Table S1. Hydrogen bonds for 4ac16r_a (6) [Å and °].

| D-H...A | d(D-H) | d(H...A) | d(D...A) | <(DHA) |
|---|---|---|---|---|
| N(1)-H(1A)...Br(4) | 0.91 | 2.82 | 3.562(11) | 140 |
| N(1)-H(1A)...Br(9) | 0.91 | 3.02 | 3.649(12) | 128 |
| N(1)-H(1B)...Br(13) | 0.91 | 2.48 | 3.382(11) | 174 |
| N(1)-H(1C)...Br(3) | 0.91 | 2.66 | 3.467(12) | 149 |
| N(2)-H(2A)...Br(1) | 0.91 | 2.87 | 3.476(11) | 126 |
| N(2)-H(2A)...Br(12)#1 | 0.91 | 3.13 | 3.783(11) | 130 |
| N(2)-H(2B)...Br(13)#1 | 0.91 | 2.55 | 3.368(11) | 150 |
| N(2)-H(2C)...Br(4) | 0.91 | 2.70 | 3.546(12) | 154 |
| N(3)-H(3A)...Br(14) | 0.91 | 2.67 | 3.432(10) | 142 |
| N(3)-H(3B)...Br(8)#3 | 0.91 | 2.79 | 3.679(10) | 167 |
| N(3)-H(3C)...Br(10)#2 | 0.91 | 2.61 | 3.421(11) | 148 |
| N(4)-H(4A)...Br(11) | 0.91 | 2.71 | 3.444(12) | 139 |
| N(4)-H(4B)...Br(12)#1 | 0.91 | 2.69 | 3.582(12) | 168 |
| N(4)-H(4C)...Br(1) | 0.91 | 2.96 | 3.558(11) | 125 |
| N(4)-H(4C)...Br(5) | 0.91 | 3.02 | 3.780(12) | 142 |
| N(5)-H(5A)...Br(5) | 0.91 | 2.95 | 3.702(11) | 140 |
| N(5)-H(5A)...Br(3) | 0.91 | 2.95 | 3.600(11) | 130 |
| N(5)-H(5B)...Br(12) | 0.91 | 2.69 | 3.591(11) | 171 |
| N(5)-H(5C)...Br(11) | 0.91 | 2.66 | 3.433(10) | 143 |
| N(6)-H(6A)...Br(10)#2 | 0.91 | 2.70 | 3.469(10) | 143 |
| N(6)-H(6B)...Br(8) | 0.91 | 2.83 | 3.708(11) | 164 |
| N(6)-H(6C)...Br(14) | 0.91 | 2.63 | 3.418(10) | 145 |
| N(7)-H(7A)...Br(15) | 0.91 | 2.70 | 3.354(13) | 129 |
| N(7)-H(7A)...Br(2) | 0.91 | 2.90 | 3.619(13) | 137 |
| N(7)-H(7B)...Br(18) | 0.91 | 2.55 | 3.445(11) | 167 |
| N(7)-H(7C)...Br(5) | 0.91 | 2.73 | 3.541(11) | 149 |
| N(8)-H(8A)...Br(5) | 0.91 | 2.76 | 3.594(15) | 152 |
| N(8)-H(8B)...Br(18)#1 | 0.91 | 2.53 | 3.431(13) | 172 |
| N(8)-H(8C)...Br(16)#1 | 0.91 | 2.71 | 3.346(16) | 128 |
| N(8)-H(8C)...Br(2) | 0.91 | 2.86 | 3.553(13) | 134 |
| N(9)-H(9A)...Br(6) | 0.91 | 2.55 | 3.385(12) | 152 |
| N(9)-H(9B)...Br(17) | 0.91 | 2.43 | 3.339(13) | 176 |

Table S2. Hydrogen bonds for $[(C_7H_{13}NH_3)_{17}Pb_7Cl_{31}]$ **(11)** [Å and °].

