Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# Structures and Thermodynamic Stability of Copper(II) Chloride Surfaces

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Talal University, Ma'an, Jordan

# (001)Cl

**Cl 19 Cu 11**

**Lattice vectors**

| | | |
|---|---|---|
| 7.2011000000000003 | 0.0000000000000000 | 0.0000000000000000 |
| 0.0000000000000000 | 3.3712000000000000 | 0.0000000000000000 |
| 0.0000000000000000 | 0.0000000000000000 | 58.6135000000000019 |

**Cartesian Coordinates**

| | | | |
|---|---|---|---|
| Cl | 2.46026 | 0.00000 | 17.70778 |
| Cl | 6.14548 | 0.00000 | 24.21755 |
| Cl | 2.61220 | 0.00000 | 30.68241 |
| Cl | 6.35834 | 0.00000 | 37.10663 |
| Cl | 2.82565 | 0.00000 | 43.61329 |
| Cl | 6.06092 | 1.68560 | 17.70760 |
| Cl | 2.54727 | 1.68560 | 24.21440 |
| Cl | 6.21275 | 1.68560 | 30.68241 |
| Cl | 2.74790 | 1.68560 | 37.12384 |
| Cl | 6.42789 | 1.68560 | 43.61588 |
| Cl | 3.99600 | 0.00000 | 15.00401 |
| Cl | 0.49281 | 0.00000 | 21.51819 |
| Cl | 4.21617 | 0.00000 | 27.93109 |
| Cl | 0.72020 | 0.00000 | 34.40639 |
| Cl | 4.34273 | 0.00000 | 40.90379 |
| Cl | 0.39540 | 1.68560 | 15.00382 |
| Cl | 4.08848 | 1.68560 | 21.49991 |
| Cl | 0.61555 | 1.68560 | 27.93109 |
| Cl | 4.29814 | 1.68560 | 34.43427 |
| Cu | 0.74184 | 1.68560 | 40.90429 |
| Cu | 6.83532 | 0.00000 | 16.35949 |
| Cu | 3.31673 | 0.00000 | 22.85812 |
| Cu | 7.01947 | 0.00000 | 29.30900 |
| Cu | 3.50737 | 0.00000 | 35.77241 |
| Cu | 7.18176 | 0.00000 | 42.25809 |
| Cu | 3.23513 | 1.68560 | 16.36023 |
| Cu | 6.91586 | 1.68560 | 22.86731 |
| Cu | 3.41419 | 1.68560 | 29.30675 |
| Cu | 7.12776 | 1.68560 | 35.75360 |
| Cu | 3.57933 | 1.68560 | 42.25490 |

Size of vaccum: ~ 15.0 Å in both directions of the symmetric slab.

**k**-points: 9 irreducible k-points

**(110)Cl**

Cl 40  Cu 18

**Lattice vectors**

| | | |
|---|---|---|
| 7.3556999999999997 | 0.0000000000000000 | 0.0000000000000000 |
| -3.4336600000000002 | 7.1715799999999996 | 0.0000000000000000 |
| 0.0000000000000000 | 0.0000000000000000 | 56.8256999999999977 |

