

Electronic supplementary information

Interface-driven spin filtering and diode effects in van der Waals junctions based on magnetic metal-organic frameworks

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1. Total energy as a function of layer distance

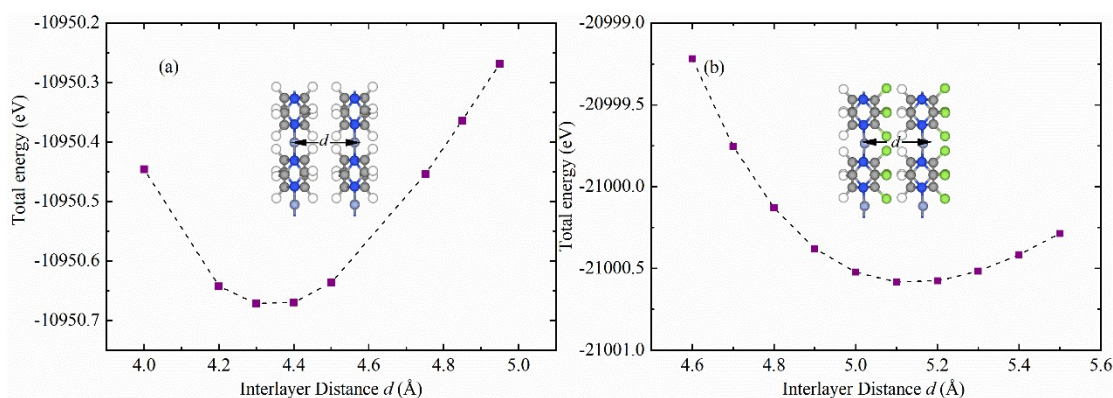


Fig. S1 Total energy as a function of layer distance for (a) $\text{Cr}(\text{pyz})_2$ and (b) $\text{Cr}(\text{h-fpyz})_2$.

2. Bias dependent transmission spectrum for $\text{Cr}(\text{pyz})_2$ -based junctions

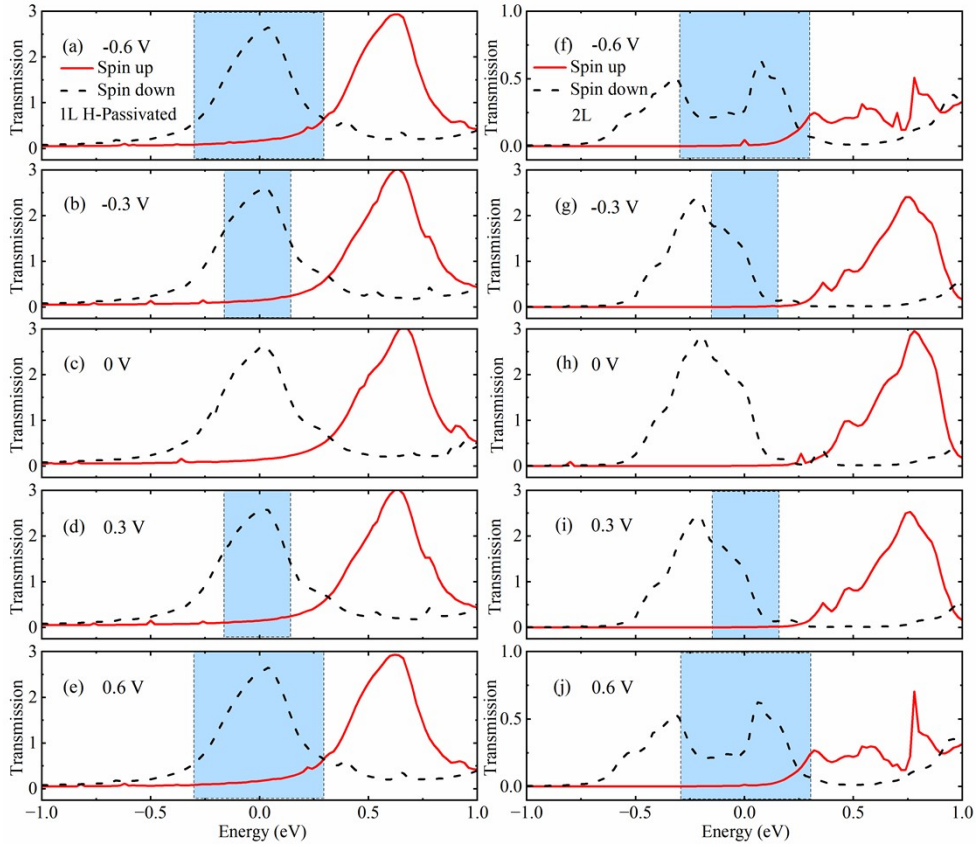


Fig. S2 Bias-dependent transmission spectrum for (a)-(e) monolayer and (f)-(j) bilayer $\text{Cr}(\text{pyz})_2$

3. Bias dependent transmission spectrum for $\text{Cr}(\text{h-fpyz})_2$ -based junctions

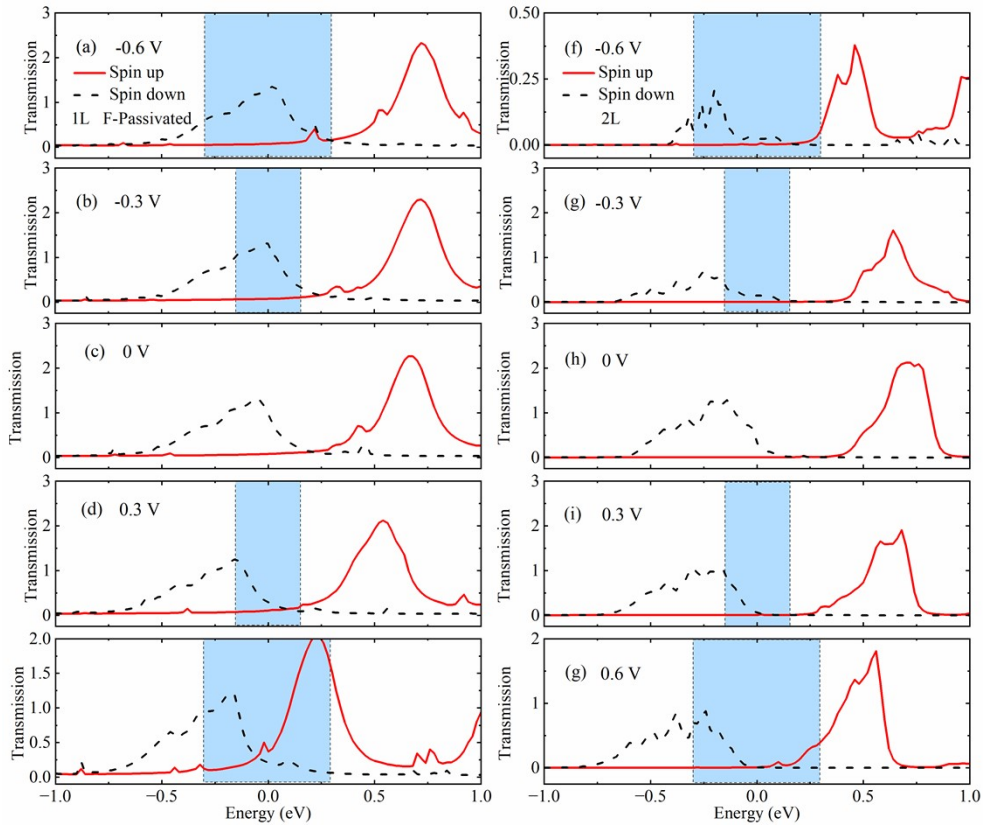


Fig. S3 Bias-dependent transmission spectrum for (a)-(e) monolayer and (f)-(j) bilayer $\text{Cr}(\text{h-fpyz})_2$

