Supplementary Information: Predicting Archetypal Nanoparticle Shapes Using a Combination of Thermodynamic Theory and Machine Learning

Tao Yan, Baichuan Sun, and Amanda S. Barnard*

Data61 CSIRO, Docklands, Victoria, Australia.

E-mail: amanda.barnard@data61.csiro.au

This file contains tables and details of archetypes and prototypes identified using theoretical data sets and machine learning, for Pt nanoparticles from 3 nm to 30 nm at room temperature; and from 3 nm to 15 nm at 100°C. The methods and results used to generate and screen this data are described in the main text. The shapes considered in this study include both low energy and high energy configurations, enclosed by different combinations of low and high index facets. These include compound shapes such as the small rhombicuboctahedron and the great rhombicuboctahedron with facets in more than one crystallographic orientation, and regular zonohedrons enclosed entirely by facets in the same crystallographic orientation such as the octahedron, cube or trapezohedron. Although they have a higher free energy (lower thermodynamic stability) the inclusion of high index shapes is important to capture all of the proposing morphologies observed experimentally. All of the shapes are symmetric, but any asymmetric closed polyhedron could be included in principle. Representations of polyhedral used herein are illustrated in Figure S1.

*To whom correspondence should be addressed

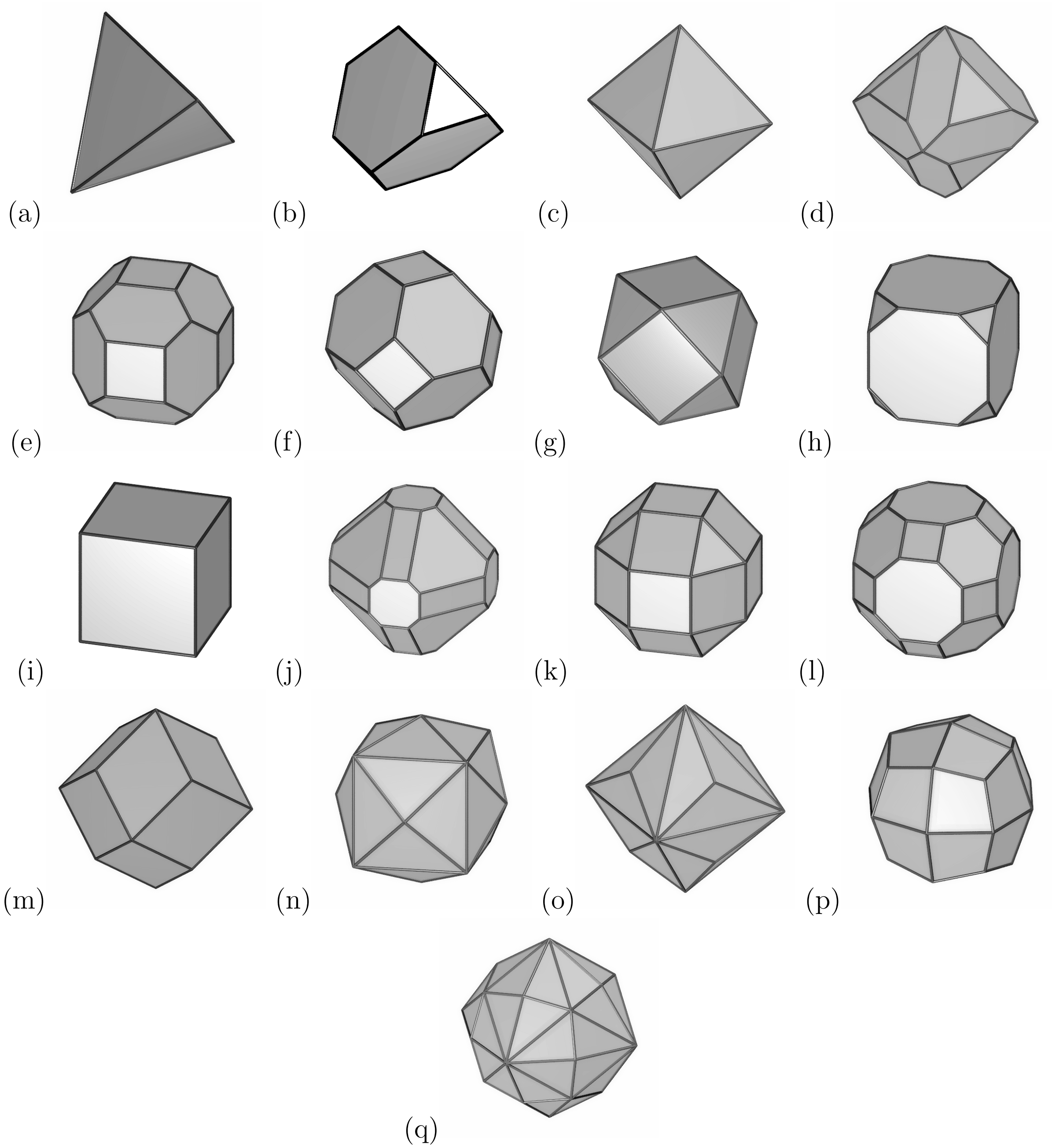


Figure S1: Schematic representations of the nanoparticle morphologies included in this study: (a) tetrahedron, (b) truncated tetrahedron, (c) octahedron, (d) rhombi-truncated octahedron, (e) rhombi-truncated cube, (f) truncated octahedron, (g) cuboctahedron, (h) truncated cube, (i) cube, (j) doubly-truncated octahedron (also known as a modified truncated octahedron) (k) small rhombicuboctahedron, (l) great rhombicuboctahedron, (m) rhombic dodecahedron, (n) tetrahexahedron, (o) trisoctahedron, (p) trapezohedron, and (q) hexoctahedron.