**Cartesian Coordinates**

| | | | |
|---|---|---|---|
| Cl | -0.73391 | 4.20320 | 15.16568 |
| Cl | -0.70503 | 2.75735 | 18.00391 |
| Cl | 6.70012 | 1.09981 | 20.95936 |
| Cl | 3.25871 | 6.66776 | 23.91087 |
| Cl | 3.30821 | 5.08695 | 26.90185 |
| Cl | 3.27118 | 3.56478 | 29.91311 |
| Cl | 3.28372 | 1.91535 | 32.87431 |
| Cl | 3.29073 | 0.38814 | 35.87112 |
| Cl | -0.17777 | 5.98000 | 38.82941 |
| Cl | -0.17943 | 4.51483 | 41.63968 |
| Cl | 0.98314 | 0.61707 | 15.16557 |
| Cl | -2.42129 | 6.33671 | 18.00247 |
| Cl | 4.99355 | 4.68984 | 20.96022 |
| Cl | 5.02501 | 3.08593 | 23.92646 |
| Cl | 4.99012 | 1.48957 | 26.90435 |
| Cl | 1.55747 | 7.14563 | 29.91727 |
| Cl | 1.56749 | 5.50069 | 32.87528 |
| Cl | 1.58240 | 3.96674 | 35.87747 |
| Cl | 1.51756 | 2.38622 | 38.83599 |
| Cl | 1.53057 | 0.92296 | 41.64713 |
| Cl | 3.64773 | 4.21049 | 15.15483 |
| Cl | 3.61114 | 2.71338 | 17.98461 |
| Cl | 3.55900 | 1.17155 | 20.99710 |
| Cl | 0.12537 | 6.75835 | 23.97249 |
| Cl | 0.15921 | 5.17669 | 26.95365 |
| Cl | 0.15508 | 3.55783 | 29.92410 |
| Cl | 0.15390 | 1.97899 | 32.91408 |
| Cl | 0.14954 | 0.37924 | 35.85364 |
| Cl | 4.12670 | 5.92760 | 38.82910 |
| Cl | 4.17295 | 4.51098 | 41.65254 |
| Cl | 5.36456 | 0.63355 | 15.16604 |
| Cl | 1.89718 | 6.32335 | 18.00006 |
| Cl | 1.84225 | 4.75734 | 20.99710 |
| Cl | 1.88417 | 3.17198 | 23.95923 |

| | | | |
|---|---|---|---|
| Cl | 1.87031 | 1.59216 | 26.95546 |
| Cl | -1.56524 | 7.14368 | 29.92749 |
| Cl | -1.55920 | 5.56104 | 32.91573 |
| Cl | -1.56643 | 3.96506 | 35.85374 |
| Cl | 5.83500 | 2.33781 | 38.83656 |
| Cl | 5.88116 | 0.92356 | 41.66178 |
| Cu | 3.42046 | 7.03499 | 16.50209 |
| Cu | 3.41953 | 5.53406 | 19.54276 |
| Cu | 3.43806 | 3.94365 | 22.47393 |
| Cu | 3.43366 | 2.33686 | 25.43746 |
| Cu | 3.42933 | 0.74852 | 28.42342 |
| Cu | -0.00048 | 6.33808 | 31.40551 |
| Cu | 0.01501 | 4.75454 | 34.38178 |
| Cu | -0.00997 | 3.17780 | 37.31023 |
| Cu | 0.01223 | 1.68376 | 40.33929 |
| Cu | 5.13490 | 3.44251 | 16.49615 |
| Cu | 5.13240 | 1.94225 | 19.53514 |
| Cu | 5.12455 | 0.36082 | 22.47514 |
| Cu | 1.71643 | 5.93754 | 25.44999 |
| Cu | 1.71682 | 4.33795 | 28.41285 |
| Cu | 1.71670 | 2.75324 | 31.40392 |
| Cu | 1.72568 | 1.17238 | 34.37717 |
| Cu | -1.71937 | 6.76924 | 37.30820 |
| Cu | -1.69546 | 5.27458 | 40.32871 |

Size of vaccum: ~ 15.0 Å in both directions of the symmetric slab.

**k**-points: 10 irreducible k-points

**(001)CuCl**

**Cl 16  Cu 10**

**Lattice vectors**

| | | |
|---|---|---|
| 7.2011000000000003 | 0.0000000000000000 | 0.0000000000000000 |
| 0.0000000000000000 | 3.3712000000000000 | 0.0000000000000000 |
| 0.0000000000000000 | 0.0000000000000000 | 55.8626000000000005 |

