

Online supporting information for:

Exploring Structural Diversity and Fluxionality of Pt_n (n=10-13)

Clusters from First Principles

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Cartesian coordinates for the putative global minimum in Figure 2:

10

Pt10

| | | | |
|----|-----------|-----------|-----------|
| Pt | 8.001540 | 9.226260 | 10.649520 |
| Pt | 8.456759 | 10.497420 | 6.323580 |
| Pt | 7.332660 | 8.952120 | 7.996861 |
| Pt | 10.679399 | 9.073979 | 10.016640 |
| Pt | 9.997560 | 8.752501 | 7.349580 |
| Pt | 8.929620 | 7.059240 | 9.249300 |
| Pt | 9.077220 | 10.941120 | 8.755380 |
| Pt | 6.467040 | 7.376400 | 9.785521 |
| Pt | 11.384460 | 7.061940 | 8.642879 |
| Pt | 9.673920 | 11.059020 | 11.230740 |

11

Pt11

| | | | |
|----|-----------|-----------|-----------|
| Pt | 9.279000 | 8.035740 | 10.140659 |
| Pt | 11.822399 | 10.585259 | 9.102600 |
| Pt | 10.109879 | 10.263420 | 11.015460 |
| Pt | 7.764480 | 9.426061 | 11.724300 |
| Pt | 10.783620 | 8.474401 | 8.126100 |
| Pt | 8.277480 | 6.004800 | 9.037260 |
| Pt | 7.800660 | 8.250480 | 7.889940 |
| Pt | 7.407900 | 10.558260 | 6.912000 |
| Pt | 6.924240 | 10.116540 | 9.418320 |
| Pt | 9.553141 | 6.609780 | 6.962760 |
| Pt | 9.277200 | 10.675260 | 8.670240 |

12

Pt12

| | | | |
|----|-----------|-----------|-----------|
| Pt | 8.665560 | 7.763220 | 6.090660 |
| Pt | 8.291700 | 6.464340 | 10.941481 |
| Pt | 10.095480 | 8.301781 | 11.283300 |
| Pt | 8.614440 | 6.972120 | 8.485200 |
| Pt | 7.422300 | 9.347940 | 7.603380 |
| Pt | 7.838460 | 8.927999 | 10.348921 |
| Pt | 8.568720 | 11.324880 | 10.118880 |
| Pt | 10.866600 | 8.938260 | 6.382440 |
| Pt | 11.026800 | 10.568340 | 10.454220 |
| Pt | 10.757880 | 8.291340 | 8.851680 |
| Pt | 9.674100 | 10.469521 | 8.039340 |
| Pt | 6.177960 | 10.630080 | 9.400320 |

13

Pt13

| | | | |
|----|-----------|-----------|-----------|
| Pt | 11.948580 | 9.295560 | 8.847900 |
| Pt | 7.190820 | 6.237720 | 8.161560 |
| Pt | 7.169400 | 8.522280 | 9.368820 |
| Pt | 11.463840 | 7.495380 | 10.596241 |
| Pt | 9.408239 | 6.745680 | 9.282060 |
| Pt | 9.809460 | 10.431900 | 9.519300 |
| Pt | 8.190900 | 10.914660 | 7.113060 |
| Pt | 7.362180 | 11.028780 | 9.550260 |
| Pt | 9.294479 | 8.673480 | 11.250540 |
| Pt | 10.827180 | 10.998000 | 7.147080 |
| Pt | 7.481520 | 8.452260 | 6.858180 |
| Pt | 9.871740 | 8.569800 | 7.622640 |
| Pt | 6.981660 | 9.634501 | 11.682361 |