.951424000		82	-2.014400000	1.821300000	-0.925800000
	82	1.987600000	1.827700000	-0.959400000		82	-1.996816000	-1.783393000	-0.951079000		82	-2.014100000	-1.821400000	-0.926300000
18.6	82	-1.242200000	-2.409000000	0.221000000	20.0	82	1.233753000	2.374230000	0.195690000	17.2	82	1.254000000	2.312400000	0.195600000
	82	0.706100000	-0.000700000	1.552500000		82	-0.694444000	0.000150000	1.513978000		82	-0.691900000	0.000100000	1.528300000
	82	-2.364100000	-0.001300000	1.925300000		82	2.347160000	0.000204000	1.903589000		82	2.442900000	0.000500000	2.001700000
	82	3.623300000	0.000500000	0.978200000		82	-3.612973000	-0.000086000	0.983803000		82	-3.707000000	-0.000600000	0.945300000
	82	-1.238800000	2.408700000	0.222900000		82	1.233379000	-2.374080000	0.195785000		82	1.253400000	-2.311900000	0.196400000
	82	-1.778300000	-2.523200000	-0.082500000		82	1.758822000	2.504779000	-0.058918000		82	1.826370000	0.041245000	2.535284000
	82	3.826000000	-0.000300000	-0.647400000		82	-3.819020000	0.000261000	-0.642259000		82	-3.942551000	0.745695000	0.000000000
	82	1.268700000	-1.734000000	-0.828800000		82	-1.263326000	1.689319000	-0.802942000		82	-1.261201000	0.771430000	1.676222000
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20.1	82	-3.381400000	-0.000100000	0.881600000	21.7	82	3.390623000	-0.000131000	0.806565000	18.6	82	3.507674000	-0.725997000	0.000000000
	82	2.489100000	0.000700000	2.022800000		82	-2.471750000	-0.000446000	1.986762000		82	-2.579418000	-1.953504000	0.000000000
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	82	-3.579369000	-0.618994000	-0.752249000		82	-3.568375000	-0.619512000	-0.763278000		82	-3.503408000	-1.072138000	-0.785130000
	82	-1.373616000	-2.091702000	0.839243000		82	-1.379464000	-2.059246000	0.829586000		82	-1.214685000	-1.972251000	1.034194000
	82	-2.129049000	1.204489000	1.394644000		82	-2.123678000	1.166395000	1.380905000		82	-2.206556000	1.157804000	1.288700000
19.7	82	-0.003702000	2.924284000	-0.000755000	22.4	82	-0.003776000	2.885738000	-0.000654000	16.0	82	-0.001432000	3.000505000	0.005046000
	82	-0.843992000	0.039747000	-1.691214000		82	-0.830744000	0.065591000	-1.626410000		82	-0.968723000	0.381426000	-1.645661000
	82	2.128177000	1.208050000	-1.392063000		82	2.123285000	1.170594000	-1.377845000		82	2.203764000	1.162904000	-1.286090000
	82	3.580113000	-0.616048000	0.754169000		82	3.568968000	-0.617401000	0.765007000		82	3.504545000	-1.069363000	0.782549000
	82	0.843373000	0.038599000	1.691164000		82	0.830559000	0.063851000	1.626680000		82	0.968018000	0.380168000	1.645366000
	82	-1.821167000	-0.971306000	-1.690918000		82	-1.854474000	-0.976189000	-1.645052000		82	-1.903971000	-1.011352000	-1.644226000
	82	-0.944001000	2.028183000	-0.001792000		82	-0.936111000	1.959678000	0.010466000		82	-0.879589000	1.893394000	0.009548000
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	82	3.287032000	-1.116125000	-0.001417000		82	3.327138000	-0.947402000	-0.017441000		82	3.353587000	-0.868315000	-0.019591000