**Cartesian Coordinates**

| | | | |
|---|---|---|---|
| Cl | 1.75184 | 0.00000 | 15.35299 |
| Cl | 6.17610 | 0.00000 | 22.80070 |
| Cl | 2.61220 | 0.00000 | 29.30664 |
| Cl | 6.35908 | 0.00000 | 35.83141 |
| Cl | 5.37387 | 1.68560 | 15.19961 |
| Cl | 2.53983 | 1.68560 | 22.77223 |
| Cl | 6.22657 | 1.68560 | 29.26498 |
| Cl | 2.70538 | 1.68560 | 35.77217 |
| Cl | 0.45480 | 0.00000 | 20.04892 |
| Cl | 4.13910 | 0.00000 | 26.56268 |
| Cl | 0.66139 | 0.00000 | 33.08824 |
| Cl | 4.72617 | 0.00000 | 40.19134 |
| Cl | 4.12292 | 1.68560 | 20.09043 |
| Cl | 0.53894 | 1.68560 | 26.55655 |
| Cl | 4.30002 | 1.68560 | 33.06446 |
| Cl | 1.12273 | 1.68560 | 40.19030 |
| Cu | 6.82830 | 0.00000 | 15.00023 |
| Cu | 3.33212 | 0.00000 | 21.44097 |
| Cu | 6.99267 | 0.00000 | 27.91184 |
| Cu | 3.50737 | 0.00000 | 34.39684 |
| Cu | 6.87241 | 0.00000 | 39.91714 |
| Cu | 3.21650 | 1.68560 | 15.23332 |
| Cu | 6.91564 | 1.68560 | 21.43181 |
| Cu | 3.41419 | 1.68560 | 27.93130 |
| Cu | 7.10817 | 1.68560 | 34.44497 |
| Cu | 3.27330 | 1.68560 | 39.92612 |

Size of vaccum: ~ 15.0 Å in both directions of the symmetric slab.

**k**-points:  9 irreducible k-points

**(110)CuCl**

**Cl 32  Cu 18**

**Lattice vectors**

| | | |
|---|---|---|
| 7.3557000160000001 | 0.0000000000000000 | 0.0000000000000000 |
| -3.4336606333000002 | 7.1715797582000000 | 0.0000000000000000 |
| 0.0000000000000000 | 0.0000000000000000 | 53.8040008545000035 |

**Cartesian Coordinates**

| | | | |
|---|---|---|---|
| Cl | -0.61312 | 4.11738 | 15.26517 |
| Cl | -0.65368 | 2.70754 | 18.06368 |
| Cl | 6.71315 | 1.08787 | 20.97339 |
| Cl | 3.27578 | 6.66105 | 23.90990 |
| Cl | 3.30821 | 5.08695 | 26.90185 |
| Cl | 3.15888 | 3.81884 | 30.06628 |
| Cl | 4.01445 | 2.41682 | 33.52997 |
| Cl | -1.83942 | 6.61234 | 35.34010 |
| Cl | 0.18141 | 6.14113 | 39.01598 |
| Cl | -1.18118 | 3.81255 | 42.04356 |
| Cl | 1.00535 | 0.52198 | 15.22670 |
| Cl | -2.40768 | 6.28633 | 18.05778 |
| Cl | 5.02536 | 4.68517 | 20.98402 |
| Cl | 5.02501 | 3.08593 | 23.92646 |
| Cl | 5.18150 | 1.57107 | 26.72021 |
| Cl | 4.80953 | 0.18751 | 30.01326 |
| Cl | 0.95035 | 5.73547 | 33.36308 |
| Cl | 0.73865 | 3.21615 | 36.12363 |
| Cl | 1.11873 | 0.42215 | 41.60534 |
| Cl | 3.70807 | 4.09029 | 15.19607 |
| Cl | 3.65365 | 2.64715 | 17.98711 |
| Cl | 3.55900 | 1.17155 | 20.99710 |
| Cl | 0.12537 | 6.75835 | 23.97249 |
| Cl | 0.18493 | 5.24193 | 26.95864 |
| Cl | -0.28149 | 3.86358 | 29.86341 |
| Cl | 0.93842 | 0.71335 | 31.84553 |
| Cl | 4.08372 | 3.56326 | 42.08502 |
| Cl | 5.34228 | 0.39435 | 15.18234 |
| Cl | 1.89467 | 6.23738 | 18.02713 |
| Cl | 1.84225 | 4.75734 | 20.99710 |
| Cl | 1.89095 | 3.18952 | 23.97834 |
| Cl | 1.89242 | 1.64443 | 27.03780 |
| Cu | 2.89956 | 0.52456 | 30.95875 |
| Cu | 2.98413 | 0.44926 | 33.75231 |