Table S1: List of diameter (in nm), geometric shape, and fractional area of each (hkl) facet of the closest matches to the six archetypal and twelve prototypical Pt nanoparticles configurations identified using archetypal analysis and k-means clustering, respectively. This set is a representative subset of a sample containing all of the shapes shown in Figure S1, at 25°C with diameters in the range 3 nm to 30 nm. Note that the ordering of the archetypes and prototypes is arbitrary.

	Size (nm)	Shape	(100)	(110)	(111)	(210)	(311)	(331)	(123)
Archetype 1	3.97	Great rhombicuboctahedron	0.337	0.194	0.469	0.000	0.000	0.000	0.000
Archetype 2	28.8	Truncated cube	0.107	0.000	0.893	0.000	0.000	0.000	0.000
Archetype 3	12.89	Truncated tetrahedron	1.000	0.000	0.000	0.000	0.000	0.000	0.000
Archetype 4	22.98	Rhombi-truncated octahedron	0.037	0.963	0.000	0.000	0.000	0.000	0.000
Archetype 5	26.28	Tetrahexahedron	0.000	0.000	0.000	0.000	1.000	0.000	0.000
Archetype 6	21.04	Trapezohedron	0.000	0.000	0.000	0.000	0.000	1.000	0.000
Prototype 1	25.7	Rhombi-truncated octahedron	0.037	0.963	0.000	0.000	0.000	0.000	0.000
Prototype 2	4.16	Great rhombicuboctahedron	0.337	0.194	0.469	0.000	0.000	0.000	0.000
Prototype 3	15.03	Cuboctahedron	0.366	0.000	0.634	0.000	0.000	0.000	0.000
Prototype 4	8.43	Hexoctahedron	0.000	0.000	0.000	0.000	0.000	0.000	1.000
Prototype 5	25.89	Tetrahexahedron	0.000	0.000	0.000	0.000	1.000	0.000	0.000
Prototype 6	26.86	Cuboctahedron	0.366	0.000	0.634	0.000	0.000	0.000	0.000
Prototype 7	11.73	Tetrahexahedron	0.000	0.000	0.000	0.000	1.000	0.000	0.000
Prototype 8	18.33	Trapezohedron	0.000	0.000	0.000	0.000	0.000	1.000	0.000
Prototype 9	18.52	Trisoctahedron	0.000	0.000	0.000	1.000	0.000	0.000	0.000
Prototype 10	13.48	Rhombi-truncated cube	0.000	0.850	0.150	0.000	0.000	0.000	0.000
Prototype 11	23.76	Hexoctahedron	0.000	0.000	0.000	0.000	0.000	0.000	1.000
Prototype 12	14.64	Truncated tetrahedron	1.000	0.000	0.000	0.000	0.000	0.000	0.000