	82	1.225965000	0.185430000	1.791160000		82	1.183547000	0.150308000	1.775543000		82	1.167684000	0.162147000	1.882005000
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	82	-2.067475000	1.727504000	-0.010778000		82	-2.070118000	1.698528000	-0.004026000		82	-2.109200000	1.722100000	-0.003900000
	82	-1.558154000	-1.177323000	-1.729265000		82	-1.560387000	-1.137346000	-1.689619000		82	-1.591200000	-1.131300000	-1.704000000
	82	0.538390000	1.331935000	1.807974000		82	0.537775000	1.308199000	1.756774000		82	0.537400000	1.349800000	1.746300000
	82	0.539647000	1.312822000	-1.819719000		82	0.538753000	1.299078000	-1.761257000		82	0.537900000	1.340200000	-1.750400000
30.9	82	3.968272000	-1.524746000	0.002854000	35.5	82	3.973392000	-1.505981000	0.000893000	29.9	82	4.077600000	-1.561400000	0.001600000
	82	1.108304000	-1.417668000	0.010861000		82	1.113518000	-1.403171000	0.005987000		82	1.137100000	-1.416000000	0.005500000
	82	-4.024845000	-0.475582000	0.000207000		82	-4.031544000	-0.488026000	-0.001616000		82	-4.137200000	-0.536100000	-0.001400000
	82	3.057837000	1.378333000	-0.003498000		82	3.061411000	1.356838000	-0.002548000		82	3.140300000	1.354300000	-0.002300000
	82	-1.561977000	-1.155274000	1.741364000		82	-1.562800000	-1.128120000	1.695412000		82	-1.592800000	-1.121600000	1.708700000
	82	-0.886971000	-0.000468000	1.735908000		82	-0.894101000	-0.000588000	1.682198000		82	-0.754811000	-0.000048000	1.690425000
	82	4.426739000	-0.001162000	-0.341620000		82	4.414953000	-0.006763000	-0.358561000		82	4.514046000	-0.004552000	-0.341218000
	82	-3.102931000	-1.463664000	-0.457663000		82	-3.076412000	-1.452378000	-0.463741000		82	-3.153207000	-1.472563000	-0.401768000
	82	-0.347019000	0.001058000	-1.653028000		82	-0.352330000	0.002283000	-1.587761000		82	-0.343881000	0.001806000	-1.590392000
31.5	82	-0.571596000	-2.917636000	0.521545000	35.7	82	-0.577117000	-2.888585000	0.525466000	29.5	82	-0.642281000	-2.972330000	0.374912000
	82	-3.105266000	1.462820000	-0.451079000		82	-3.073612000	1.457276000	-0.462947000		82	-3.148041000	1.477850000	-0.401368000
	82	2.079602000	1.649574000	0.057383000		82	2.068861000	1.618958000	0.067001000		82	2.084315000	1.645160000	0.148537000
	82	-0.571706000	2.916687000	0.523378000		82	-0.569820000	2.886809000	0.528488000		82	-0.633217000	2.972641000	0.377071000
	82	2.079148000	-1.647209000	0.065177000		82	2.059578000	-1.617012000	0.069856000		82	2.077076000	-1.647965000	0.143799000
	82	-2.888012000	-1.996516000	-0.622211000		82	-2.875442000	-1.983418000	-0.680275000		82	0.820100000	-2.122100000	-2.659800000
	82	0.007178000	3.173022000	-1.208311000		82	0.000194000	3.205206000	-1.093116000		82	1.193200000	3.198900000	0.000000000
	82	2.877487000	-2.009239000	-0.621711000		82	2.875420000	-1.983487000	-0.680165000		82	0.820100000	-2.122100000	2.659800000