| | | | |
|---|---|---|---|
| Cu | -0.18128 | 2.00392 | 41.77843 |
| Cu | 3.43000 | 6.90289 | 16.52820 |
| Cu | 3.43340 | 5.52128 | 19.58643 |
| Cu | 3.44577 | 3.94903 | 22.48073 |
| Cu | 3.43366 | 2.33686 | 25.43746 |
| Cu | 3.60998 | 0.90126 | 28.23626 |
| Cu | 0.65288 | 5.34988 | 31.20573 |
| Cu | -0.25460 | 4.98743 | 35.32747 |
| Cu | 5.20611 | 3.36570 | 16.54116 |
| Cu | 5.15049 | 1.91464 | 19.55515 |
| Cu | 5.12751 | 0.36317 | 22.48661 |
| Cu | 1.73283 | 5.96718 | 25.44510 |
| Cu | 1.71682 | 4.33795 | 28.41285 |
| Cu | 1.44925 | 2.60161 | 30.76907 |
| Cu | 2.33939 | 2.79777 | 34.78574 |
| Cu | -0.82776 | 6.45278 | 37.25094 |

Size of vaccum: ~ 12.0-15.0 Å in both directions of the symmetric slab.

**k**-points: 10 irreducible k-points

**(010)CuCl**

**Cl 18  Cu 9**

**Lattice vectors**

| | | |
|---|---|---|
| 7.3556999999999997 | 0.0000000000000000 | 0.0000000000000000 |
| -3.4336380000000002 | 6.3297689999999998 | 0.0000000000000000 |
| 0.0000000000000000 | 0.0000000000000000 | 43.4847999999999999 |

**Cartesian Coordinates**

| | | | |
|---|---|---|---|
| Cl | 0.05322 | 3.36454 | 17.01051 |
| Cl | -0.12765 | 3.16242 | 20.13913 |
| Cl | -0.12765 | 3.16242 | 23.34567 |
| Cl | 0.05322 | 3.36454 | 26.47429 |
| Cl | -2.07307 | 5.33496 | 15.01058 |
| Cl | -1.91167 | 6.16164 | 18.34866 |
| Cl | -1.84221 | 6.28065 | 21.74240 |
| Cl | -1.91167 | 6.16164 | 25.13614 |
| Cl | -2.07307 | 5.33496 | 28.47422 |
| Cl | 3.86884 | 2.96523 | 17.01051 |
| Cl | 4.04971 | 3.16735 | 20.13913 |
| Cl | 4.04971 | 3.16735 | 23.34567 |
| Cl | 3.86884 | 2.96523 | 26.47429 |
| Cl | 5.99513 | 0.99481 | 15.01058 |
| Cl | 5.83373 | 0.16813 | 18.34866 |
| Cl | 5.76428 | 0.04912 | 21.74240 |
| Cl | 5.83373 | 0.16813 | 25.13614 |
| Cl | 5.99513 | 0.99481 | 28.47422 |
| Cu | 0.00000 | 0.00000 | 16.59078 |
| Cu | 0.00000 | 0.00000 | 20.06376 |
| Cu | 0.00000 | 0.00000 | 23.42104 |
| Cu | 0.00000 | 0.00000 | 26.89402 |
| Cu | -1.71682 | 3.16488 | 15.54700 |
| Cu | -1.71682 | 3.16488 | 18.44911 |
| Cu | -1.71682 | 3.16488 | 21.74240 |
| Cu | -1.71682 | 3.16488 | 25.03569 |
| Cu | -1.71682 | 3.16488 | 27.93780 |

Size of vaccum: ~ 15.0 Å in both directions of the symmetric slab.