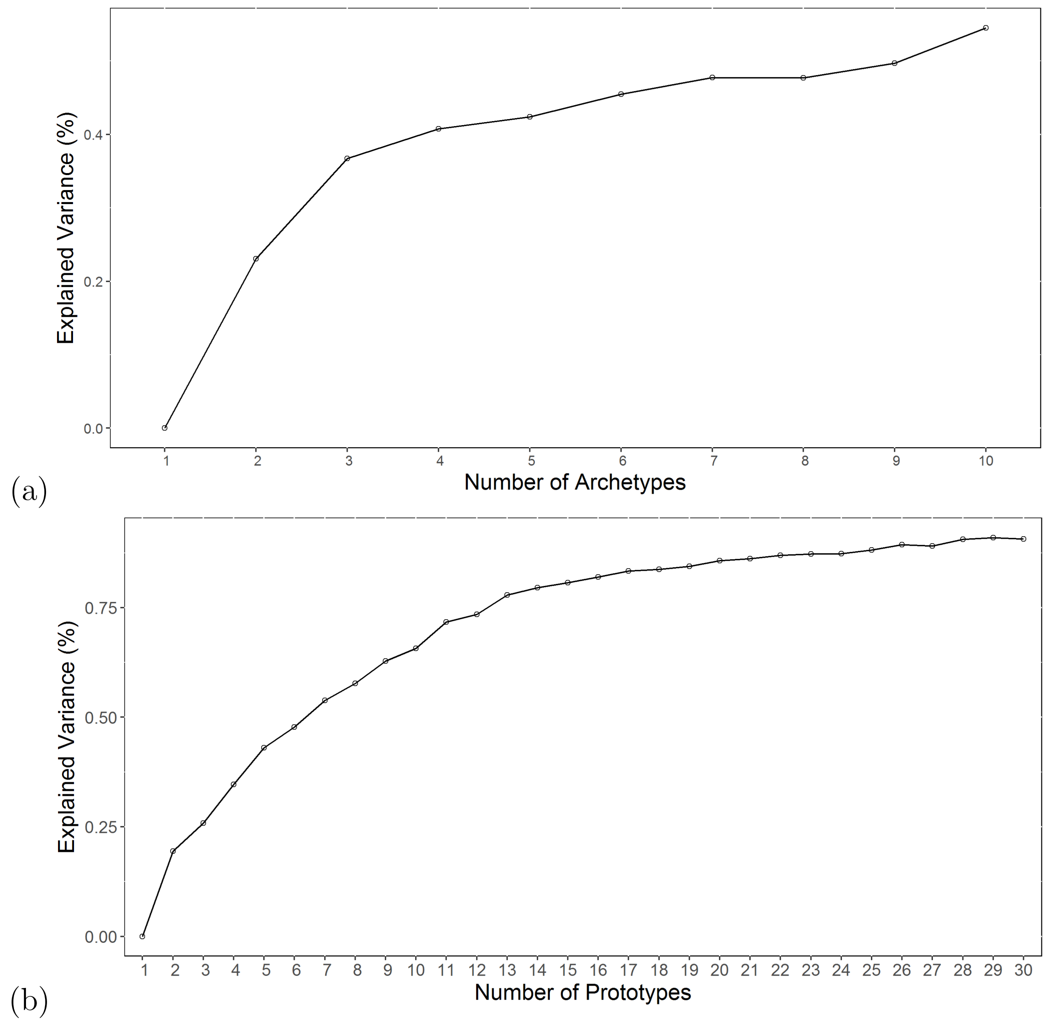
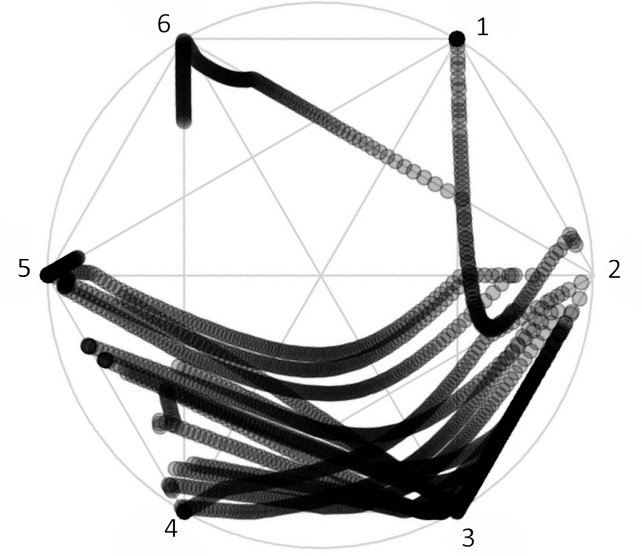
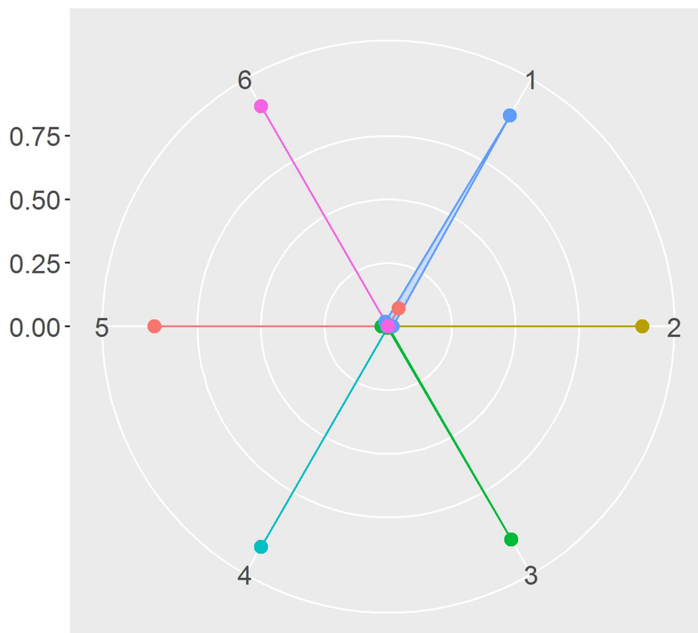