| D-H...A | d(D-H) | d(H...A) | d(D...A) | <(DHA) |
|---|---|---|---|---|
| N(1)-H(1A)...Cl(23) | 0.91 | 2.55 | 3.358(15) | 148 |
| N(1)-H(1B)...Cl(25)#2 | 0.91 | 2.76 | 3.468(14) | 136 |
| N(1)-H(1C)...Cl(9)#2 | 0.91 | 2.46 | 3.348(14) | 167 |
| N(2)-H(2A)...Cl(27) | 0.91 | 2.51 | 3.338(14) | 151 |
| N(2)-H(2B)...Cl(7) | 0.91 | 2.38 | 3.273(14) | 167 |
| N(2)-H(2C)...Cl(30) | 0.91 | 2.78 | 3.432(14) | 130 |
| N(2)-H(2C)...Cl(23) | 0.91 | 2.79 | 3.549(14) | 142 |
| N(3)-H(3A)...Cl(9) | 0.91 | 2.47 | 3.305(13) | 152 |
| N(3)-H(3B)...O(1)#1 | 0.91 | 1.95 | 2.847(16) | 171 |
| N(3)-H(3C)...Cl(13)#1 | 0.91 | 2.33 | 3.193(12) | 159 |
| N(4)-H(4A)...Cl(16) | 0.91 | 2.62 | 3.338(16) | 137 |
| N(4)-H(4B)...Cl(5) | 0.91 | 2.41 | 3.286(16) | 163 |
| N(4)-H(4C)...Cl(21) | 0.91 | 2.67 | 3.483(17) | 149 |
| N(5)-H(5A)...Cl(30) | 0.91 | 2.62 | 3.338(14) | 137 |
| N(5)-H(5B)...Cl(24) | 0.91 | 2.59 | 3.301(13) | 135 |
| N(5)-H(5C)...Cl(10) | 0.91 | 2.38 | 3.285(15) | 177 |
| N(6)-H(6A)...Cl(25) | 0.91 | 2.78 | 3.568(17) | 146 |
| N(6)-H(6B)...Cl(8)#1 | 0.91 | 2.36 | 3.249(16) | 166 |
| N(6)-H(6C)...Cl(23)#1 | 0.91 | 2.57 | 3.379(15) | 148 |
| N(7)-H(7A)...O(1)#1 | 0.91 | 2.00 | 2.873(17) | 161 |
| N(7)-H(7B)...Cl(12) | 0.91 | 2.37 | 3.272(17) | 174 |
| N(7)-H(7C)...Cl(10) | 0.91 | 2.34 | 3.239(15) | 169 |
| N(8)-H(8A)...Cl(29) | 0.91 | 2.64 | 3.317(13) | 132 |
| N(8)-H(8A)...Cl(31) | 0.91 | 2.70 | 3.332(12) | 127 |
| N(8)-H(8B)...Cl(11) | 0.91 | 2.32 | 3.219(12) | 169 |
| N(8)-H(8C)...Cl(13) | 0.91 | 2.39 | 3.248(12) | 158 |
| N(9)-H(9A)...Cl(17) | 0.91 | 2.62 | 3.251(12) | 127 |
| N(9)-H(9A)...Cl(15) | 0.91 | 2.78 | 3.474(12) | 134 |
| N(9)-H(9B)...Cl(3) | 0.91 | 2.37 | 3.229(12) | 158 |
| N(9)-H(9C)...Cl(1) | 0.91 | 2.38 | 3.258(12) | 163 |
| N(10)-H(10A)...Cl(14) | 0.91 | 2.74 | 3.209(14) | 113 |
| N(10)-H(10B)...Cl(29) | 0.91 | 2.52 | 3.302(11) | 144 |

| | | | | |
|---|---|---|---|---|
| N(10)-H(10B)...Cl(12) | 0.91 | 2.70 | 3.240(13) | 119 |
| N(10)-H(10C)...Cl(31) | 0.91 | 2.54 | 3.428(12) | 165 |
| N(11)-H(11A)...Cl(6) | 0.91 | 2.48 | 3.353(13) | 161 |
| N(11)-H(11B)...Cl(2)#2 | 0.91 | 2.29 | 3.192(13) | 169 |
| N(11)-H(11C)...O(2) | 0.91 | 1.99 | 2.882(17) | 165 |
| N(12)-H(12A)...Cl(4) | 0.91 | 2.43 | 3.192(16) | 142 |
| N(12)-H(12B)...Cl(17) | 0.91 | 2.41 | 3.254(15) | 155 |
| N(12)-H(12C)...Cl(2) | 0.91 | 2.38 | 3.239(16) | 158 |
| N(13)-H(13A)...Cl(5) | 0.91 | 2.26 | 3.167(14) | 175 |
| N(13)-H(13B)...Cl(3) | 0.91 | 2.32 | 3.218(15) | 170 |
| N(13)-H(13C)...O(2) | 0.91 | 2.00 | 2.833(17) | 151 |
| N(14)-H(14A)...Cl(25) | 0.91 | 2.71 | 3.460(15) | 140 |
| N(14)-H(14C)...Cl(6)#1 | 0.91 | 2.44 | 3.313(14) | 161 |
| N(14)-H(14B)...Cl(22) | 0.91 | 2.50 | 3.357(14) | 157 |
| N(15)-H(15A)...Cl(22) | 0.91 | 2.48 | 3.320(15) | 154 |
| N(15)-H(15B)...Cl(7) | 0.91 | 2.42 | 3.291(16) | 161 |
| N(15)-H(15C)...Cl(25) | 0.91 | 2.77 | 3.627(16) | 158 |
| N(16)-H(16A)...Cl(11) | 0.91 | 2.49 | 3.251(12) | 141 |
| N(16)-H(16C)...Cl(28) | 0.91 | 2.33 | 3.203(13) | 161 |
| N(17)-H(17A)...Cl(19) | 0.91 | 2.55 | 3.330(14) | 144 |
| N(17)-H(17B)...Cl(16) | 0.91 | 2.60 | 3.342(13) | 139 |
| N(17)-H(17C)...Cl(8) | 0.91 | 2.39 | 3.300(13) | 179 |
| O(1)-H(1AA)...Cl(31) | 0.85 | 2.34 | 3.188(10) | 180 |
| O(1)-H(1AB)...Cl(28)#2 | 0.85 | 2.40 | 3.149(11) | 146 |
| O(2)-H(2AA)...Cl(18) | 0.85 | 2.29 | 3.142(11) | 179.0 |
| O(2)-H(2AB)...Cl(15)#2 | 0.85 | 2.35 | 3.203(11) | 179 |