4. Spin-resolved transmission spectrum for junctions based on 1L/2L two sides dual-side fluorinated

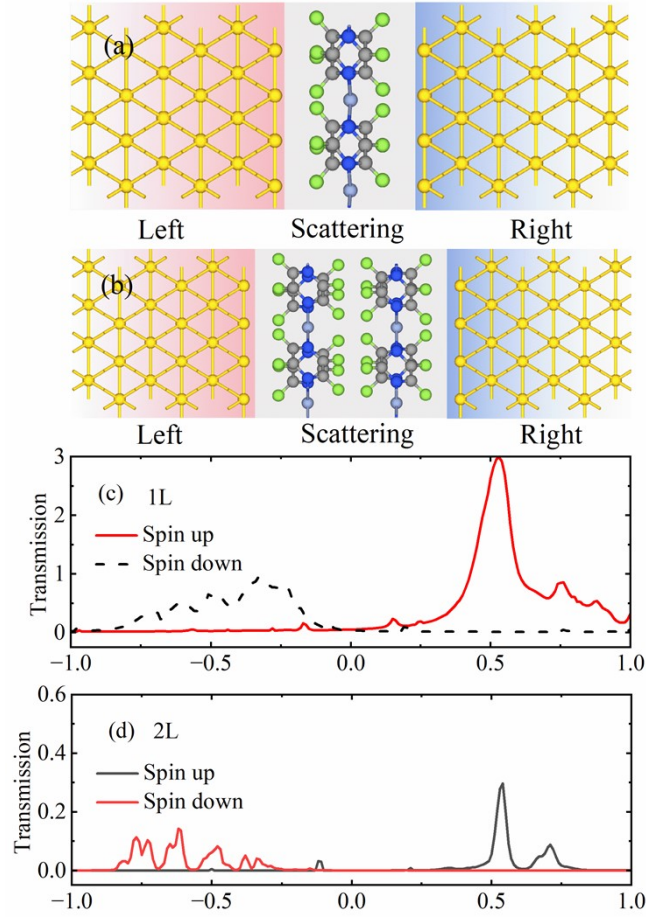


Fig. S4. Spin-resolved transmission spectrum for (a)-(e) monolayer and (f)-(j) bilayer $\text{Cr}(\text{h-fpyz})_2$ under zero bias.

5. Bias dependent PLDOS for $\text{Cr}(\text{pyz})_2$ and $\text{Cr}(\text{h-fpyz})_2$ -based junctions

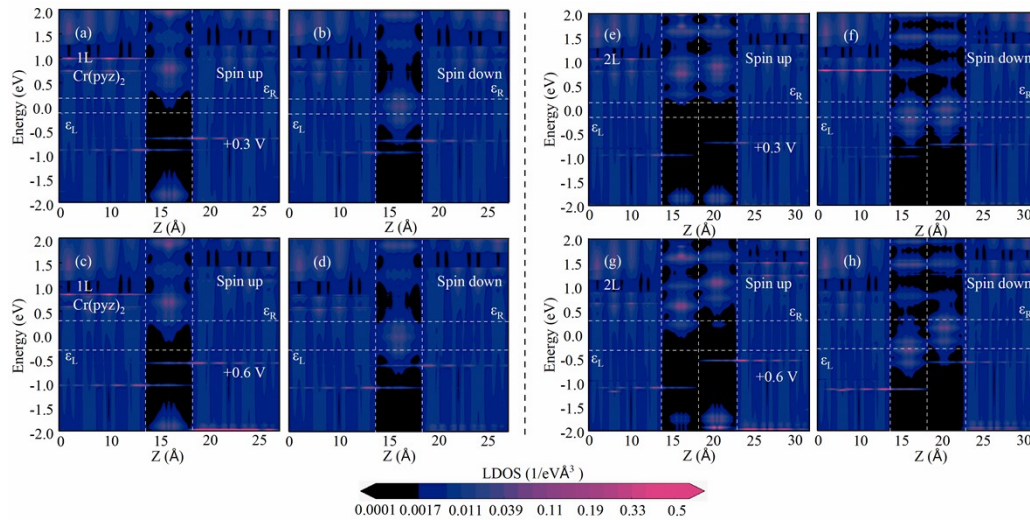


Fig. S5. Spin-resolved projected local density of states (PLDOS) for the junctions based on monolayer (1L) (a)-(d) and bilayer (2L) (e)-(f) $\text{Cr}(\text{pyz})_2$ under biases of 0.3 V and 0.6 V.

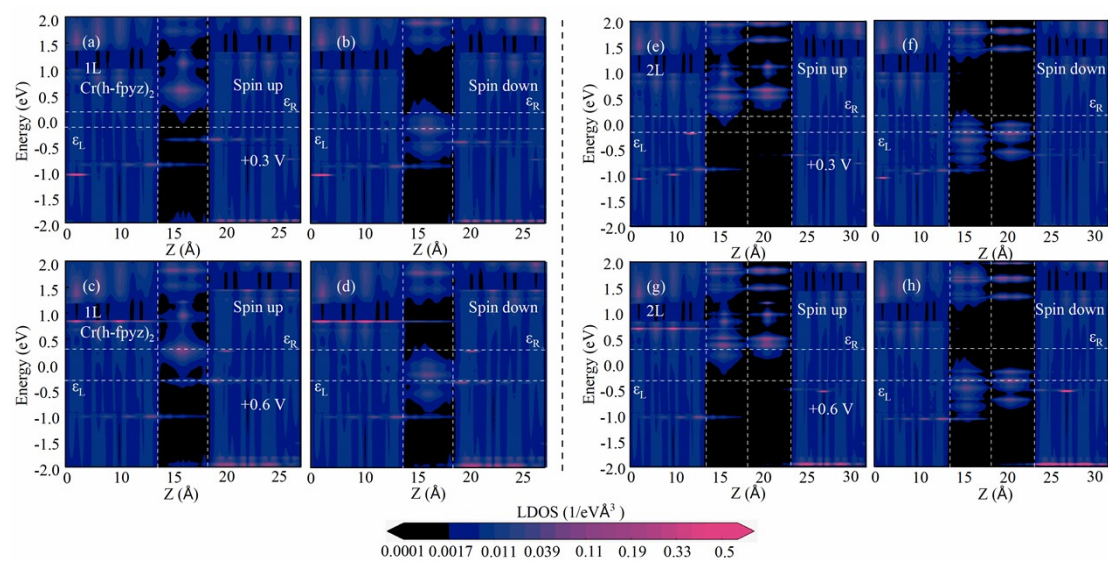


Fig. S6. Spin-resolved projected local density of states (PLDOS) for the junctions based on monolayer (1L) (a)-(d) and bilayer (2L) (e)-(f) $\text{Cr}(\text{h-fpyz})_2$ under biases of 0.3 V and 0.6 V.