Figure S2: The elbow plot identifying (a) how many archetypes are required to maximise the explained variance (the first six have been chosen in this example); and the elbow plot identifying how many prototypes are required to maximise the explained variance (the first twelve have been chosen in this example). Both for the case of a sample containing all of the shapes shown in Figure S1, at 25°C with diameters in the range 3 nm to 30 nm.

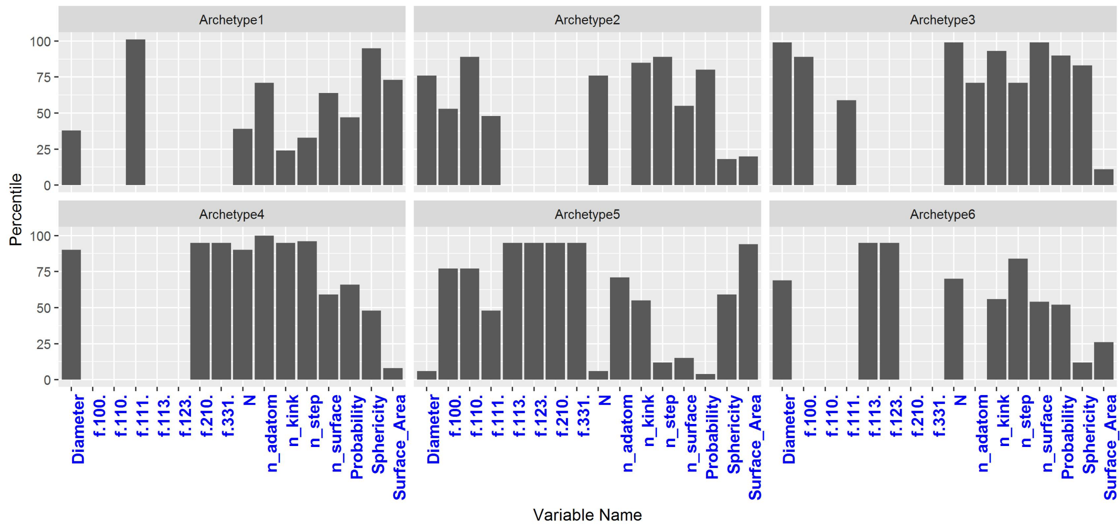


(a)

