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Theoretical assessment of thermodynamic stability of 2D octane-1,8-diammonium lead halide perovskites

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Supporting information

Calculated charges in *.cif file with P1 symmetry

$(NH_3C_8H_{16}NH_3)MA_{n-1}Pb_nI_{3n+1}$ (n =1)

generated using pymatgen

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H H109 1 0.039295 0.152581 0.774515 1.0 0.0727

H H110 1 0.039295 0.847419 0.274515 1.0 0.0728

H H111 1 0.539295 0.652581 0.774515 1.0 0.0727

H H112 1 0.539295 0.347419 0.274515 1.0 0.0728

Pb Pb113 1 0.816140 0.251500 0.748900 1.0 0.7338

Pb Pb114 1 0.816140 0.748500 0.248900 1.0 0.7336

Pb Pb115 1 0.316140 0.751500 0.748900 1.0 0.7338

Pb Pb116 1 0.316140 0.248500 0.248900 1.0 0.7336

Pb Pb117 1 0.146360 0.748500 0.749000 1.0 0.7591

Pb Pb118 1 0.146360 0.251500 0.249000 1.0 0.7587

Pb Pb119 1 0.646360 0.248500 0.749000 1.0 0.7591

Pb Pb120 1 0.646360 0.751500 0.249000 1.0 0.7587

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C C122 1 0.739000 0.260000 0.218000 1.0 -0.2791

C C123 1 0.239000 0.240000 0.718000 1.0 -0.2788

C C124 1 0.239000 0.760000 0.218000 1.0 -0.2791

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C C126 1 0.897900 0.186000 0.207000 1.0 -0.0178

C C127 1 0.397900 0.314000 0.707000 1.0 -0.0195

C C128 1 0.397900 0.686000 0.207000 1.0 -0.0178

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C C130 1 0.934700 0.217000 0.258000 1.0 -0.1434

C C131 1 0.434700 0.283000 0.758000 1.0 -0.1451

C C132 1 0.434700 0.717000 0.258000 1.0 -0.1434

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C C134 1 0.939400 0.383000 0.281000 1.0 -0.1699

C C135 1 0.439400 0.117000 0.781000 1.0 -0.17

C C136 1 0.439400 0.883000 0.281000 1.0 -0.1699

C C137 1 0.971400 0.590000 0.875000 1.0 -0.1725

C C138 1 0.971400 0.410000 0.375000 1.0 -0.1725

C C139 1 0.471400 0.090000 0.875000 1.0 -0.1725

C C140 1 0.471400 0.910000 0.375000 1.0 -0.1725

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C C142 1 0.981200 0.573000 0.367000 1.0 -0.17

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C C147 1 0.502400 0.899000 0.729000 1.0 -0.155

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C C150 1 0.040400 0.619000 0.270000 1.0 -0.1442

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C C152 1 0.540400 0.119000 0.270000 1.0 -0.1442

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C C154 1 0.052800 0.772000 0.224000 1.0 0.0287

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C C156 1 0.552800 0.272000 0.224000 1.0 0.0287

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I I167 1 0.157700 0.004500 0.991400 1.0 -0.421

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I I170 1 0.139200 0.508700 0.497300 1.0 -0.4155

I I171 1 0.639200 0.991300 0.997300 1.0 -0.4162

I I172 1 0.639200 0.008700 0.497300 1.0 -0.4155

I I173 1 0.066330 0.810000 0.759000 1.0 -0.4231

I I174 1 0.066330 0.190000 0.259000 1.0 -0.424

I I175 1 0.566330 0.310000 0.759000 1.0 -0.4231

I I176 1 0.566330 0.690000 0.259000 1.0 -0.424

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I I178 1 0.730100 0.793800 0.253600 1.0 -0.3984

I I179 1 0.230100 0.706200 0.753600 1.0 -0.399

I I180 1 0.230100 0.293800 0.253600 1.0 -0.3984

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I I182 1 0.895030 0.689200 0.259800 1.0 -0.3883

I I183 1 0.395030 0.810800 0.759800 1.0 -0.3869

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N N187 1 0.226400 0.298000 0.867000 1.0 -0.4665

N N188 1 0.226400 0.702000 0.367000 1.0 -0.4664

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N N190 1 0.874000 0.307000 0.264000 1.0 -0.4109