6. The coordinates of the isolated molecule and junctions

Isolated 1L- $\text{Cr}(\text{pyz})_2$ molecule

42

Bulk

C	8.414293e+00	2.545384e+00	6.520332e+00
C	1.384698e+00	7.243031e+00	6.519644e+00
C	3.518044e+00	2.347153e+00	6.523080e+00
C	6.280897e+00	7.441951e+00	6.521922e+00
C	2.549050e+00	1.380841e+00	6.518800e+00
C	7.249998e+00	8.408133e+00	6.517361e+00
C	7.446545e+00	3.512744e+00	6.521759e+00
C	2.352312e+00	6.275652e+00	6.521295e+00
C	7.255115e+00	1.382927e+00	8.143506e+00
C	2.543487e+00	8.405471e+00	8.143129e+00
C	2.354296e+00	3.507384e+00	8.144543e+00
C	7.444683e+00	6.281999e+00	8.143539e+00
C	1.385448e+00	2.541275e+00	8.140284e+00
C	8.413608e+00	7.248020e+00	8.138990e+00
C	6.287310e+00	2.350079e+00	8.144869e+00
C	3.511168e+00	7.438195e+00	8.144820e+00
Cr	-8.028851e-05	9.790695e+00	7.325646e+00
Cr	4.899533e+00	4.894396e+00	7.335695e+00

H	9.276413e+00	2.640907e+00	5.861100e+00
H	5.225958e-01	7.147506e+00	5.860491e+00
H	4.382581e+00	2.252098e+00	5.866734e+00
H	5.416149e+00	7.537128e+00	5.865985e+00
H	2.644563e+00	5.192530e-01	5.858619e+00
H	7.154486e+00	9.269659e+00	5.857174e+00
H	7.540313e+00	4.375495e+00	5.863075e+00
H	2.258451e+00	5.412729e+00	5.862941e+00
H	7.161245e+00	5.201577e-01	8.802159e+00
H	2.637039e+00	9.268016e+00	8.802179e+00
H	2.259517e+00	4.368427e+00	8.805324e+00
H	7.539412e+00	5.421168e+00	8.804619e+00
H	5.211980e-01	2.636084e+00	8.796629e+00
H	9.277787e+00	7.153433e+00	8.795474e+00
H	5.425009e+00	2.254351e+00	8.803744e+00
H	4.373049e+00	7.533445e+00	8.804262e+00
N	8.376987e+00	1.421851e+00	7.330849e+00
N	1.422121e+00	8.366756e+00	7.329852e+00
N	6.320073e+00	6.319931e+00	7.334578e+00
N	3.478864e+00	3.469289e+00	7.335558e+00
N	8.375345e+00	8.369219e+00	7.325443e+00
N	1.423825e+00	1.419729e+00	7.327167e+00
N	6.324414e+00	3.473387e+00	7.334055e+00
N	3.474291e+00	6.315128e+00	7.333659e+00

Isolated 2L-Cr(py₂)₂ molecule

84

Bulk

H	7.729165e+00	4.728285e+00	9.693828e+00
H	2.237752e+00	5.713791e+00	9.696146e+00
H	9.487451e+00	2.988647e+00	9.700406e+00
H	4.820574e-01	7.455811e+00	9.701261e+00
H	5.475042e+00	7.983428e+00	9.719731e+00
H	2.737834e+00	7.184759e-01	9.716365e+00
H	7.229421e+00	9.726218e+00	9.717650e+00
H	4.494138e+00	2.459150e+00	9.719982e+00
C	7.606156e+00	3.832761e+00	1.032510e+01
C	2.363610e+00	6.610198e+00	1.032518e+01
C	8.591396e+00	2.858294e+00	1.032895e+01
C	1.379293e+00	7.585531e+00	1.032872e+01
C	6.378860e+00	7.845845e+00	1.033543e+01
C	7.362367e+00	8.822247e+00	1.033395e+01
C	2.606761e+00	1.621189e+00	1.033490e+01
C	3.591646e+00	2.596182e+00	1.033752e+01
N	6.461245e+00	6.704003e+00	1.110012e+01

N	1.464029e+00	1.711817e+00	1.109748e+01
N	3.499508e+00	6.692836e+00	1.109921e+01
N	6.471330e+00	3.749724e+00	1.109989e+01
N	8.505008e+00	8.732028e+00	1.109748e+01
Cr	4.985065e+00	5.219338e+00	1.099706e+01
N	3.510238e+00	3.737352e+00	1.110320e+01
Cr	9.991921e+00	2.399593e-01	1.099979e+01
N	1.453900e+00	8.718303e+00	1.110697e+01
N	8.517834e+00	1.725500e+00	1.110783e+01
C	7.606909e+00	6.613741e+00	1.186781e+01
C	1.381806e+00	2.856610e+00	1.186681e+01
C	8.587663e+00	7.587508e+00	1.186681e+01
C	2.363901e+00	3.828996e+00	1.186956e+01
C	3.574639e+00	7.828910e+00	1.188205e+01
C	6.398231e+00	2.615493e+00	1.188541e+01
C	2.592414e+00	8.801416e+00	1.188610e+01
C	7.380828e+00	1.643451e+00	1.188902e+01
H	7.725260e+00	5.704318e+00	1.247531e+01
H	4.723322e-01	2.980396e+00	1.247340e+01
H	9.496287e+00	7.465126e+00	1.247511e+01
H	2.246112e+00	4.738502e+00	1.247710e+01
H	4.477485e+00	7.944883e+00	1.250027e+01
H	5.496869e+00	2.501220e+00	1.250602e+01
H	2.702514e+00	9.703108e+00	1.250676e+01
H	7.272130e+00	7.427400e-01	1.251127e+01
H	7.705183e+00	4.718339e+00	1.446365e+01
H	2.266882e+00	5.723771e+00	1.446547e+01
H	9.479172e+00	2.958751e+00	1.446934e+01
H	4.907061e-01	7.481189e+00	1.447167e+01
H	5.485556e+00	7.957684e+00	1.449458e+01
H	2.715745e+00	7.269883e-01	1.449544e+01
H	7.257758e+00	9.717381e+00	1.449565e+01
H	4.488136e+00	2.486129e+00	1.450041e+01
C	7.596121e+00	3.817881e+00	1.508630e+01
C	2.375869e+00	6.624997e+00	1.508691e+01
C	8.577736e+00	2.844808e+00	1.509000e+01
C	1.392768e+00	7.596496e+00	1.509105e+01
C	6.393703e+00	7.834494e+00	1.510328e+01
C	7.375060e+00	8.807622e+00	1.510287e+01
C	2.596996e+00	1.635874e+00	1.510366e+01
C	3.578474e+00	2.608925e+00	1.510702e+01
N	6.475107e+00	6.689824e+00	1.587288e+01
N	1.450472e+00	1.726073e+00	1.587012e+01
N	3.513732e+00	6.708030e+00	1.586666e+01

N	6.459236e+00	3.736674e+00	1.586792e+01
N	8.519962e+00	8.716554e+00	1.587142e+01
Cr	4.985370e+00	5.220103e+00	1.597456e+01
N	3.495661e+00	3.752938e+00	1.587715e+01
Cr	9.991991e+00	2.392872e-01	1.597754e+01
N	1.466143e+00	8.731322e+00	1.587567e+01
N	8.503700e+00	1.710274e+00	1.587507e+01
C	7.616766e+00	6.599461e+00	1.663713e+01
C	1.367608e+00	2.867766e+00	1.663509e+01
C	8.601046e+00	7.575032e+00	1.663656e+01
C	2.351734e+00	3.843489e+00	1.663879e+01
C	3.588343e+00	7.842118e+00	1.664366e+01
C	6.384772e+00	2.604586e+00	1.664712e+01
C	2.602471e+00	8.816039e+00	1.664814e+01
C	7.368571e+00	1.628662e+00	1.665041e+01
H	7.747157e+00	5.696435e+00	1.725532e+01
H	4.627945e-01	3.005509e+00	1.724915e+01
H	9.502655e+00	7.438293e+00	1.725548e+01
H	2.218271e+00	4.747152e+00	1.725539e+01
H	4.485697e+00	7.974148e+00	1.726998e+01
H	5.488276e+00	2.476178e+00	1.727605e+01
H	2.726266e+00	9.712551e+00	1.727785e+01
H	7.242927e+00	7.329009e-01	1.728056e+01