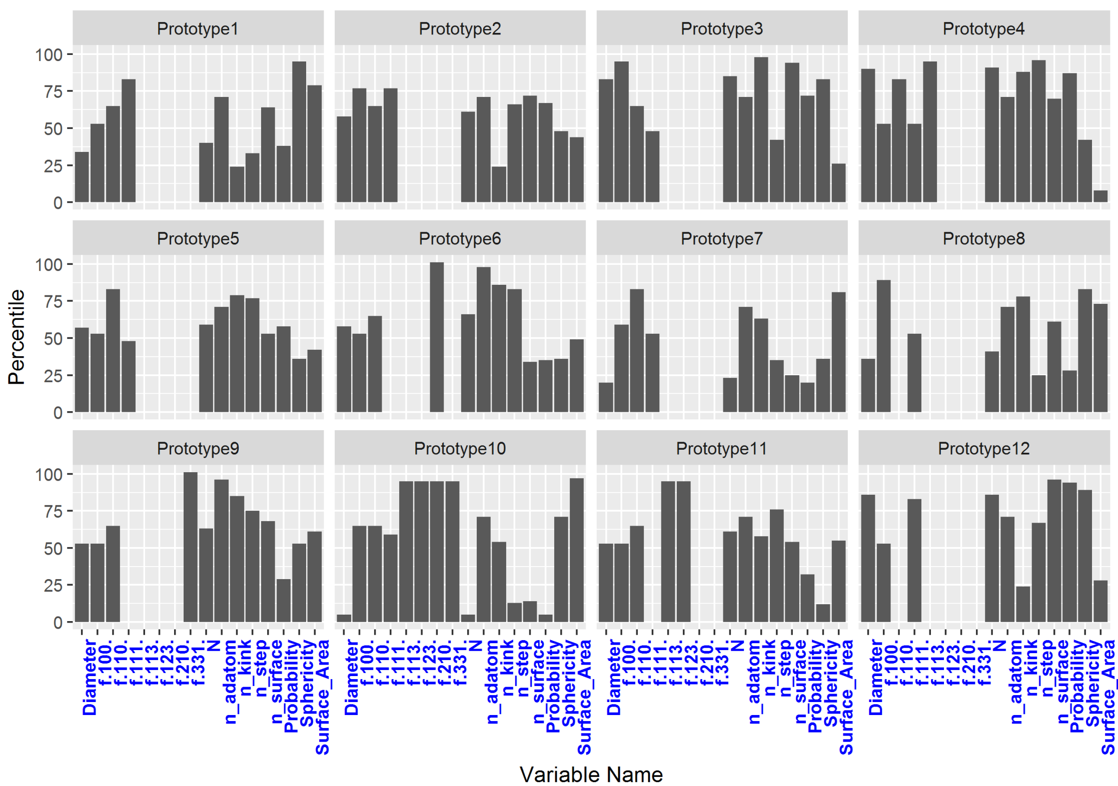


(b)

Figure S3: (a) The simplex plot showing the relationship of all of the nanoparticle configurations in the set to the six archetypes, and (b) a radar plot showing the closest matches from the data set to the six archetypes; both for the case of a sample containing all of the shapes shown in Figure S1, at 25°C with diameters in the range 3 nm to 30 nm.



(a)

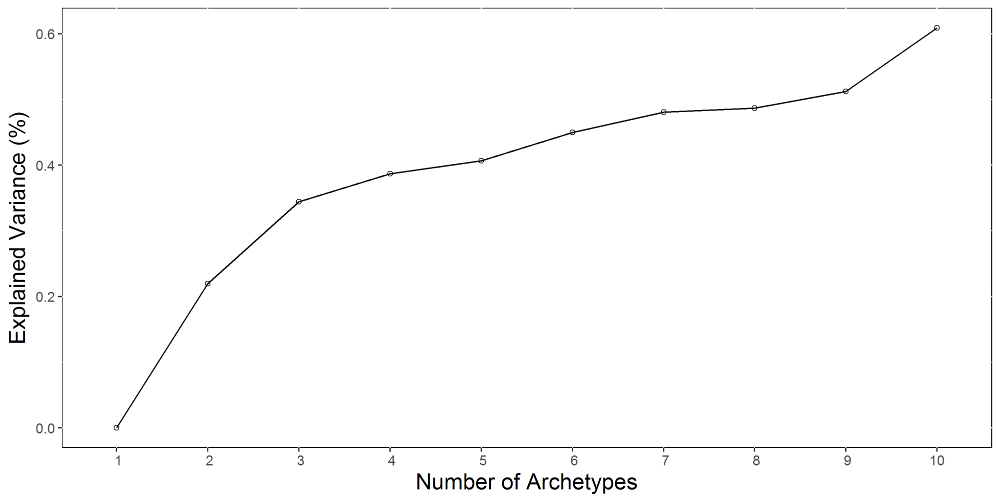


(b)