N N191 1 0.374000 0.193000 0.764000 1.0 -0.4114

N N192 1 0.374000 0.807000 0.264000 1.0 -0.4109

N N193 1 0.090800 0.210000 0.764000 1.0 -0.4589

N N194 1 0.090800 0.790000 0.264000 1.0 -0.4591

N N195 1 0.590800 0.710000 0.764000 1.0 -0.4589

N N196 1 0.590800 0.290000 0.264000 1.0 -0.4591

$(NH_3C_8H_{16}NH_3)MA_{n-1}PbnI_{3n+1}$ (n =3)

generated using pymatgen

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_cell_length_b 8.91060000

_cell_length_c 8.91590000

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_cell_angle_beta 100.02400000

_cell_angle_gamma 90.00000000

_symmetry_Int_Tables_number 1

_chemical_formula_structural H34Pb3C10(I5N2)2

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1 'x, y, z'

loop_

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H H2 1 0.421318 0.122833 0.955730 1.0 0.2796

H H3 1 0.398821 0.773160 0.546981 1.0 0.2988

H H4 1 0.398821 0.226840 0.046981 1.0 0.298

H H5 1 0.425599 0.720555 0.430579 1.0 0.2853

H H6 1 0.425599 0.279445 0.930579 1.0 0.2858

H H7 1 0.634554 0.701131 0.384199 1.0 0.2874

H H8 1 0.634554 0.298869 0.884199 1.0 0.2871

H H9 1 0.621732 0.590427 0.486521 1.0 0.2908

H H10 1 0.621732 0.409573 0.986521 1.0 0.2958

H H11 1 0.582293 0.691771 0.415621 1.0 0.2814

H H12 1 0.582293 0.308229 0.915621 1.0 0.2813

H H13 1 0.195110 0.317120 0.846705 1.0 0.3127

H H14 1 0.195110 0.682880 0.346705 1.0 0.3127

H H15 1 0.158129 0.322239 0.947985 1.0 0.2389

H H16 1 0.158129 0.677761 0.447985 1.0 0.2386

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H H18 1 0.164332 0.811573 0.366262 1.0 0.2392

H H19 1 0.867711 0.776638 0.685669 1.0 0.2856

H H20 1 0.867711 0.223362 0.185669 1.0 0.2854

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H H24 1 0.895062 0.285592 0.074878 1.0 0.2384

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H H66 1 0.956123 0.509871 0.069085 1.0 0.0696

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H H68 1 0.992429 0.493114 0.945773 1.0 0.0786

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Pb Pb71 1 0.247400 0.250900 0.381700 1.0 0.7443

Pb Pb72 1 0.247400 0.749100 0.881700 1.0 0.7447

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C C76 1 0.122400 0.662000 0.235000 1.0 -0.0153

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C C78 1 0.939100 0.290000 0.279000 1.0 -0.06

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C C80 1 0.354000 0.205000 0.845000 1.0 -0.2578

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C C82 1 0.630100 0.211000 0.084000 1.0 -0.2402

C C83 1 0.080800 0.219000 0.699000 1.0 -0.1704

C C84 1 0.080800 0.781000 0.199000 1.0 -0.1691

C C85 1 0.992800 0.730000 0.738000 1.0 -0.1774

C C86 1 0.992800 0.270000 0.238000 1.0 -0.1748

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C C88 1 0.027800 0.709000 0.150000 1.0 -0.2023

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C C90 1 0.990400 0.304000 0.072000 1.0 -0.1613

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C C92 1 0.033900 0.542000 0.156000 1.0 -0.181

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$(NH_3C_8H_{16}NH_3)MA_{n-1}PbnI_{3n+1}$ (n =4)

generated using pymatgen

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H H7 1 0.061026 0.275017 0.542109 1.0 0.2896

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H H63 1 0.437302 0.277143 0.110403 1.0 0.0924

H H64 1 0.437302 0.722857 0.610403 1.0 0.0924

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H H66 1 0.957017 0.116966 0.624241 1.0 0.093

H H67 1 0.457017 0.383034 0.124241 1.0 0.0957

H H68 1 0.457017 0.616966 0.624241 1.0 0.093

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H H70 1 0.959235 0.273586 0.545676 1.0 0.0963

H H71 1 0.459235 0.226414 0.045676 1.0 0.0961

H H72 1 0.459235 0.773586 0.545676 1.0 0.0963

H H73 1 0.844360 0.336941 0.578664 1.0 0.0877

H H74 1 0.844360 0.663059 0.078664 1.0 0.0876

H H75 1 0.344360 0.836941 0.578664 1.0 0.0877

H H76 1 0.344360 0.163059 0.078664 1.0 0.0876

H H77 1 0.848905 0.168077 0.615931 1.0 0.1008

H H78 1 0.848905 0.831923 0.115931 1.0 0.1034

H H79 1 0.348905 0.668077 0.615931 1.0 0.1008

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H H81 1 0.840960 0.276777 0.742328 1.0 0.0935