Isolated 1L-Cr(f-hpyz)₂ molecule

42

Bulk

C	2.533435e+00	1.499003e+00	6.553500e+00
C	3.494070e+00	2.480701e+00	6.552623e+00
C	2.477449e+00	3.480901e+00	8.360801e+00
C	1.513881e+00	2.498005e+00	8.360499e+00
C	7.457307e+00	6.560264e+00	8.360715e+00
C	8.421002e+00	7.543128e+00	8.360371e+00
C	7.401416e+00	8.542209e+00	6.553420e+00
C	6.440746e+00	7.560629e+00	6.552600e+00
C	1.476357e+00	7.501219e+00	6.548994e+00
C	2.432283e+00	6.515165e+00	6.557240e+00
C	3.445994e+00	7.512268e+00	8.368440e+00
C	2.488018e+00	8.500915e+00	8.360370e+00
C	6.488742e+00	2.528599e+00	8.368278e+00
C	7.446506e+00	1.539919e+00	8.359983e+00
C	8.458725e+00	2.540113e+00	6.549331e+00
C	7.502701e+00	3.526183e+00	6.557609e+00
Cr	4.967439e+00	5.020568e+00	7.546794e+00

Cr	0.000000e+00	0.000000e+00	7.536320e+00
F	5.542358e+00	2.562280e+00	9.319024e+00
F	5.591978e-01	2.472035e+00	9.303123e+00
F	9.375663e+00	7.569025e+00	9.302958e+00
F	4.392111e+00	7.478159e+00	9.319366e+00
F	2.484631e+00	4.434853e+00	9.304191e+00
F	2.477982e+00	9.456550e+00	9.302053e+00
F	7.456095e+00	5.838982e-01	9.301369e+00
F	7.450044e+00	5.606358e+00	9.304085e+00
H	2.589348e+00	6.628363e-01	5.842437e+00
H	2.374647e+00	5.675708e+00	5.850233e+00
H	7.560487e+00	4.365780e+00	5.850865e+00
H	7.345530e+00	9.378514e+00	5.842452e+00
H	6.433249e-01	7.463881e+00	5.833189e+00
H	5.604919e+00	7.599263e+00	5.840292e+00
H	4.329862e+00	2.442130e+00	5.840302e+00
H	9.291864e+00	2.577725e+00	5.833722e+00
N	3.489655e+00	3.547517e+00	7.441155e+00
N	1.467143e+00	1.483672e+00	7.442120e+00
N	8.467810e+00	8.557411e+00	7.441958e+00
N	6.445112e+00	6.493739e+00	7.441063e+00
N	3.495404e+00	6.498770e+00	7.449434e+00
N	1.482680e+00	8.571425e+00	7.433435e+00
N	8.452448e+00	1.469878e+00	7.433724e+00
N	6.439642e+00	3.542565e+00	7.449835e+00

Isolated 2L-Cr(f-hpyz)₂ molecule

84

Bulk

H	7.153660e+00	9.238161e-01	9.423095e+00
H	2.279939e+00	9.596230e+00	9.423628e+00
H	7.288680e+00	5.898519e+00	9.430198e+00
H	2.144705e+00	4.621119e+00	9.430208e+00
H	3.699554e-01	2.876354e+00	9.432343e+00
H	9.063388e+00	7.643381e+00	9.432358e+00
H	5.370042e+00	2.660080e+00	9.440139e+00
H	4.063439e+00	7.859911e+00	9.440771e+00
C	7.190900e+00	1.759047e+00	1.013890e+01
C	2.242425e+00	8.760894e+00	1.013924e+01
C	7.250143e+00	6.736566e+00	1.014251e+01
C	2.183180e+00	3.783107e+00	1.014253e+01
C	8.229216e+00	7.699582e+00	1.014333e+01
C	1.203989e+00	2.820125e+00	1.014341e+01
C	6.207358e+00	2.717701e+00	1.014715e+01
C	3.225983e+00	7.802141e+00	1.014751e+01

N	8.258376e+00	1.765171e+00	1.102334e+01
N	1.174920e+00	8.754814e+00	1.102363e+01
N	6.185973e+00	6.741158e+00	1.103097e+01
N	3.247276e+00	3.778466e+00	1.103106e+01
N	8.244375e+00	8.768797e+00	1.103186e+01
N	1.188701e+00	1.751013e+00	1.103203e+01
N	6.191002e+00	3.783639e+00	1.103934e+01
N	3.242326e+00	6.736264e+00	1.103974e+01
Cr	9.724297e+00	2.788880e-01	1.112622e+01
Cr	4.716565e+00	5.259868e+00	1.113670e+01
C	1.244786e+00	7.746195e+00	1.194989e+01
C	8.188043e+00	2.773185e+00	1.195028e+01
C	7.232680e+00	8.722068e+00	1.195028e+01
C	2.200446e+00	1.797672e+00	1.195041e+01
C	6.252326e+00	7.756019e+00	1.195062e+01
C	3.180833e+00	2.763594e+00	1.195071e+01
C	2.230947e+00	6.785697e+00	1.195818e+01
C	7.201915e+00	3.733896e+00	1.195835e+01
F	2.912030e-01	7.756001e+00	1.289128e+01
F	9.141241e+00	2.762931e+00	1.289196e+01
F	7.258507e+00	9.679251e+00	1.289286e+01
F	2.174546e+00	8.404666e-01	1.289303e+01
F	5.300852e+00	7.748928e+00	1.289399e+01
F	4.132351e+00	2.770604e+00	1.289410e+01
F	2.264545e+00	5.836802e+00	1.290893e+01
F	7.167889e+00	4.682523e+00	1.290927e+01
H	7.153660e+00	9.238161e-01	1.452310e+01
H	2.279939e+00	9.596230e+00	1.452363e+01
H	7.288680e+00	5.898519e+00	1.453020e+01
H	2.144705e+00	4.621119e+00	1.453021e+01
H	3.699554e-01	2.876354e+00	1.453234e+01
H	9.063388e+00	7.643381e+00	1.453236e+01
H	5.370042e+00	2.660080e+00	1.454014e+01
H	4.063439e+00	7.859911e+00	1.454077e+01
C	7.190900e+00	1.759047e+00	1.523890e+01
C	2.242425e+00	8.760894e+00	1.523924e+01
C	7.250143e+00	6.736566e+00	1.524251e+01
C	2.183180e+00	3.783107e+00	1.524253e+01
C	8.229216e+00	7.699582e+00	1.524333e+01
C	1.203989e+00	2.820125e+00	1.524341e+01
C	6.207358e+00	2.717701e+00	1.524715e+01
C	3.225983e+00	7.802141e+00	1.524751e+01
N	8.258376e+00	1.765171e+00	1.612334e+01
N	1.174920e+00	8.754814e+00	1.612363e+01

N	6.185973e+00	6.741158e+00	1.613097e+01
N	3.247276e+00	3.778466e+00	1.613106e+01
N	8.244375e+00	8.768797e+00	1.613186e+01
N	1.188701e+00	1.751013e+00	1.613203e+01
N	6.191002e+00	3.783639e+00	1.613934e+01
N	3.242326e+00	6.736264e+00	1.613974e+01
Cr	9.724297e+00	2.788880e-01	1.622622e+01
Cr	4.716565e+00	5.259868e+00	1.623670e+01
C	1.244786e+00	7.746195e+00	1.704989e+01
C	8.188043e+00	2.773185e+00	1.705028e+01
C	7.232680e+00	8.722068e+00	1.705028e+01
C	2.200446e+00	1.797672e+00	1.705041e+01
C	6.252326e+00	7.756019e+00	1.705062e+01
C	3.180833e+00	2.763594e+00	1.705071e+01
C	2.230947e+00	6.785697e+00	1.705818e+01
C	7.201915e+00	3.733896e+00	1.705835e+01
F	2.912030e-01	7.756001e+00	1.799128e+01
F	9.141241e+00	2.762931e+00	1.799196e+01
F	7.258507e+00	9.679251e+00	1.799286e+01
F	2.174546e+00	8.404666e-01	1.799303e+01
F	5.300852e+00	7.748928e+00	1.799399e+01
F	4.132351e+00	2.770604e+00	1.799410e+01
F	2.264545e+00	5.836802e+00	1.800893e+01
F	7.167889e+00	4.682523e+00	1.800927e+01