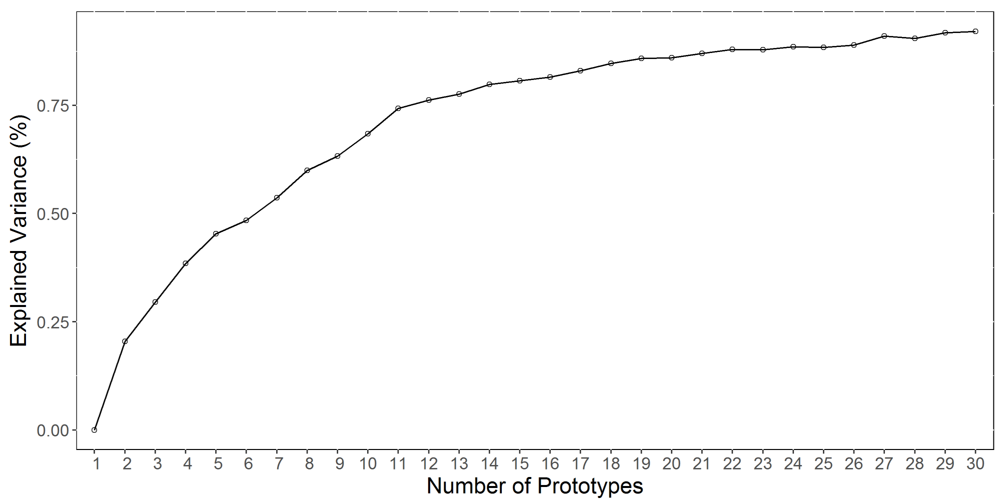
Figure S4: The (a) histograms of the importance of each structural feature to the definition of the first six archetypes, and (b) histograms of the importance of each structural feature to the definition of the first twelve prototypes; both for the case of a sample containing all of the shapes shown in Figure S1, at 25°C with diameters in the range 3 nm to 30 nm.

Table S2: List of diameter (in nm), geometric shape, and fractional area of each (hkl) facet of the closest matches to the six archetypal and twelve prototypical Pt nanoparticles configurations identified using archetypal analysis and k-means clustering, respectively. This set is a representative subset of a sample containing all of the shapes shown in Figure S1, at 100°C with diameters in the range 3 nm to 15 nm. Note that the ordering of the archetypes and prototypes is arbitrary.

	Size (nm)	Shape	(100)	(110)	(111)	(210)	(311)	(331)	(123)
Archetype 1	12.89	Cube	0.000	0.000	1.000	0.000	0.000	0.000	0.000
Archetype 2	11.34	Hexoctahedron	0.000	0.000	0.000	0.000	0.000	0.000	1.000
Archetype 3	11.34	Tetrahexahedron	0.000	0.000	0.000	0.000	1.000	0.000	0.000
Archetype 4	3.39	Doubly-truncated octahedron	0.460	0.245	0.296	0.000	0.000	0.000	0.000
Archetype 5	12.89	Truncated tetrahedron	1.000	0.000	0.000	0.000	0.000	0.000	0.000
Archetype 6	14.45	Rhombi-truncated octahedron	0.037	0.963	0.000	0.000	0.000	0.000	0.000
Prototype 1	5.91	Truncated tetrahedron	1.000	0.000	0.000	0.000	0.000	0.000	0.000
Prototype 2	12.7	Truncated tetrahedron	1.000	0.000	0.000	0.000	0.000	0.000	0.000
Prototype 3	11.73	Great rhombicuboctahedron	0.337	0.194	0.469	0.000	0.000	0.000	0.000
Prototype 4	5.91	Rhombi-truncated cube	0.000	0.850	0.150	0.000	0.000	0.000	0.000
Prototype 5	12.7	Rhombi-truncated octahedron	0.037	0.963	0.000	0.000	0.000	0.000	0.000
Prototype 6	9.21	Trapezohedron	0.000	0.000	0.000	0.000	0.000	1.000	0.000
Prototype 7	12.31	Trisoctahedron	0.000	0.000	0.000	1.000	0.000	0.000	0.000
Prototype 8	5.91	Trisoctahedron	0.000	0.000	0.000	1.000	0.000	0.000	0.000
Prototype 9	11.73	Cube	0.000	0.000	1.000	0.000	0.000	0.000	0.000
Prototype 10	5.33	Cuboctahedron	0.366	0.000	0.634	0.000	0.000	0.000	0.000
Prototype 11	9.01	Hexoctahedron	0.000	0.000	0.000	0.000	0.000	0.000	1.000
Prototype 12	9.4	Tetrahexahedron	0.000	0.000	0.000	0.000	1.000	0.000	0.000