H H82 1 0.840960 0.723223 0.242328 1.0 0.0938

H H83 1 0.340960 0.776777 0.742328 1.0 0.0935

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H H85 1 0.544987 0.648318 0.777736 1.0 0.0926

H H86 1 0.544987 0.351682 0.277736 1.0 0.0956

H H87 1 0.044987 0.148318 0.777736 1.0 0.0926

H H88 1 0.044987 0.851682 0.277736 1.0 0.0956

H H89 1 0.553975 0.804971 0.826155 1.0 0.0966

H H90 1 0.553975 0.195029 0.326155 1.0 0.0952

H H91 1 0.053975 0.304971 0.826155 1.0 0.0966

H H92 1 0.053975 0.695029 0.326155 1.0 0.0952

H H93 1 0.536475 0.795053 0.701718 1.0 0.0942

H H94 1 0.536475 0.204947 0.201718 1.0 0.0938

H H95 1 0.036475 0.295053 0.701718 1.0 0.0942

H H96 1 0.036475 0.704947 0.201718 1.0 0.0938

H H97 1 0.291283 0.285615 0.930375 1.0 0.0773

H H98 1 0.291283 0.714385 0.430375 1.0 0.077

H H99 1 0.791283 0.785615 0.930375 1.0 0.0773

H H100 1 0.791283 0.214385 0.430375 1.0 0.077

H H101 1 0.272520 0.388966 0.981014 1.0 0.0662

H H102 1 0.272520 0.611034 0.481014 1.0 0.0643

H H103 1 0.772520 0.888966 0.981014 1.0 0.0662

H H104 1 0.772520 0.111034 0.481014 1.0 0.0643

H H105 1 0.264872 0.144331 0.856618 1.0 0.116

H H106 1 0.264872 0.855669 0.356618 1.0 0.1168

H H107 1 0.764872 0.644331 0.856618 1.0 0.116

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H H109 1 0.267148 0.083830 0.021148 1.0 0.0733