1L-Cr(py_z)₂ molecular junction

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Device

Au	1.252185e+00	1.245013e+00	1.019562e+00
Au	3.756065e+00	1.245013e+00	1.019562e+00
Au	6.259945e+00	1.245013e+00	1.019562e+00
Au	8.763825e+00	1.245013e+00	1.019562e+00
Au	1.252675e+00	3.735041e+00	1.019562e+00
Au	3.756555e+00	3.735041e+00	1.019562e+00
Au	6.260435e+00	3.735041e+00	1.019562e+00
Au	8.764315e+00	3.735041e+00	1.019562e+00
Au	1.253165e+00	6.225069e+00	1.019562e+00
Au	3.757045e+00	6.225069e+00	1.019562e+00
Au	6.260925e+00	6.225069e+00	1.019562e+00
Au	8.764805e+00	6.225069e+00	1.019562e+00
Au	1.253655e+00	8.715098e+00	1.019562e+00
Au	3.757535e+00	8.715098e+00	1.019562e+00
Au	6.261415e+00	8.715098e+00	1.019562e+00
Au	8.765295e+00	8.715098e+00	1.019562e+00
Au	0.000000e+00	0.000000e+00	3.058688e+00

Au	2.503880e+00	1.900000e-11	3.058688e+00
Au	5.007760e+00	3.800000e-11	3.058688e+00
Au	7.511640e+00	5.800000e-11	3.058688e+00
Au	4.899026e-04	2.490027e+00	3.058688e+00
Au	2.504370e+00	2.490027e+00	3.058688e+00
Au	5.008250e+00	2.490027e+00	3.058688e+00
Au	7.512130e+00	2.490027e+00	3.058688e+00
Au	9.798054e-04	4.980055e+00	3.058688e+00
Au	2.504860e+00	4.980055e+00	3.058688e+00
Au	5.008740e+00	4.980055e+00	3.058688e+00
Au	7.512620e+00	4.980055e+00	3.058688e+00
Au	1.469708e-03	7.470083e+00	3.058688e+00
Au	2.505350e+00	7.470083e+00	3.058688e+00
Au	5.009230e+00	7.470083e+00	3.058688e+00
Au	7.513110e+00	7.470083e+00	3.058688e+00
Au	1.252185e+00	1.245013e+00	5.097813e+00
Au	3.756065e+00	1.245013e+00	5.097813e+00
Au	6.259945e+00	1.245013e+00	5.097813e+00
Au	8.763825e+00	1.245013e+00	5.097813e+00
Au	1.252675e+00	3.735041e+00	5.097813e+00
Au	3.756555e+00	3.735041e+00	5.097813e+00
Au	6.260435e+00	3.735041e+00	5.097813e+00
Au	8.764315e+00	3.735041e+00	5.097813e+00
Au	1.253165e+00	6.225069e+00	5.097813e+00
Au	3.757045e+00	6.225069e+00	5.097813e+00
Au	6.260925e+00	6.225069e+00	5.097813e+00
Au	8.764805e+00	6.225069e+00	5.097813e+00
Au	1.253655e+00	8.715098e+00	5.097813e+00
Au	3.757535e+00	8.715098e+00	5.097813e+00
Au	6.261415e+00	8.715098e+00	5.097813e+00
Au	8.765295e+00	8.715098e+00	5.097813e+00
Au	0.000000e+00	0.000000e+00	7.136938e+00
Au	2.503880e+00	1.900000e-11	7.136938e+00
Au	5.007760e+00	3.800000e-11	7.136938e+00
Au	7.511640e+00	5.800000e-11	7.136938e+00
Au	4.899026e-04	2.490027e+00	7.136938e+00
Au	2.504370e+00	2.490027e+00	7.136938e+00
Au	5.008250e+00	2.490027e+00	7.136938e+00
Au	7.512130e+00	2.490027e+00	7.136938e+00
Au	9.798054e-04	4.980055e+00	7.136938e+00
Au	2.504860e+00	4.980055e+00	7.136938e+00
Au	5.008740e+00	4.980055e+00	7.136938e+00
Au	7.512620e+00	4.980055e+00	7.136938e+00
Au	1.469708e-03	7.470083e+00	7.136938e+00

Au	2.505350e+00	7.470083e+00	7.136938e+00
Au	5.009230e+00	7.470083e+00	7.136938e+00
Au	7.513110e+00	7.470083e+00	7.136938e+00
H	7.681710e+00	4.470140e+00	9.697417e+00
H	9.440233e+00	2.720868e+00	9.702441e+00
H	2.237859e+00	5.505429e+00	9.700064e+00
H	4.796595e-01	7.254481e+00	9.705074e+00
H	5.469626e+00	7.722166e+00	9.727707e+00
H	2.699173e+00	5.036861e-01	9.731230e+00
H	7.222580e+00	9.475105e+00	9.731630e+00
H	4.454198e+00	2.254716e+00	9.734413e+00
C	7.567545e+00	3.585111e+00	1.034520e+01
C	8.553488e+00	2.604991e+00	1.034838e+01
C	2.353419e+00	6.391289e+00	1.034623e+01
C	1.367473e+00	7.371326e+00	1.034976e+01
C	6.365115e+00	7.596580e+00	1.035961e+01
C	7.348924e+00	8.578877e+00	1.036075e+01
C	3.557542e+00	2.380525e+00	1.036436e+01
C	2.572941e+00	1.398982e+00	1.036175e+01
N	6.456956e+00	6.472634e+00	1.113345e+01
N	1.446597e+00	1.494145e+00	1.113361e+01
N	3.469250e+00	6.476777e+00	1.113419e+01
Cr	4.960641e+00	4.989616e+00	1.113625e+01
N	6.452938e+00	3.500837e+00	1.113464e+01
N	3.464862e+00	3.503780e+00	1.113971e+01
N	8.473553e+00	8.483793e+00	1.113554e+01
N	8.473081e+00	1.493934e+00	1.114179e+01
Cr	9.967219e+00	9.738589e-03	1.114045e+01
N	1.448407e+00	8.483340e+00	1.114174e+01
C	7.581729e+00	6.376949e+00	1.190737e+01
C	1.353258e+00	2.617846e+00	1.190761e+01
C	2.337724e+00	3.599031e+00	1.191099e+01
C	8.565423e+00	7.359235e+00	1.190897e+01
C	3.551307e+00	7.589745e+00	1.192486e+01
C	2.564955e+00	8.569565e+00	1.192826e+01
C	6.372377e+00	2.389539e+00	1.192778e+01
C	7.357959e+00	1.409167e+00	1.193100e+01
H	7.706846e+00	5.480352e+00	1.253618e+01
H	4.556891e-01	2.743483e+00	1.253645e+01
H	2.209811e+00	4.494604e+00	1.254080e+01
H	9.460658e+00	7.232826e+00	1.254064e+01
H	4.439666e+00	7.707842e+00	1.256819e+01
H	2.680721e+00	9.456093e+00	1.257367e+01
H	5.484978e+00	2.274247e+00	1.257357e+01