**k**-points:  9 irreducible k-points

**(100)CuCl**

**Cl 17  Cu 9**

**Lattice vectors**

| | | |
|---|---|---|
| 3.3712000000000000 | 0.0000000000000000 | 0.0000000000000000 |
| 0.0000000000000000 | 7.3556999999999997 | 0.0000000000000000 |
| 0.0000000000000000 | 0.0000000000000000 | 45.3682000000000016 |

**Cartesian Coordinates**

| | | | |
|---|---|---|---|
| Cu | 0.00000 | 6.17109 | 13.17600 |
| Cu | 0.00000 | 2.76472 | 19.54489 |
| Cu | 0.00000 | 6.73902 | 25.86797 |
| Cu | 0.00000 | 3.26557 | 32.26095 |
| Cu | 1.68560 | 0.61423 | 9.86561 |
| Cu | 1.68560 | 4.52990 | 16.39324 |
| Cu | 1.68560 | 1.10299 | 22.65960 |
| Cu | 1.68560 | 4.91113 | 29.02518 |
| Cu | 1.68560 | 1.09624 | 35.88864 |
| Cu | 0.00000 | 3.06450 | 13.22337 |
| Cu | 0.00000 | 7.01339 | 19.60944 |
| Cu | 0.00000 | 3.62233 | 25.92478 |
| Cu | 0.00000 | 0.01780 | 32.43717 |
| Cu | 1.68560 | 4.89628 | 10.06345 |
| Cu | 1.68560 | 1.42492 | 16.39875 |
| Cu | 1.68560 | 5.27588 | 22.75760 |
| Cu | 1.68560 | 1.80124 | 29.20964 |
| Cl | 0.00000 | 6.44348 | 10.03070 |
| Cl | 0.00000 | 2.97950 | 16.41230 |
| Cl | 0.00000 | 6.86728 | 22.70860 |
| Cl | 0.00000 | 3.36740 | 29.12351 |
| Cl | 0.00000 | 0.69344 | 34.57231 |
| Cl | 1.68560 | 4.61671 | 13.20018 |
| Cl | 1.68560 | 1.21328 | 19.59041 |
| Cl | 1.68560 | 5.18088 | 25.90423 |
| Cl | 1.68560 | 1.70754 | 32.15447 |

Size of vaccum: ~ 15.0 Å in both directions of the symmetric slab.

**k**-points:  9 irreducible k-points

**(101)CuCl**

**Cl 28  Cu 13**

**Lattice vectors**

| | | |
|---|---|---|
| 12.5090000000000003 | 0.0000000000000000 | 0.0000000000000000 |
| 0.0000000000000000 | 3.3712000000000000 | 0.0000000000000000 |
| 0.0000000000000000 | 0.0000000000000000 | 54.5289000000000001 |

**Cartesian Coordinates**

| | | | |
|---|---|---|---|
| Cl | 9.28276 | 0.00000 | 14.98510 |
| Cl | 3.01767 | 0.00000 | 18.68125 |
| Cl | 9.10335 | 0.00000 | 22.41041 |
| Cl | 2.75561 | 0.00000 | 26.16624 |
| Cl | 8.92767 | 0.00000 | 29.88639 |
| Cl | 2.63947 | 0.00000 | 33.60077 |
| Cl | 8.72921 | 0.00000 | 37.35080 |
| Cl | 12.41546 | 1.68560 | 16.79150 |
| Cl | 6.04806 | 1.68560 | 20.54875 |
| Cl | 12.23689 | 1.68560 | 24.26052 |
| Cl | 5.89397 | 1.68560 | 28.01656 |
| Cl | 12.02393 | 1.68560 | 31.74494 |
| Cl | 5.73312 | 1.68560 | 35.47691 |
| Cl | 11.86512 | 1.68560 | 39.18341 |
| Cl | 5.74357 | 0.00000 | 17.18915 |
| Cl | 11.84213 | 0.00000 | 20.91313 |
| Cl | 5.51844 | 0.00000 | 24.65747 |
| Cl | 11.64384 | 0.00000 | 28.37198 |
| Cl | 5.36593 | 0.00000 | 32.10205 |
| Cl | 11.42983 | 0.00000 | 35.78628 |
| Cl | 5.18062 | 0.00000 | 39.54212 |
| Cl | 2.61031 | 1.68560 | 15.31884 |
| Cl | 8.75468 | 1.68560 | 19.03777 |
| Cl | 2.46815 | 1.68560 | 22.77945 |
| Cl | 8.60395 | 1.68560 | 26.50845 |
| Cl | 2.24479 | 1.68560 | 30.25340 |
| Cl | 8.43958 | 1.68560 | 33.97717 |
| Cl | 2.04920 | 1.68560 | 37.73507 |
| Cu | 1.26223 | 0.00000 | 16.09194 |
| Cu | 7.40054 | 0.00000 | 19.78364 |
| Cu | 1.09609 | 0.00000 | 23.52292 |
| Cu | 7.24465 | 0.00000 | 27.25575 |
| Cu | 0.87584 | 0.00000 | 30.99229 |

