

Table 1 Cluster connectivities (Å)

| | 1 cage A | 1 cage B | 3 cage A | 3 cage B | 4 cage A | 4 cage B | 4 cage C ^a | 4 cage D ^a | 6 cage A | 6 cage B | 7 cage A | 7 cage B | 8 cage A | 8 cage B |
|---------|------------|------------|----------|-----------|------------|------------|-----------------------|-----------------------|-----------|----------|-----------|-----------|----------|----------|
| C1–B2 | 1.5289(14) | 1.5243(15) | 1.557(8) | 1.524(7) | 1.530(3) | 1.517(3) | 1.521(3) | 1.521(3) | 1.597(7) | 1.574(6) | 1.536(9) | 1.480(16) | 1.539(4) | 1.535(4) |
| C1–B3 | 1.5276(14) | 1.5324(15) | 1.527(8) | 1.521(8) | 1.536(3) | 1.534(3) | 1.535(3) | 1.537(3) | 1.588(7) | 1.559(7) | 1.543(10) | 1.580(11) | 1.534(4) | 1.543(4) |
| C1–M4 | 2.0897(9) | 2.0826(9) | 2.012(5) | 2.060(5) | 2.0772(19) | 2.0679(19) | 2.0721(19) | 2.0655(19) | 2.208(4) | 2.171(4) | 2.063(6) | 2.088(7) | 2.062(3) | 2.058(2) |
| C1–B5 | 1.7594(15) | 1.7571(14) | 1.770(8) | 1.761(8) | 1.738(3) | 1.729(3) | 1.741(3) | 1.720(3) | 1.692(8) | 1.754(6) | 1.751(9) | 1.705(10) | 1.758(4) | 1.752(4) |
| B2–M4 | 2.2885(11) | 2.2931(11) | 2.205(6) | 2.219(6) | 2.267(2) | 2.260(2) | 2.264(2) | 2.254(2) | 2.420(5) | 2.435(5) | 2.279(6) | 2.272(10) | 2.309(3) | 2.300(3) |
| B2–B5 | 1.9993(16) | 2.0290(16) | 1.963(8) | 1.967(9) | 2.060(3) | 2.053(3) | 2.069(3) | 2.067(3) | 1.893(10) | 1.984(7) | 1.992(10) | 2.226(14) | 1.985(4) | 2.012(4) |
| B2–B6 | 1.8414(16) | 1.8340(15) | 1.850(8) | 1.853(9) | 1.781(3) | 1.783(3) | 1.782(3) | 1.780(3) | 1.780(7) | 1.768(7) | 1.807(10) | 1.74(2) | 1.826(4) | 1.817(4) |
| B2–B9 | 1.7933(16) | 1.8025(16) | 1.770(9) | 1.791(8) | 1.813(3) | 1.815(3) | 1.824(3) | 1.826(3) | 1.784(7) | 1.800(7) | 1.777(10) | 1.681(15) | 1.775(4) | 1.803(5) |
| B3–M4 | 2.2596(11) | 2.2517(11) | 2.231(5) | 2.231(6) | 2.248(2) | 2.236(2) | 2.241(2) | 2.230(2) | 2.397(5) | 2.411(5) | 2.290(7) | 2.273(7) | 2.274(3) | 2.275(3) |
| B3–B5 | 2.0239(15) | 1.9943(16) | 2.086(8) | 2.095(8) | 2.001(3) | 1.994(3) | 1.994(3) | 1.978(3) | 2.239(7) | 2.008(7) | 2.002(10) | 1.903(11) | 2.022(4) | 1.979(4) |
| B3–B7 | 1.8267(16) | 1.8247(14) | 1.870(8) | 1.846(9) | 1.800(3) | 1.796(3) | 1.800(3) | 1.796(3) | 1.785(7) | 1.778(9) | 1.811(11) | 1.813(9) | 1.809(4) | 1.817(4) |
| B3–B8 | 1.8040(16) | 1.7949(16) | 1.815(8) | 1.824(8) | 1.793(3) | 1.794(3) | 1.795(3) | 1.794(3) | 1.790(7) | 1.790(8) | 1.784(10) | 1.780(10) | 1.798(4) | 1.780(4) |
| M4–B6 | 2.2147(10) | 2.2218(11) | 2.277(6) | 2.212(6) | 2.223(2) | 2.231(2) | 2.221(2) | 2.220(2) | 2.399(6) | 2.382(5) | 2.242(7) | 2.209(10) | 2.235(3) | 2.247(3) |
| M4–B7 | 2.2044(10) | 2.1972(11) | 2.472(5) | 2.306(6) | 2.203(2) | 2.204(2) | 2.203(2) | 2.206(2) | 2.407(5) | 2.392(5) | 2.240(7) | 2.254(7) | 2.231(3) | 2.233(3) |
| M4–C10 | 2.1745(9) | 2.1618(9) | 2.662(5) | 2.389(5) | 2.1350(19) | 2.149(2) | 2.1343(19) | 2.146(2) | 2.244(5) | 2.285(4) | 2.173(6) | 2.111(6) | 2.164(3) | 2.159(3) |
| B5–B8 | 1.8929(15) | 1.8960(16) | 1.935(9) | 1.926(8) | 1.903(3) | 1.905(3) | 1.907(3) | 1.907(3) | 2.204(8) | 1.933(8) | 1.917(11) | 1.830(10) | 1.899(4) | 1.910(4) |