H	7.243076e+00	5.237296e-01	1.257808e+01
Au	-3.940000e-10	4.881287e-06	1.513694e+01
Au	2.503880e+00	4.881306e-06	1.513694e+01
Au	5.007760e+00	4.881325e-06	1.513694e+01
Au	7.511640e+00	4.881344e-06	1.513694e+01
Au	4.899022e-04	2.490032e+00	1.513694e+01
Au	2.504370e+00	2.490032e+00	1.513694e+01
Au	5.008250e+00	2.490032e+00	1.513694e+01
Au	7.512130e+00	2.490032e+00	1.513694e+01
Au	9.798050e-04	4.980060e+00	1.513694e+01
Au	2.504860e+00	4.980060e+00	1.513694e+01
Au	5.008740e+00	4.980060e+00	1.513694e+01
Au	7.512620e+00	4.980060e+00	1.513694e+01
Au	1.469708e-03	7.470088e+00	1.513694e+01
Au	2.505350e+00	7.470088e+00	1.513694e+01
Au	5.009230e+00	7.470088e+00	1.513694e+01
Au	7.513110e+00	7.470088e+00	1.513694e+01
Au	1.252185e+00	1.245018e+00	1.717606e+01
Au	3.756065e+00	1.245018e+00	1.717606e+01
Au	6.259945e+00	1.245018e+00	1.717606e+01
Au	8.763825e+00	1.245018e+00	1.717606e+01
Au	1.252675e+00	3.735046e+00	1.717606e+01
Au	3.756555e+00	3.735046e+00	1.717606e+01
Au	6.260435e+00	3.735046e+00	1.717606e+01
Au	8.764315e+00	3.735046e+00	1.717606e+01
Au	1.253165e+00	6.225074e+00	1.717606e+01
Au	3.757045e+00	6.225074e+00	1.717606e+01
Au	6.260925e+00	6.225074e+00	1.717606e+01
Au	8.764805e+00	6.225074e+00	1.717606e+01
Au	1.253655e+00	8.715102e+00	1.717606e+01
Au	3.757535e+00	8.715102e+00	1.717606e+01
Au	6.261415e+00	8.715102e+00	1.717606e+01
Au	8.765295e+00	8.715102e+00	1.717606e+01
Au	-3.940000e-10	4.881287e-06	1.921519e+01
Au	2.503880e+00	4.881306e-06	1.921519e+01
Au	5.007760e+00	4.881325e-06	1.921519e+01
Au	7.511640e+00	4.881344e-06	1.921519e+01
Au	4.899022e-04	2.490032e+00	1.921519e+01
Au	2.504370e+00	2.490032e+00	1.921519e+01
Au	5.008250e+00	2.490032e+00	1.921519e+01
Au	7.512130e+00	2.490032e+00	1.921519e+01
Au	9.798050e-04	4.980060e+00	1.921519e+01
Au	2.504860e+00	4.980060e+00	1.921519e+01
Au	5.008740e+00	4.980060e+00	1.921519e+01

Au	7.512620e+00	4.980060e+00	1.921519e+01
Au	1.469708e-03	7.470088e+00	1.921519e+01
Au	2.505350e+00	7.470088e+00	1.921519e+01
Au	5.009230e+00	7.470088e+00	1.921519e+01
Au	7.513110e+00	7.470088e+00	1.921519e+01
Au	1.252185e+00	1.245018e+00	2.125431e+01
Au	3.756065e+00	1.245018e+00	2.125431e+01
Au	6.259945e+00	1.245018e+00	2.125431e+01
Au	8.763825e+00	1.245018e+00	2.125431e+01
Au	1.252675e+00	3.735046e+00	2.125431e+01
Au	3.756555e+00	3.735046e+00	2.125431e+01
Au	6.260435e+00	3.735046e+00	2.125431e+01
Au	8.764315e+00	3.735046e+00	2.125431e+01
Au	1.253165e+00	6.225074e+00	2.125431e+01
Au	3.757045e+00	6.225074e+00	2.125431e+01
Au	6.260925e+00	6.225074e+00	2.125431e+01
Au	8.764805e+00	6.225074e+00	2.125431e+01
Au	1.253655e+00	8.715102e+00	2.125431e+01
Au	3.757535e+00	8.715102e+00	2.125431e+01
Au	6.261415e+00	8.715102e+00	2.125431e+01
Au	8.765295e+00	8.715102e+00	2.125431e+01

2L-Cr(py_z)₂ molecular junction

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Device

Au	1.277305e+00	1.487515e+00	1.019562e+00
Au	3.781185e+00	1.487515e+00	1.019562e+00
Au	6.285065e+00	1.487515e+00	1.019562e+00
Au	8.788946e+00	1.487515e+00	1.019562e+00
Au	1.277795e+00	3.977543e+00	1.019562e+00
Au	3.781675e+00	3.977543e+00	1.019562e+00
Au	6.285555e+00	3.977543e+00	1.019562e+00
Au	8.789435e+00	3.977543e+00	1.019562e+00
Au	1.278285e+00	6.467572e+00	1.019562e+00
Au	3.782165e+00	6.467572e+00	1.019562e+00
Au	6.286045e+00	6.467572e+00	1.019562e+00
Au	8.789925e+00	6.467572e+00	1.019562e+00
Au	1.278775e+00	8.957600e+00	1.019562e+00
Au	3.782655e+00	8.957600e+00	1.019562e+00
Au	6.286535e+00	8.957600e+00	1.019562e+00
Au	8.790415e+00	8.957600e+00	1.019562e+00
Au	2.512040e-02	2.425023e-01	3.058688e+00
Au	2.529000e+00	2.425023e-01	3.058688e+00
Au	5.032880e+00	2.425023e-01	3.058688e+00
Au	7.536761e+00	2.425023e-01	3.058688e+00

Au	2.561031e-02	2.732529e+00	3.058688e+00
Au	2.529490e+00	2.732529e+00	3.058688e+00
Au	5.033370e+00	2.732529e+00	3.058688e+00
Au	7.537250e+00	2.732529e+00	3.058688e+00
Au	2.610021e-02	5.222557e+00	3.058688e+00
Au	2.529980e+00	5.222557e+00	3.058688e+00
Au	5.033860e+00	5.222557e+00	3.058688e+00
Au	7.537740e+00	5.222557e+00	3.058688e+00
Au	2.659011e-02	7.712586e+00	3.058688e+00
Au	2.530470e+00	7.712586e+00	3.058688e+00
Au	5.034350e+00	7.712586e+00	3.058688e+00
Au	7.538230e+00	7.712586e+00	3.058688e+00
Au	1.277305e+00	1.487515e+00	5.097813e+00
Au	3.781185e+00	1.487515e+00	5.097813e+00
Au	6.285065e+00	1.487515e+00	5.097813e+00
Au	8.788946e+00	1.487515e+00	5.097813e+00
Au	1.277795e+00	3.977543e+00	5.097813e+00
Au	3.781675e+00	3.977543e+00	5.097813e+00
Au	6.285555e+00	3.977543e+00	5.097813e+00
Au	8.789435e+00	3.977543e+00	5.097813e+00
Au	1.278285e+00	6.467572e+00	5.097813e+00
Au	3.782165e+00	6.467572e+00	5.097813e+00
Au	6.286045e+00	6.467572e+00	5.097813e+00
Au	8.789925e+00	6.467572e+00	5.097813e+00
Au	1.278775e+00	8.957600e+00	5.097813e+00
Au	3.782655e+00	8.957600e+00	5.097813e+00
Au	6.286535e+00	8.957600e+00	5.097813e+00
Au	8.790415e+00	8.957600e+00	5.097813e+00
Au	2.512040e-02	2.425023e-01	7.136938e+00
Au	2.529000e+00	2.425023e-01	7.136938e+00
Au	5.032880e+00	2.425023e-01	7.136938e+00
Au	7.536761e+00	2.425023e-01	7.136938e+00
Au	2.561031e-02	2.732529e+00	7.136938e+00
Au	2.529490e+00	2.732529e+00	7.136938e+00
Au	5.033370e+00	2.732529e+00	7.136938e+00
Au	7.537250e+00	2.732529e+00	7.136938e+00
Au	2.610021e-02	5.222557e+00	7.136938e+00
Au	2.529980e+00	5.222557e+00	7.136938e+00
Au	5.033860e+00	5.222557e+00	7.136938e+00
Au	7.537740e+00	5.222557e+00	7.136938e+00
Au	2.659011e-02	7.712586e+00	7.136938e+00
Au	2.530470e+00	7.712586e+00	7.136938e+00
Au	5.034350e+00	7.712586e+00	7.136938e+00
Au	7.538230e+00	7.712586e+00	7.136938e+00