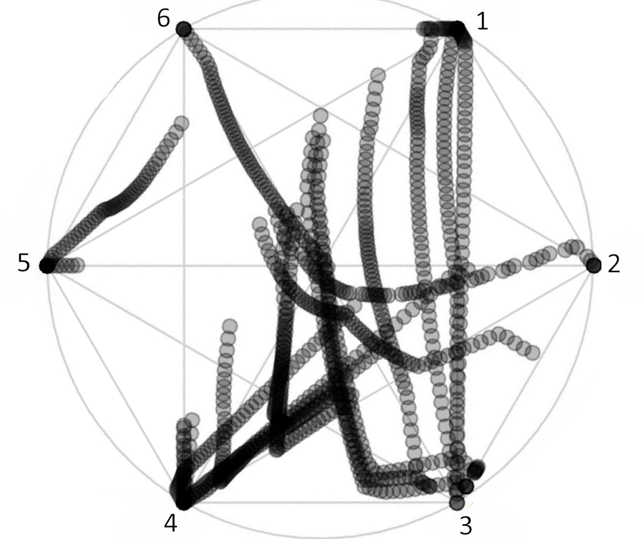


(a)

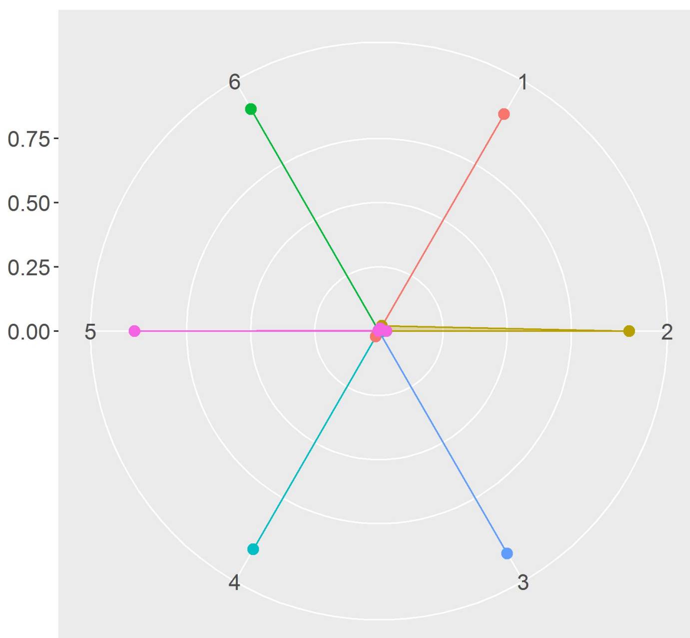


(b)

Figure S5: The elbow plot identifying (a) how many archetypes are required to maximise the explained variance (the first six have been chosen in this example); and the elbow plot identifying how many prototypes are required to maximise the explained variance (the first twelve have been chosen in this example). Both for the case of a sample containing all of the shapes shown in Figure S1, at 100°C with diameters in the range 3 nm to 15 nm.