Symmetry transformations used to generate equivalent atoms:

#1 x-1,y,z  #2 x+1,y,z

| | | | | |
|---|---|---|---|---|
| N(9)-H(9C)...Br(15) | 0.91 | 2.66 | 3.341(13) | 132 |
| N(10)-H(10A)...Br(17) | 0.91 | 2.66 | 3.350(13) | 134 |
| N(10)-H(10B)...Br(6)#3 | 0.91 | 2.50 | 3.361(12) | 158 |
| N(10)-H(10C)...Br(16) | 0.91 | 2.45 | 3.296(13) | 154 |

Symmetry transformations used to generate equivalent atoms:

#1 x-1,y,z  #2 -x+1,-y+1,-z+1  #3 x+1,y,z

Table S3. Hydrogen bonds for $[(C_8H_{15}NH_3)_{18}Pb_{11}Cl_{40}]$ (**12**) [Å and °].

| D-H...A | d(D-H) | d(H...A) | d(D...A) | <(DHA) |
|---|---|---|---|---|
| N(1)-H(1A)...Cl(13) | 0.91 | 2.42 | 3.270(13) | 156 |
| N(1)-H(1C)...Cl(21) | 0.91 | 2.35 | 3.230(13) | 161 |
| N(1)-H(1B)...Cl(17) | 0.91 | 2.66 | 3.253(13) | 124 |
| N(2)-H(2A)...Cl(14) | 0.91 | 2.38 | 3.284(14) | 175 |
| N(2)-H(2C)...Cl(13)#5 | 0.91 | 2.43 | 3.296(14) | 160 |
| N(2)-H(2B)...Cl(17) | 0.91 | 2.35 | 3.234(13) | 163 |
| N(3)-H(3A)...Cl(1)#1 | 0.91 | 2.57 | 3.328(17) | 141 |
| N(3)-H(3C)...Cl(20) | 0.91 | 2.57 | 3.169(15) | 124 |
| N(3)-H(3B)...Cl(2)#6 | 0.91 | 2.35 | 3.241(14) | 165 |
| N(4)-H(4A)...Cl(11) | 0.91 | 2.63 | 3.314(14) | 132 |
| N(4)-H(4C)...Cl(15)#1 | 0.91 | 2.31 | 3.208(14) | 168 |
| N(4)-H(4B)...Cl(18) | 0.91 | 2.41 | 3.237(14) | 151 |
| N(5)-H(5A)...Cl(14) | 0.91 | 2.55 | 3.343(16) | 146 |
| N(5)-H(5C)...Cl(20) | 0.91 | 2.62 | 3.375(15) | 141 |
| N(5)-H(5B)...Cl(16)#1 | 0.91 | 2.37 | 3.270(17) | 172 |
| N(6)-H(6A)...Cl(21)#2 | 0.91 | 2.27 | 3.155(16) | 165 |
| N(6)-H(6C)...Cl(1) | 0.91 | 2.38 | 3.26(2) | 162 |
| N(6)-H(6B)...Cl(6)#4 | 0.91 | 2.52 | 3.294(19) | 143 |
| N(7)-H(7A)...Cl(7) | 0.91 | 2.63 | 3.28(2) | 128 |
| N(7)-H(7C)...Cl(16) | 0.91 | 2.41 | 3.28(2) | 159 |
| N(7)-H(7B)...Cl(9) | 0.91 | 2.40 | 3.26(2) | 158 |
| N(8)-H(8A)...Cl(8) | 0.91 | 2.38 | 3.252(15) | 161 |
| N(8)-H(8B)...Cl(6) | 0.91 | 2.34 | 3.204(14) | 158 |
| N(8)-H(8C)...Cl(5)#4 | 0.91 | 2.55 | 3.223(15) | 131 |
| N(9)-H(9A)...Cl(12) | 0.91 | 2.67 | 3.343(15) | 132 |
| N(9)-H(9C)...Cl(15) | 0.91 | 2.31 | 3.208(18) | 168 |
| N(9)-H(9A)...Cl(9) | 0.91 | 2.89 | 3.390(16) | 116 |

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y,-z #2 x,y,z+1 #3 -x+2,-y,-z+1

#4 -x+1,-y,-z+1 #5 -x+1,-y,-z #6 x,y,z-1