H H110 1 0.267148 0.916170 0.521148 1.0 0.0698

H H111 1 0.767148 0.583830 0.021148 1.0 0.0733

H H112 1 0.767148 0.416170 0.521148 1.0 0.0698

H H113 1 0.231854 0.148527 0.961109 1.0 0.0733

H H114 1 0.231854 0.851473 0.461109 1.0 0.0741

H H115 1 0.731854 0.648527 0.961109 1.0 0.0733

H H116 1 0.731854 0.351473 0.461109 1.0 0.0741

H H117 1 0.239212 0.315783 0.945509 1.0 0.0627

H H118 1 0.239212 0.684217 0.445509 1.0 0.0617

H H119 1 0.739212 0.815783 0.945509 1.0 0.0627

H H120 1 0.739212 0.184217 0.445509 1.0 0.0617

H H121 1 0.246501 0.162583 0.213354 1.0 0.0662

H H122 1 0.246501 0.837417 0.713354 1.0 0.0652

H H123 1 0.746501 0.662583 0.213354 1.0 0.0662

H H124 1 0.746501 0.337417 0.713354 1.0 0.0652

H H125 1 0.245628 0.336937 0.190927 1.0 0.0755

H H126 1 0.245628 0.663063 0.690927 1.0 0.0747

H H127 1 0.745628 0.836937 0.190927 1.0 0.0755

H H128 1 0.745628 0.163063 0.690927 1.0 0.0747

H H129 1 0.209158 0.168525 0.142720 1.0 0.0763

H H130 1 0.209158 0.831475 0.642720 1.0 0.0764

H H131 1 0.709158 0.668525 0.142720 1.0 0.0763

H H132 1 0.709158 0.331475 0.642720 1.0 0.0764

H H133 1 0.210461 0.339545 0.182829 1.0 0.0614

H H134 1 0.210461 0.660455 0.682829 1.0 0.0592

H H135 1 0.710461 0.839545 0.182829 1.0 0.0614

H H136 1 0.710461 0.160455 0.682829 1.0 0.0592

H H137 1 0.218834 0.287751 0.425192 1.0 0.0639

H H138 1 0.218834 0.712249 0.925192 1.0 0.0665

H H139 1 0.718834 0.787751 0.425192 1.0 0.0639

H H140 1 0.718834 0.212249 0.925192 1.0 0.0665

H H141 1 0.222141 0.117283 0.388700 1.0 0.0632

H H142 1 0.222141 0.882717 0.888700 1.0 0.0628

H H143 1 0.722141 0.617283 0.388700 1.0 0.0632

H H144 1 0.722141 0.382717 0.888700 1.0 0.0628

H H145 1 0.182577 0.254921 0.358550 1.0 0.1078

H H146 1 0.182577 0.745079 0.858550 1.0 0.107

H H147 1 0.682577 0.754921 0.358550 1.0 0.1078

H H148 1 0.682577 0.245079 0.858550 1.0 0.107

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H H150 1 0.186921 0.918222 0.854996 1.0 0.0539

H H151 1 0.686921 0.581778 0.354996 1.0 0.0509

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H H154 1 0.198393 0.770665 0.114991 1.0 0.0676

H H155 1 0.698393 0.729335 0.614991 1.0 0.0672

H H156 1 0.698393 0.270665 0.114991 1.0 0.0676

H H157 1 0.189410 0.066120 0.599319 1.0 0.063

H H158 1 0.189410 0.933880 0.099319 1.0 0.0641

H H159 1 0.689410 0.566120 0.599319 1.0 0.063

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Pb Pb161 1 0.115880 0.249400 0.179800 1.0 0.7255