	82	0.004105000	1.874622000	1.657089000		82	-0.000072000	1.779223000	1.637791000		82	-1.468800000	1.553100000	0.000000000
31.9	82	2.263987000	-0.235605000	1.843089000	38.4	82	2.275369000	-0.280005000	1.787925000	31.4	82	-1.667500000	-0.103400000	2.671300000
	82	-2.265313000	-0.227051000	1.842589000		82	-2.275550000	-0.279824000	1.787808000		82	-1.667500000	-0.103400000	-2.671300000
	82	1.770343000	0.773223000	-1.216011000		82	1.736747000	0.791754000	-1.189764000		82	1.361900000	0.724800000	1.792200000
	82	-1.764356000	0.780021000	-1.216011000		82	-1.736630000	0.791837000	-1.189868000		82	1.361900000	0.724800000	-1.792200000
	82	-0.005419000	-2.132477000	-0.458511000		82	-0.000036000	-2.041285000	-0.380339000		82	-0.753400000	-1.750600000	0.000000000
								Pb_{10}						
	82	-1.191595000	0.526417000	-1.971335000		82	-1.186802000	1.389197000	-1.432008000		82	-1.016504000	-1.763487000	-1.198970000
0.0	82	0.334249000	-2.204938000	-2.200779000	0.0	82	0.314485000	-0.862035000	-2.979218000	1.6	82	-3.134204000	0.000201000	0.339348000
	82	-3.425706000	-0.035825000	-0.008446000		82	-3.428164000	-0.013716000	0.007278000		82	0.014412000	-0.000212000	-3.506338000
	82	1.994452000	1.327622000	1.315273000		82	1.989626000	0.515818000	1.760549000		82	1.864435000	-0.000044000	2.025696000

	82	-1.171371000	-1.974439000	0.537388000		82	-1.170445000	-1.944123000	-0.466558000		82	-1.015869000	1.761999000	-1.198026000
	82	-1.210235000	1.445657000	1.437495000		82	-1.175375000	0.560688000	1.927038000		82	2.044478000	0.000133000	-1.189164000
	82	0.313165000	3.014993000	-0.810509000		82	0.340649000	3.013629000	0.740362000		82	1.559860000	-2.718081000	0.347444000
	82	2.022363000	-1.794276000	0.487332000		82	1.989384000	-1.793829000	-0.452625000		82	-0.938412000	1.621016000	2.015972000
	82	2.006688000	0.485521000	-1.802703000		82	1.976149000	1.276680000	-1.345350000		82	-0.937910000	-1.619934000	2.014703000
	82	0.327989000	-0.790732000	3.016284000		82	0.350493000	-2.142310000	2.240532000		82	1.559714000	2.717911000	0.348837000
	82	2.387616000	0.244902000	-0.169543000		82	-2.305682000	-0.505010000	-0.172597000		82	-2.440332000	-0.534280000	-0.152429000
	82	0.832359000	1.715189000	2.165111000		82	-0.616892000	-1.767847000	2.146267000		82	-0.621389000	-1.782114000	2.123528000
	82	1.166122000	-1.494181000	2.178042000		82	-1.307340000	1.361943000	2.138351000		82	-1.314598000	1.369862000	2.116373000
	82	1.716658000	-2.450757000	-1.310615000		82	-2.000723000	2.243931000	-1.268175000		82	-2.013075000	2.258965000	-1.297109000
1.0	82	-3.029918000	-0.319285000	-1.204039000	0.7	82	2.982129000	0.653028000	-1.187156000	4.5	82	3.003958000	0.657724000	-1.226859000
	82	-1.782034000	-0.177067000	2.278841000		82	1.756127000	0.393407000	2.231418000		82	1.764204000	0.395256000	2.216949000
	82	-1.414637000	1.927949000	-0.050908000		82	1.594914000	-1.719419000	-0.065740000		82	1.688429000	-1.816131000	-0.039761000