| | | | |
|---|---|---|---|
| Cu | 7.08146 | 0.00000 | 34.73603 |
| Cu | 0.69736 | 0.00000 | 38.41602 |
| Cu | 4.38479 | 1.68560 | 17.94176 |
| Cu | 10.46969 | 1.68560 | 21.65189 |
| Cu | 4.15299 | 1.68560 | 25.40338 |
| Cu | 10.28648 | 1.68560 | 29.13123 |
| Cu | 3.99978 | 1.68560 | 32.84337 |
| Cu | 10.07150 | 1.68560 | 36.55408 |

Size of vaccum: ~ 12.0-15.0 Å in both directions of the symmetric slab.

**k**-points: 10 irreducible k-points

**(111)CuCl**

**Cl 28  Cu 13**

**Lattice vectors**

| | | |
|---|---|---|
| 7.9512000000000000 | 0.0000000000000000 | 0.0000000000000000 |
| 1.7471350000000001 | 7.9005239999999999 | 0.0000000000000000 |
| 0.0000000000000000 | 0.0000000000000000 | 50.4664000000000001 |

**Cartesian Coordinates**

| | | | |
|---|---|---|---|
| Cl | 9.28276 | 0.00000 | 14.98510 |
| Cl | 3.01767 | 0.00000 | 18.68125 |
| Cl | 9.10335 | 0.00000 | 22.41041 |
| Cl | 2.75561 | 0.00000 | 26.16624 |
| Cl | 8.92767 | 0.00000 | 29.88639 |
| Cl | 2.63947 | 0.00000 | 33.60077 |
| Cl | 8.72921 | 0.00000 | 37.35080 |
| Cl | 12.41546 | 1.68560 | 16.79150 |
| Cl | 6.04806 | 1.68560 | 20.54875 |
| Cl | 12.23689 | 1.68560 | 24.26052 |
| Cl | 5.89397 | 1.68560 | 28.01656 |
| Cl | 12.02393 | 1.68560 | 31.74494 |
| Cl | 5.73312 | 1.68560 | 35.47691 |
| Cl | 11.86512 | 1.68560 | 39.18341 |
| Cl | 5.74357 | 0.00000 | 17.18915 |
| Cl | 11.84213 | 0.00000 | 20.91313 |
| Cl | 5.51844 | 0.00000 | 24.65747 |
| Cl | 11.64384 | 0.00000 | 28.37198 |
| Cl | 5.36593 | 0.00000 | 32.10205 |
| Cl | 11.42983 | 0.00000 | 35.78628 |
| Cl | 5.18062 | 0.00000 | 39.54212 |
| Cl | 2.61031 | 1.68560 | 15.31884 |
| Cl | 8.75468 | 1.68560 | 19.03777 |
| Cl | 2.46815 | 1.68560 | 22.77945 |
| Cl | 8.60395 | 1.68560 | 26.50845 |
| Cl | 2.24479 | 1.68560 | 30.25340 |
| Cl | 8.43958 | 1.68560 | 33.97717 |
| Cl | 2.04920 | 1.68560 | 37.73507 |
| Cu | 1.26223 | 0.00000 | 16.09194 |
| Cu | 7.40054 | 0.00000 | 19.78364 |
| Cu | 1.09609 | 0.00000 | 23.52292 |
| Cu | 7.24465 | 0.00000 | 27.25575 |
| Cu | 0.87584 | 0.00000 | 30.99229 |

| | | | |
|---|---|---|---|
| Cu | 7.08146 | 0.00000 | 34.73603 |
| Cu | 0.69736 | 0.00000 | 38.41602 |
| Cu | 4.38479 | 1.68560 | 17.94176 |
| Cu | 10.46969 | 1.68560 | 21.65189 |
| Cu | 4.15299 | 1.68560 | 25.40338 |
| Cu | 10.28648 | 1.68560 | 29.13123 |
| Cu | 3.99978 | 1.68560 | 32.84337 |
| Cu | 10.07150 | 1.68560 | 36.55408 |

Size of vaccum: ~ 12.0-15.0 Å in both directions of the symmetric slab.