H	7.728816e+00	4.736896e+00	9.693828e+00
H	2.237403e+00	5.722401e+00	9.696146e+00
H	9.487102e+00	2.997258e+00	9.700406e+00
H	4.817090e-01	7.464422e+00	9.701261e+00
H	5.474693e+00	7.992039e+00	9.719731e+00
H	2.737486e+00	7.270866e-01	9.716365e+00
H	7.229072e+00	9.734829e+00	9.717650e+00
H	4.493789e+00	2.467761e+00	9.719982e+00
C	7.605808e+00	3.841371e+00	1.032510e+01
C	2.363262e+00	6.618808e+00	1.032518e+01
C	8.591047e+00	2.866905e+00	1.032895e+01
C	1.378945e+00	7.594141e+00	1.032872e+01
C	6.378512e+00	7.854456e+00	1.033543e+01
C	7.362018e+00	8.830858e+00	1.033395e+01
C	2.606412e+00	1.629800e+00	1.033490e+01
C	3.591298e+00	2.604793e+00	1.033752e+01
N	6.460897e+00	6.712614e+00	1.110012e+01
N	1.463681e+00	1.720428e+00	1.109748e+01
N	3.499159e+00	6.701446e+00	1.109921e+01
N	6.470982e+00	3.758335e+00	1.109989e+01
N	8.504660e+00	8.740639e+00	1.109748e+01
Cr	4.984716e+00	5.227949e+00	1.099706e+01
N	3.509890e+00	3.745963e+00	1.110320e+01
Cr	9.991573e+00	2.485700e-01	1.099979e+01
N	1.453551e+00	8.726914e+00	1.110697e+01
N	8.517485e+00	1.734111e+00	1.110783e+01
C	7.606561e+00	6.622352e+00	1.186781e+01
C	1.381458e+00	2.865220e+00	1.186681e+01
C	8.587315e+00	7.596118e+00	1.186681e+01
C	2.363553e+00	3.837606e+00	1.186956e+01
C	3.574291e+00	7.837521e+00	1.188205e+01
C	6.397883e+00	2.624104e+00	1.188541e+01
C	2.592066e+00	8.810026e+00	1.188610e+01
C	7.380479e+00	1.652062e+00	1.188902e+01
H	7.724912e+00	5.712929e+00	1.247531e+01
H	4.719839e-01	2.989006e+00	1.247340e+01
H	9.495939e+00	7.473737e+00	1.247511e+01
H	2.245764e+00	4.747113e+00	1.247710e+01
H	4.477137e+00	7.953494e+00	1.250027e+01
H	5.496521e+00	2.509831e+00	1.250602e+01
H	2.702166e+00	9.711719e+00	1.250676e+01
H	7.271782e+00	7.513507e-01	1.251127e+01
H	7.704834e+00	4.726949e+00	1.446365e+01
H	2.266534e+00	5.732382e+00	1.446547e+01

H	9.478824e+00	2.967362e+00	1.446934e+01
H	4.903578e-01	7.489800e+00	1.447167e+01
H	5.485208e+00	7.966295e+00	1.449458e+01
H	2.715397e+00	7.355990e-01	1.449544e+01
H	7.257410e+00	9.725992e+00	1.449565e+01
H	4.487788e+00	2.494740e+00	1.450041e+01
C	7.595773e+00	3.826491e+00	1.508630e+01
C	2.375521e+00	6.633608e+00	1.508691e+01
C	8.577388e+00	2.853418e+00	1.509000e+01
C	1.392419e+00	7.605106e+00	1.509105e+01
C	6.393355e+00	7.843105e+00	1.510328e+01
C	7.374711e+00	8.816233e+00	1.510287e+01
C	2.596648e+00	1.644485e+00	1.510366e+01
C	3.578125e+00	2.617536e+00	1.510702e+01
N	6.474759e+00	6.698435e+00	1.587288e+01
N	1.450124e+00	1.734683e+00	1.587012e+01
N	3.513383e+00	6.716641e+00	1.586666e+01
N	6.458888e+00	3.745284e+00	1.586792e+01
N	8.519614e+00	8.725165e+00	1.587142e+01
Cr	4.985022e+00	5.228714e+00	1.597456e+01
N	3.495313e+00	3.761548e+00	1.587715e+01
Cr	9.991643e+00	2.478979e-01	1.597754e+01
N	1.465795e+00	8.739933e+00	1.587567e+01
N	8.503352e+00	1.718885e+00	1.587507e+01
C	7.616418e+00	6.608072e+00	1.663713e+01
C	1.367260e+00	2.876377e+00	1.663509e+01
C	8.600697e+00	7.583643e+00	1.663656e+01
C	2.351386e+00	3.852100e+00	1.663879e+01
C	3.587995e+00	7.850729e+00	1.664366e+01
C	6.384423e+00	2.613197e+00	1.664712e+01
C	2.602123e+00	8.824650e+00	1.664814e+01
C	7.368223e+00	1.637273e+00	1.665041e+01
H	7.746809e+00	5.705045e+00	1.725532e+01
H	4.624462e-01	3.014120e+00	1.724915e+01
H	9.502307e+00	7.446903e+00	1.725548e+01
H	2.217923e+00	4.755762e+00	1.725539e+01
H	4.485348e+00	7.982759e+00	1.726998e+01
H	5.487928e+00	2.484789e+00	1.727605e+01
H	2.725918e+00	9.721162e+00	1.727785e+01
H	7.242579e+00	7.415116e-01	1.728056e+01
Au	2.512040e-02	2.425072e-01	1.983694e+01
Au	2.529000e+00	2.425072e-01	1.983694e+01
Au	5.032880e+00	2.425072e-01	1.983694e+01
Au	7.536761e+00	2.425072e-01	1.983694e+01

Au	2.561031e-02	2.732534e+00	1.983694e+01
Au	2.529490e+00	2.732534e+00	1.983694e+01
Au	5.033370e+00	2.732534e+00	1.983694e+01
Au	7.537250e+00	2.732534e+00	1.983694e+01
Au	2.610021e-02	5.222562e+00	1.983694e+01
Au	2.529980e+00	5.222562e+00	1.983694e+01
Au	5.033860e+00	5.222562e+00	1.983694e+01
Au	7.537740e+00	5.222562e+00	1.983694e+01
Au	2.659011e-02	7.712591e+00	1.983694e+01
Au	2.530470e+00	7.712591e+00	1.983694e+01
Au	5.034350e+00	7.712591e+00	1.983694e+01
Au	7.538230e+00	7.712591e+00	1.983694e+01
Au	1.277305e+00	1.487520e+00	2.187606e+01
Au	3.781185e+00	1.487520e+00	2.187606e+01
Au	6.285065e+00	1.487520e+00	2.187606e+01
Au	8.788946e+00	1.487520e+00	2.187606e+01
Au	1.277795e+00	3.977548e+00	2.187606e+01
Au	3.781675e+00	3.977548e+00	2.187606e+01
Au	6.285555e+00	3.977548e+00	2.187606e+01
Au	8.789435e+00	3.977548e+00	2.187606e+01
Au	1.278285e+00	6.467576e+00	2.187606e+01
Au	3.782165e+00	6.467576e+00	2.187606e+01
Au	6.286045e+00	6.467576e+00	2.187606e+01
Au	8.789925e+00	6.467576e+00	2.187606e+01
Au	1.278775e+00	8.957605e+00	2.187606e+01
Au	3.782655e+00	8.957605e+00	2.187606e+01
Au	6.286535e+00	8.957605e+00	2.187606e+01
Au	8.790415e+00	8.957605e+00	2.187606e+01
Au	2.512040e-02	2.425072e-01	2.391519e+01
Au	2.529000e+00	2.425072e-01	2.391519e+01
Au	5.032880e+00	2.425072e-01	2.391519e+01
Au	7.536761e+00	2.425072e-01	2.391519e+01
Au	2.561031e-02	2.732534e+00	2.391519e+01
Au	2.529490e+00	2.732534e+00	2.391519e+01
Au	5.033370e+00	2.732534e+00	2.391519e+01
Au	7.537250e+00	2.732534e+00	2.391519e+01
Au	2.610021e-02	5.222562e+00	2.391519e+01
Au	2.529980e+00	5.222562e+00	2.391519e+01
Au	5.033860e+00	5.222562e+00	2.391519e+01
Au	7.537740e+00	5.222562e+00	2.391519e+01
Au	2.659011e-02	7.712591e+00	2.391519e+01
Au	2.530470e+00	7.712591e+00	2.391519e+01
Au	5.034350e+00	7.712591e+00	2.391519e+01
Au	7.538230e+00	7.712591e+00	2.391519e+01