	82	-0.070245000	-0.013481000	-2.529240000		82	0.048911000	-0.000425000	-2.497597000		82	0.045087000	-0.000343000	-2.416117000
	82	-0.985857000	-2.175588000	-0.035903000		82	0.721329000	2.222828000	-0.077328000		82	0.766342000	2.353526000	-0.054088000
	82	1.179936000	2.742319000	-1.321746000		82	-0.872773000	-2.882436000	-1.247443000		82	-0.878627000	-2.902464000	-1.270488000
	82	1.341736000	-1.743929000	1.638235000		82	1.345042000	-1.720434000	1.606289000		82	1.350000000	-1.655500000	1.631600000
	82	1.340560000	1.741819000	1.639551000		82	1.342881000	1.709652000	1.612179000		82	1.349200000	1.648700000	1.640700000
	82	-1.318037000	0.001630000	-1.929007000		82	-1.311247000	0.006256000	-1.886396000		82	-1.352500000	0.005200000	-2.291500000
	82	3.403128000	0.001393000	-0.001868000		82	3.397845000	0.003138000	-0.009003000		82	3.491700000	0.001100000	-0.009100000
3.6	82	1.339098000	1.743081000	-1.638632000	1.1	82	1.330246000	1.719073000	-1.608629000	0.0	82	1.338500000	1.655400000	-1.637200000
	82	1.339622000	-1.743600000	-1.638851000		82	1.332738000	-1.707780000	-1.612616000		82	1.340100000	-1.646300000	-1.646700000
	82	-3.596512000	-0.000228000	0.001897000		82	-3.588113000	0.001065000	0.011154000		82	-3.488400000	-0.001900000	0.009500000
	82	-1.266909000	2.617694000	0.001743000		82	-1.279372000	2.581758000	0.011985000		82	-1.346500000	2.368800000	0.009100000
	82	-1.267976000	-2.616337000	-0.000554000		82	-1.277295000	-2.583545000	-0.006487000		82	-1.344400000	-2.370000000	-0.002800000
	82	-1.314710000	-0.001523000	1.927485000		82	-1.292726000	-0.009183000	1.881524000		82	-1.337700000	-0.005500000	2.296500000
	82	3.090186000	-1.586207000	-0.743890000		82	3.083850000	-1.574942000	-0.725300000		82	3.165260000	-1.597082000	-0.717312000
	82	0.485784000	-2.635701000	0.601210000		82	0.477998000	-2.603881000	0.600688000		82	0.485634000	-2.615202000	0.624557000
	82	-4.092310000	-0.001390000	0.418410000		82	-4.088509000	-0.000109000	0.413041000		82	-4.210262000	0.018438000	0.409894000
	82	-2.129406000	1.768605000	-1.117190000		82	-2.118837000	1.727145000	-1.108005000		82	-2.163819000	1.734823000	-1.104314000
18.1	82	0.483390000	-0.001101000	-1.479890000	13.9	82	0.502393000	0.000090000	-1.428863000	12.3	82	0.517764000	-0.006485000	-1.462909000
	82	-1.239510000	0.002703000	1.665710000		82	-1.239066000	-0.000272000	1.617586000		82	-1.256618000	-0.009397000	1.630429000
	82	0.483496000	2.636999000	0.597810000		82	0.477427000	2.603737000	0.601134000		82	0.479028000	2.613742000	0.617174000
	82	-2.129014000	-1.770395000	-1.115790000		82	-2.118599000	-1.727321000	-1.108162000		82	-2.161898000	-1.738506000	-1.091117000
	82	1.957090000	0.000495000	1.916110000		82	1.940132000	0.000101000	1.863655000		82	1.995204000	0.008399000	1.832892000
	82	3.090294000	1.585993000	-0.742490000		82	3.083213000	1.575453000	-0.725772000		82	3.150207000	1.591269000	-0.739291000

Table ESI-2. HOMO-LUMO gap for Pb_n (n = 3 - 10) isomers. Energy in eV at PBE0 level of theory.