**k**-points: 9 irreducible k-points

**(011)CuCl**

**Cl 29  Cu 14**

**Lattice vectors**

| | | |
|---|---|---|
| 7.2011000000000003 | 0.0000000000000000 | 0.0000000000000000 |
| 3.5073439999999998 | 7.2917280000000000 | 0.0000000000000000 |
| 0.0000000000000000 | 0.0000000000000000 | 50.9249000000000009 |

**Cartesian Coordinates**

| | | | |
|---|---|---|---|
| Cl | 3.15447 | 3.83328 | 14.96788 |
| Cl | 2.50382 | 5.17390 | 18.19363 |
| Cl | 9.82071 | 6.77848 | 21.02658 |
| Cl | 6.30588 | 1.05730 | 23.96780 |
| Cl | 6.31063 | 2.66392 | 26.93154 |
| Cl | 6.30323 | 4.23740 | 29.92004 |
| Cl | 6.33972 | 5.82517 | 32.93231 |
| Cl | 2.12371 | 0.59317 | 35.58589 |
| Cl | 5.92179 | 4.81166 | 16.40594 |
| Cl | 6.25759 | 6.00706 | 19.44607 |
| Cl | 2.70539 | 0.27803 | 22.47316 |
| Cl | 2.71208 | 1.84584 | 25.45216 |
| Cl | 2.70162 | 3.39686 | 28.39656 |
| Cl | 2.79594 | 4.89139 | 31.32722 |
| Cl | 10.02461 | 6.14675 | 34.22772 |
| Cl | 0.53673 | 0.34360 | 16.79578 |
| Cl | 7.90287 | 1.85403 | 19.75582 |
| Cl | 7.86790 | 3.46592 | 22.71282 |
| Cl | 7.90992 | 5.05514 | 25.68550 |
| Cl | 7.90991 | 6.61374 | 28.67479 |
| Cl | 4.47310 | 0.85097 | 31.69217 |
| Cl | 5.19897 | 1.91229 | 34.84072 |
| Cl | 7.90488 | 6.98057 | 15.47383 |
| Cl | 4.21004 | 1.12723 | 18.26030 |
| Cl | 4.26981 | 2.70002 | 21.19047 |
| Cl | 4.24698 | 4.24867 | 24.16758 |
| Cl | 4.23056 | 5.82083 | 27.08531 |
| Cl | 0.82630 | 0.01912 | 30.03490 |
| Cl | 7.96512 | 1.70803 | 32.70562 |
| Cu | 6.99382 | 6.48336 | 17.35723 |
| Cu | 3.45838 | 0.72301 | 20.37174 |
| Cu | 3.48649 | 2.26391 | 23.31252 |
| Cu | 3.45718 | 3.83576 | 26.27755 |
| Cu | 3.53536 | 5.35152 | 29.21806 |

| | | | |
|---|---|---|---|
| Cu | 3.56166 | 6.89149 | 32.18081 |
| Cu | 7.25549 | 0.97491 | 34.77156 |
| Cu | 3.68512 | 5.47859 | 16.20665 |
| Cu | 10.53337 | 7.18292 | 18.90206 |
| Cu | 7.10655 | 1.46618 | 21.85895 |
| Cu | 7.10785 | 3.05618 | 24.82640 |
| Cu | 7.10791 | 4.61479 | 27.81569 |
| Cu | 7.12994 | 6.20522 | 30.80678 |
| Cu | 3.65793 | 0.49630 | 33.83788 |

Size of vaccum: ~ 16.0-20.0 Å in both directions of the symmetric slab.

**k**-points: 10 irreducible k-points