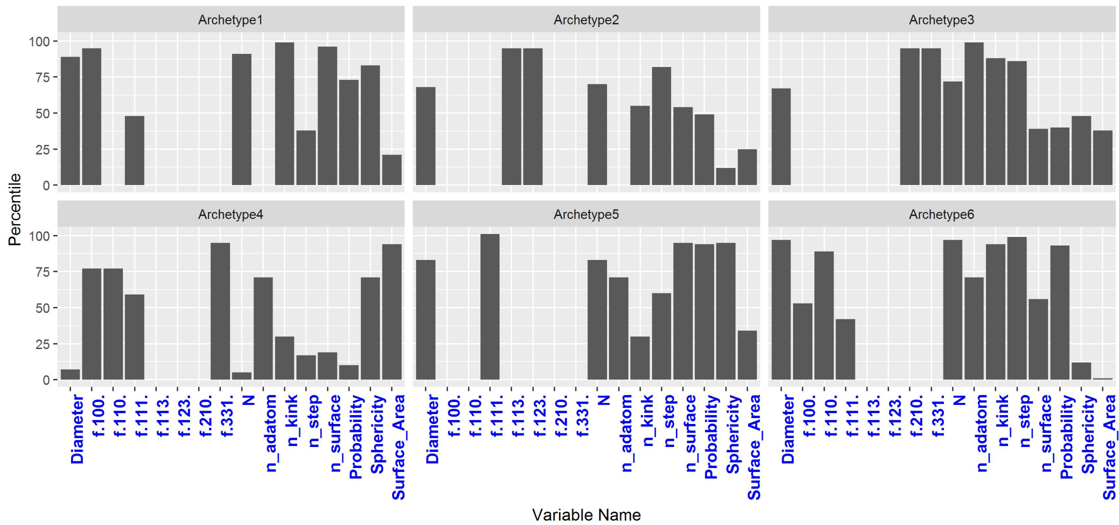


(a)

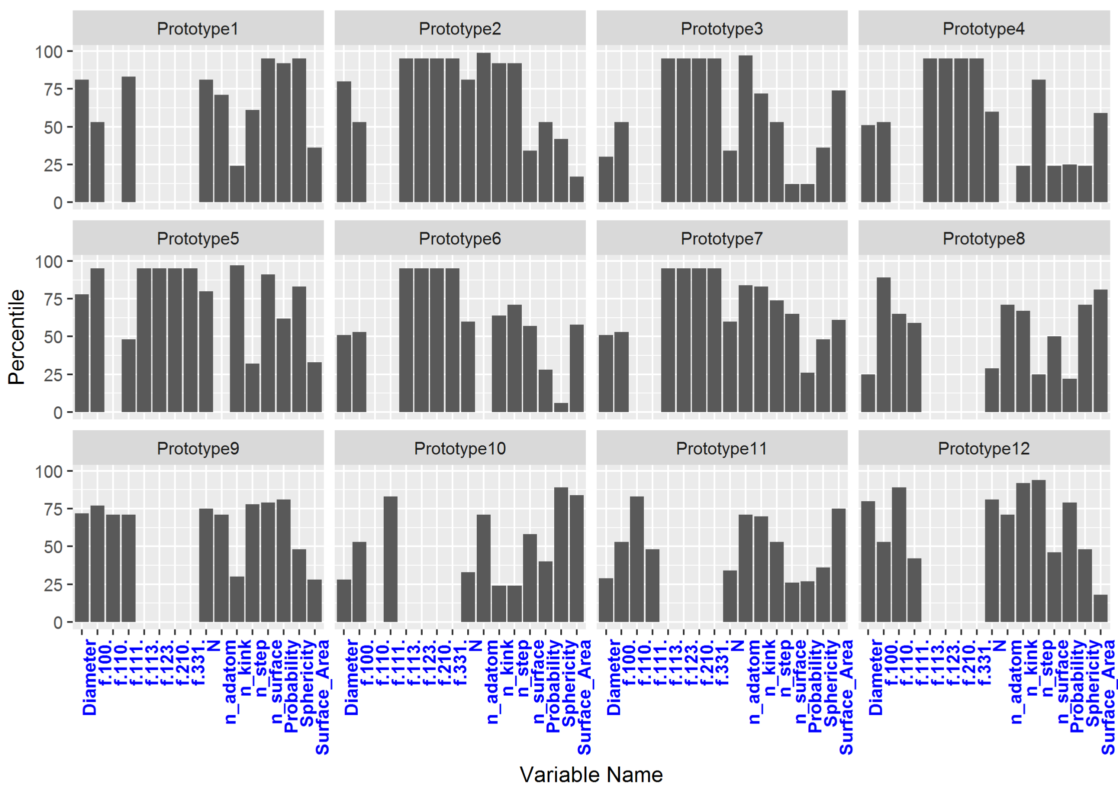


(b)

Figure S6: (a) The simplex plot showing the relationship of all of the nanoparticle configurations in the set to the six archetypes, and (b) a radar plot showing the closest matches from the data set to the six archetypes; both for the case of a sample containing all of the shapes shown in Figure S1, at 100°C with diameters in the range 3 nm to 15 nm.



(a)



(b)

Figure S7: The (a) histograms of the importance of each structural feature to the definition of the first six archetypes, and (b) histograms of the importance of each structural feature to the definition of the first twelve prototypes; both for the case of a sample containing all of the shapes shown in Figure S1, at 100°C with diameters in the range 3 nm to 15 nm.