	ISOMERS	LANL2DZ-SR	DEF2TZVP-SR	ZORA-SR/TZ2P	CRENBL-SO	ZORA-SO/TZ2P
Pb3	Isomer01	1.95	1.88 (0.72)	1.88 (0.75)	2.10 (0.78)	2.24 (0.89)
	Isomer02	1.88	1.89 (0.89)	1.87 (0.89)		
Pb4	Isomer01	2.35	2.36 (1.12)	2.37 (1.23)	2.52 (1.48)	2.73 (1.50)
	Isomer02	1.74	1.80 (0.68)	1.81 (0.67)	2.01 (0.78)	2.11 (0.84)
Pb5	Isomer01	2.74	2.66 (1.48)	2.71 (1.50)	1.30 (0.29)	1.37 (0.29)
	Isomer02	2.19	2.21 (0.97)	2.22 (0.97)	2.00 (0.86)	2.11 (0.98)
	Isomer03	1.38	1.38 (0.24)	1.38 (0.24)	1.41 (0.21)	1.51 (0.24)
	Isomer04	0.96	1.02 (0.12)	1.02 (0.12)	1.80 (0.61)	1.87 (0.67)
Pb6	Isomer01	2.73	2.73 (1.56)	2.72 (1.56)	1.81 (0.83)	1.91 (0.88)
	Isomer02	2.30	2.32 (1.15)	2.32 (1.15)	1.81 (0.83)	1.91 (0.88)
	Isomer03	2.06	1.94 (0.91)	1.96 (0.88)	1.81 (0.83)	1.91 (0.88)
	Isomer04	1.91	1.80 (0.75)	1.82 (0.74)	1.81 (0.83)	1.91 (0.88)
Pb7	Isomer01	2.47	2.46 (1.24)	2.44 (1.25)	1.94 (0,78)	2.02 (0.91)
	Isomer02	2.03	2.11 (1.01)	2.11 (0.99)	1.94 (0.78)	2.02 (0.91)
	Isomer03	1.80	1.78 (0.63)	1.77 (0.63)	1.48 (0.50)	1.65 (0.56)
	Isomer04	2.70	2.64 (1.53)	2.11 (1.51)	1.94 (0.78)	2.02 (0.91)
Pb8	Isomer01	2.20	2.21 (1.09)	2.21 (1.10)	1.68 (0.80)	1.79 (0.81)
	Isomer02	1.90	1.89 (0.84)	1.89 (0.82)	1.26 (0.38)	1.40 (0.43)
	Isomer03	1.85	1.88 (0.78)	1.90 (0.80)	1.48 (0.51)	1.61 (0.56)
	Isomer04	1.49	1.35 (0.32)	1.35 (0.34)	1.68 (0.80)	1.79 (0.81)
	Isomer05	1.78	1.75 (0.67)	1.76 (0.68)	1.68 (0.80)	1.79 (0.81)
	Isomer06	1.69	1.65 (0.61)	1.65 (0.60)	1.68 (0.80)	1.79 (0.81)
	Isomer07	1.72	1.66 (0.60)	1.66 (0.59)	1.36 (0.39)	1.41 (0.43)
	Isomer08	1.48	1.43 (0.45)	1.44 (0.46)	1.75 (0.73)	1.84 (0.79)
Pb9	Isomer01	2.42	2.42 (1.29)	2.42 (1.30)	(0.92)	(0.99)
	Isomer02	2.07	2.04 (0.98)	2.03 (0.98)	(0.60)	(0.62)
	Isomer03	1.88	1.92 (0.86)	1.92 (0.87)	(0.62)	(0.64)
	Isomer04	1.80	1.74 (0.70)	1.74 (0.69)	(0.53)	(0.57)
	Isomer05	1.77	1.76 (0.77)	1.75 (0.77)	(0.65)	(0.70)
	Isomer06	1.58	1.56 (0.53)	1.56 (0.54)	(0.40)	(0.45)
	Isomer07	2.25	2.22 (1.10)	2.21 (1.10)	(0.89)	(0.93)
	Isomer08	1.89	1.98 (1.02)	1.98 (1.02)	(0.52)	(0.59)
	Isomer09	1.96	1.91 (0.93)	1.91 (0.93)	(0.85)	(0.90)
	Isomer10	1.78	1.74 (0.66)	1.74 (0.68)	(0.47)	(0.52)
Pb10	Isomer01	2.53	2.56 (1.45)	(1.46)	(0.95)	(1.03)
	Isomer02	2.67	2.71 (1.58)	(1.59)	(0.91)	(0.96)
	Isomer03	1.90	1.99 (0.92)	(0.94)	(0.56)	(0.61)
	Isomer04	1.87	1.84 (0.76)	(0.74)	(0.62)	(0.68)