| B5–B9 | 1.8947(15) | 1.9067(16) | 1.876(8) | 1.877(9) | 1.920(3) | 1.906(3) | 1.913(3) | 1.907(3) | 1.816(9) | 1.914(7) | 1.914(11) | 2.062(16) | 1.902(4) | 1.914(4) |
| B5–B11 | 1.7966(15) | 1.7879(15) | 1.789(9) | 1.801(9) | 1.801(3) | 1.798(3) | 1.794(3) | 1.794(3) | 1.752(13) | 1.832(7) | 1.808(10) | 1.761(12) | 1.814(4) | 1.817(4) |
| B6–B9 | 1.7611(15) | 1.7631(16) | 1.789(8) | 1.792(9) | 1.769(3) | 1.759(3) | 1.773(3) | 1.773(3) | 1.778(7) | 1.780(7) | 1.757(10) | 1.831(16) | 1.765(4) | 1.761(4) |
| B6–C10 | 1.6736(14) | 1.6707(15) | 1.679(7) | 1.673(8) | 1.687(3) | 1.689(3) | 1.682(3) | 1.676(3) | 1.637(8) | 1.686(7) | 1.677(10) | 1.701(15) | 1.671(4) | 1.672(4) |
| B6–B12 | 1.7616(15) | 1.7580(16) | 1.817(8) | 1.794(9) | 1.764(3) | 1.763(3) | 1.758(3) | 1.762(3) | 1.748(9) | 1.787(7) | 1.770(10) | 1.620(16) | 1.756(4) | 1.761(4) |
| B7–B8 | 1.7616(15) | 1.7621(16) | 1.745(8) | 1.767(9) | 1.769(3) | 1.771(3) | 1.767(3) | 1.771(3) | 1.755(7) | 1.772(7) | 1.755(10) | 1.767(9) | 1.763(4) | 1.763(4) |
| B7–C10 | 1.6748(14) | 1.6776(15) | 1.621(7) | 1.637(8) | 1.685(3) | 1.680(3) | 1.682(3) | 1.676(3) | 1.640(7) | 1.671(8) | 1.671(10) | 1.622(10) | 1.671(4) | 1.675(4) |
| B7–B13 | 1.7613(15) | 1.7612(16) | 1.792(8) | 1.784(9) | 1.762(3) | 1.774(3) | 1.768(3) | 1.779(3) | 1.761(8) | 1.762(8) | 1.758(10) | 1.843(12) | 1.771(4) | 1.761(4) |
| B8–B11 | 1.7541(15) | 1.7605(16) | 1.787(8) | 1.763(8) | 1.761(3) | 1.760(3) | 1.759(3) | 1.753(3) | 1.738(9) | 1.760(8) | 1.756(10) | 1.738(11) | 1.759(4) | 1.765(4) |
| B8–B13 | 1.7427(16) | 1.7364(16) | 1.740(9) | 1.740(9) | 1.724(3) | 1.730(3) | 1.729(3) | 1.726(3) | 1.738(9) | 1.748(8) | 1.722(11) | 1.796(12) | 1.739(4) | 1.739(4) |
| B9–B11 | 1.7533(15) | 1.7521(16) | 1.776(8) | 1.776(9) | 1.758(3) | 1.752(3) | 1.756(3) | 1.756(3) | 1.714(8) | 1.756(8) | 1.762(10) | 1.679(14) | 1.758(4) | 1.754(4) |
| B9–B12 | 1.7426(16) | 1.7436(16) | 1.739(8) | 1.745(10) | 1.730(3) | 1.738(3) | 1.728(3) | 1.741(3) | 1.675(10) | 1.745(8) | 1.732(10) | 1.58(2) | 1.742(4) | 1.744(4) |
| C10–B12 | 1.7145(14) | 1.7188(15) | 1.684(8) | 1.692(9) | 1.723(3) | 1.733(3) | 1.721(3) | 1.730(3) | 1.881(9) | 1.736(7) | 1.738(9) | 1.988(16) | 1.734(4) | 1.731(4) |
| C10–B13 | 1.7241(14) | 1.7201(15) | 1.694(7) | 1.718(8) | 1.721(3) | 1.725(3) | 1.720(3) | 1.724(3) | 1.725(9) | 1.763(7) | 1.730(9) | 1.661(11) | 1.743(4) | 1.736(4) |
| B11–B12 | 1.7867(16) | 1.7841(16) | 1.795(8) | 1.809(9) | 1.777(3) | 1.777(3) | 1.778(3) | 1.783(3) | 1.926(12) | 1.781(7) | 1.776(10) | 1.782(16) | 1.785(4) | 1.784(4) |
| B11–B13 | 1.7869(15) | 1.7866(16) | 1.775(9) | 1.787(10) | 1.778(3) | 1.785(3) | 1.777(3) | 1.776(3) | 1.759(13) | 1.782(7) | 1.772(10) | 1.764(13) | 1.779(4) | 1.782(4) |
| B12–B13 | 1.7478(15) | 1.7448(17) | 1.762(8) | 1.767(9) | 1.759(3) | 1.753(3) | 1.755(3) | 1.753(3) | 1.616(13) | 1.750(8) | 1.738(11) | 1.608(19) | 1.755(4) | 1.745(5) |

^a In **4** there are two crystallographically independent molecules in the asymmetric fraction of the unit cell