Pb Pb162 1 0.115880 0.750600 0.679800 1.0 0.7253

Pb Pb163 1 0.615880 0.749400 0.179800 1.0 0.7255

Pb Pb164 1 0.615880 0.250600 0.679800 1.0 0.7253

Pb Pb165 1 0.015250 0.250100 0.180200 1.0 0.7126

Pb Pb166 1 0.015250 0.749900 0.680200 1.0 0.7129

Pb Pb167 1 0.515250 0.750100 0.180200 1.0 0.7126

Pb Pb168 1 0.515250 0.249900 0.680200 1.0 0.7129

Pb Pb169 1 0.914890 0.250600 0.181700 1.0 0.7342

Pb Pb170 1 0.914890 0.749400 0.681700 1.0 0.7339

Pb Pb171 1 0.414890 0.750600 0.181700 1.0 0.7342

Pb Pb172 1 0.414890 0.249400 0.681700 1.0 0.7339

Pb Pb173 1 0.814140 0.249300 0.181200 1.0 0.816

Pb Pb174 1 0.814140 0.750700 0.681200 1.0 0.8161

Pb Pb175 1 0.314140 0.749300 0.181200 1.0 0.816

Pb Pb176 1 0.314140 0.250700 0.681200 1.0 0.8161

C C177 1 0.952300 0.781000 0.125000 1.0 -0.2464

C C178 1 0.952300 0.219000 0.625000 1.0 -0.2465

C C179 1 0.452300 0.281000 0.125000 1.0 -0.2464

C C180 1 0.452300 0.719000 0.625000 1.0 -0.2465

C C181 1 0.849500 0.269000 0.654000 1.0 -0.228

C C182 1 0.849500 0.731000 0.154000 1.0 -0.2284

C C183 1 0.349500 0.769000 0.654000 1.0 -0.228

C C184 1 0.349500 0.231000 0.154000 1.0 -0.2284

C C185 1 0.548700 0.747000 0.743000 1.0 -0.2407

C C186 1 0.548700 0.253000 0.243000 1.0 -0.2403

C C187 1 0.048700 0.247000 0.743000 1.0 -0.2407

C C188 1 0.048700 0.753000 0.243000 1.0 -0.2403

C C189 1 0.279300 0.294000 0.996000 1.0 -0.0337

C C190 1 0.279300 0.706000 0.496000 1.0 -0.0332

C C191 1 0.779300 0.794000 0.996000 1.0 -0.0337

C C192 1 0.779300 0.206000 0.496000 1.0 -0.0332

C C193 1 0.263900 0.170000 0.961000 1.0 -0.1527

C C194 1 0.263900 0.830000 0.461000 1.0 -0.1548

C C195 1 0.763900 0.670000 0.961000 1.0 -0.1527

C C196 1 0.763900 0.330000 0.461000 1.0 -0.1548

C C197 1 0.241800 0.222000 0.996000 1.0 -0.1809

C C198 1 0.241800 0.778000 0.496000 1.0 -0.1806

C C199 1 0.741800 0.722000 0.996000 1.0 -0.1809

C C200 1 0.741800 0.278000 0.496000 1.0 -0.1806

C C201 1 0.239500 0.243000 0.162000 1.0 -0.1664

C C202 1 0.239500 0.757000 0.662000 1.0 -0.1664

C C203 1 0.739500 0.743000 0.162000 1.0 -0.1664

C C204 1 0.739500 0.257000 0.662000 1.0 -0.1664

C C205 1 0.216400 0.242000 0.202000 1.0 -0.1521

C C206 1 0.216400 0.758000 0.702000 1.0 -0.1528

C C207 1 0.716400 0.742000 0.202000 1.0 -0.1521

C C208 1 0.716400 0.258000 0.702000 1.0 -0.1528

C C209 1 0.214000 0.205000 0.366000 1.0 -0.1786

C C210 1 0.214000 0.795000 0.866000 1.0 -0.1781

C C211 1 0.714000 0.705000 0.366000 1.0 -0.1786

C C212 1 0.714000 0.295000 0.866000 1.0 -0.1781

C C213 1 0.191100 0.175000 0.399000 1.0 -0.145

C C214 1 0.191100 0.825000 0.899000 1.0 -0.1446

C C215 1 0.691100 0.675000 0.399000 1.0 -0.145

C C216 1 0.691100 0.325000 0.899000 1.0 -0.1446

C C217 1 0.188000 0.168000 0.566000 1.0 -0.0105

C C218 1 0.188000 0.832000 0.066000 1.0 -0.0107

C C219 1 0.688000 0.668000 0.566000 1.0 -0.0105

C C220 1 0.688000 0.332000 0.066000 1.0 -0.0107

I I221 1 0.121200 0.498000 0.438000 1.0 -0.3048

I I222 1 0.121200 0.502000 0.938000 1.0 -0.3047

I I223 1 0.621200 0.998000 0.438000 1.0 -0.3048

I I224 1 0.621200 0.002000 0.938000 1.0 -0.3047

I I225 1 0.112800 0.996000 0.427000 1.0 -0.203

I I226 1 0.112800 0.004000 0.927000 1.0 -0.2036

I I227 1 0.612800 0.496000 0.427000 1.0 -0.203

I I228 1 0.612800 0.504000 0.927000 1.0 -0.2036

I I229 1 0.012800 0.498000 0.922000 1.0 -0.3908

I I230 1 0.012800 0.502000 0.422000 1.0 -0.3905

I I231 1 0.512800 0.998000 0.922000 1.0 -0.3908

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I I233 1 0.020600 0.997000 0.437000 1.0 -0.3299

I I234 1 0.020600 0.003000 0.937000 1.0 -0.3297

I I235 1 0.520600 0.497000 0.437000 1.0 -0.3299

I I236 1 0.520600 0.503000 0.937000 1.0 -0.3297

I I237 1 0.921000 0.495000 0.936000 1.0 -0.3174

I I238 1 0.921000 0.505000 0.436000 1.0 -0.3172

I I239 1 0.421000 0.995000 0.936000 1.0 -0.3174

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I I241 1 0.912400 0.001000 0.422000 1.0 -0.3936

I I242 1 0.912400 0.999000 0.922000 1.0 -0.3936

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I I246 1 0.811600 0.496000 0.925000 1.0 -0.426

I I247 1 0.311600 0.004000 0.425000 1.0 -0.4267

I I248 1 0.311600 0.996000 0.925000 1.0 -0.426

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I I250 1 0.821500 0.005000 0.938000 1.0 -0.4064

I I251 1 0.321500 0.495000 0.438000 1.0 -0.4066

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I I254 1 0.766600 0.801000 0.659000 1.0 -0.4433

I I255 1 0.266600 0.699000 0.159000 1.0 -0.4435

I I256 1 0.266600 0.301000 0.659000 1.0 -0.4433

I I257 1 0.866000 0.289000 0.168000 1.0 -0.4017

I I258 1 0.866000 0.711000 0.668000 1.0 -0.4006

I I259 1 0.366000 0.789000 0.168000 1.0 -0.4017

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N N274 1 0.565600 0.265000 0.125000 1.0 -0.5892

N N275 1 0.065600 0.235000 0.625000 1.0 -0.5891

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N N278 1 0.957800 0.290000 0.773000 1.0 -0.5617

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N N282 1 0.872000 0.692000 0.192000 1.0 -0.5139

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N N290 1 0.166300 0.776000 0.105000 1.0 -0.4259

N N291 1 0.666300 0.724000 0.605000 1.0 -0.4248

N N292 1 0.666300 0.276000 0.105000 1.0 -0.4259