Au	1.277305e+00	1.487520e+00	2.595431e+01
Au	3.781185e+00	1.487520e+00	2.595431e+01
Au	6.285065e+00	1.487520e+00	2.595431e+01
Au	8.788946e+00	1.487520e+00	2.595431e+01
Au	1.277795e+00	3.977548e+00	2.595431e+01
Au	3.781675e+00	3.977548e+00	2.595431e+01
Au	6.285555e+00	3.977548e+00	2.595431e+01
Au	8.789435e+00	3.977548e+00	2.595431e+01
Au	1.278285e+00	6.467576e+00	2.595431e+01
Au	3.782165e+00	6.467576e+00	2.595431e+01
Au	6.286045e+00	6.467576e+00	2.595431e+01
Au	8.789925e+00	6.467576e+00	2.595431e+01
Au	1.278775e+00	8.957605e+00	2.595431e+01
Au	3.782655e+00	8.957605e+00	2.595431e+01
Au	6.286535e+00	8.957605e+00	2.595431e+01
Au	8.790415e+00	8.957605e+00	2.595431e+01

1L-Cr(h-pyz)₂ molecular junction

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Device

Au	8.590125e+00	1.488083e+00	1.019562e+00
Au	6.086245e+00	1.488576e+00	1.019562e+00
Au	3.582365e+00	1.489068e+00	1.019562e+00
Au	1.078485e+00	1.489561e+00	1.019562e+00
Au	8.590125e+00	3.978112e+00	1.019562e+00
Au	6.086245e+00	3.978604e+00	1.019562e+00
Au	3.582365e+00	3.979097e+00	1.019562e+00
Au	1.078485e+00	3.979589e+00	1.019562e+00
Au	8.590125e+00	6.468140e+00	1.019562e+00
Au	6.086245e+00	6.468632e+00	1.019562e+00
Au	3.582365e+00	6.469125e+00	1.019562e+00
Au	1.078485e+00	6.469618e+00	1.019562e+00
Au	8.590125e+00	8.958168e+00	1.019562e+00
Au	6.086245e+00	8.958661e+00	1.019562e+00
Au	3.582365e+00	8.959153e+00	1.019562e+00
Au	1.078485e+00	8.959646e+00	1.019562e+00
Au	9.842065e+00	2.428242e-01	3.058688e+00
Au	7.338185e+00	2.433168e-01	3.058688e+00
Au	4.834305e+00	2.438094e-01	3.058688e+00
Au	2.330425e+00	2.443021e-01	3.058688e+00
Au	9.842065e+00	2.732851e+00	3.058688e+00
Au	7.338185e+00	2.733344e+00	3.058688e+00
Au	4.834305e+00	2.733836e+00	3.058688e+00
Au	2.330425e+00	2.734329e+00	3.058688e+00
Au	9.842065e+00	5.222879e+00	3.058688e+00

Au	7.338185e+00	5.223372e+00	3.058688e+00
Au	4.834305e+00	5.223865e+00	3.058688e+00
Au	2.330425e+00	5.224357e+00	3.058688e+00
Au	9.842065e+00	7.712908e+00	3.058688e+00
Au	7.338185e+00	7.713400e+00	3.058688e+00
Au	4.834305e+00	7.713893e+00	3.058688e+00
Au	2.330425e+00	7.714386e+00	3.058688e+00
Au	8.590125e+00	1.488083e+00	5.097813e+00
Au	6.086245e+00	1.488576e+00	5.097813e+00
Au	3.582365e+00	1.489068e+00	5.097813e+00
Au	1.078485e+00	1.489561e+00	5.097813e+00
Au	8.590125e+00	3.978112e+00	5.097813e+00
Au	6.086245e+00	3.978604e+00	5.097813e+00
Au	3.582365e+00	3.979097e+00	5.097813e+00
Au	1.078485e+00	3.979589e+00	5.097813e+00
Au	8.590125e+00	6.468140e+00	5.097813e+00
Au	6.086245e+00	6.468632e+00	5.097813e+00
Au	3.582365e+00	6.469125e+00	5.097813e+00
Au	1.078485e+00	6.469618e+00	5.097813e+00
Au	8.590125e+00	8.958168e+00	5.097813e+00
Au	6.086245e+00	8.958661e+00	5.097813e+00
Au	3.582365e+00	8.959153e+00	5.097813e+00
Au	1.078485e+00	8.959646e+00	5.097813e+00
Au	9.842065e+00	2.428242e-01	7.136938e+00
Au	7.338185e+00	2.433168e-01	7.136938e+00
Au	4.834305e+00	2.438094e-01	7.136938e+00
Au	2.330425e+00	2.443021e-01	7.136938e+00
Au	9.842065e+00	2.732851e+00	7.136938e+00
Au	7.338185e+00	2.733344e+00	7.136938e+00
Au	4.834305e+00	2.733836e+00	7.136938e+00
Au	2.330425e+00	2.734329e+00	7.136938e+00
Au	9.842065e+00	5.222879e+00	7.136938e+00
Au	7.338185e+00	5.223372e+00	7.136938e+00
Au	4.834305e+00	5.223865e+00	7.136938e+00
Au	2.330425e+00	5.224357e+00	7.136938e+00
Au	9.842065e+00	7.712908e+00	7.136938e+00
Au	7.338185e+00	7.713400e+00	7.136938e+00
Au	4.834305e+00	7.713893e+00	7.136938e+00
Au	2.330425e+00	7.714386e+00	7.136938e+00
H	7.444845e+00	6.435283e-01	9.423095e+00
H	2.571124e+00	9.315943e+00	9.423628e+00
H	7.579865e+00	5.618231e+00	9.430198e+00
H	2.435890e+00	4.340831e+00	9.430208e+00
H	6.611405e-01	2.596066e+00	9.432343e+00

H	9.354573e+00	7.363094e+00	9.432358e+00
H	5.661227e+00	2.379792e+00	9.440139e+00
H	4.354624e+00	7.579623e+00	9.440771e+00
C	7.482085e+00	1.478759e+00	1.013890e+01
C	2.533610e+00	8.480606e+00	1.013924e+01
C	7.541328e+00	6.456278e+00	1.014251e+01
C	2.474365e+00	3.502819e+00	1.014253e+01
C	8.520401e+00	7.419294e+00	1.014333e+01
C	1.495174e+00	2.539837e+00	1.014341e+01
C	6.498543e+00	2.437413e+00	1.014715e+01
C	3.517168e+00	7.521853e+00	1.014751e+01
N	8.549561e+00	1.484883e+00	1.102334e+01
N	1.466105e+00	8.474526e+00	1.102363e+01
N	6.477158e+00	6.460870e+00	1.103097e+01
N	3.538461e+00	3.498178e+00	1.103106e+01
N	8.535560e+00	8.488509e+00	1.103186e+01
N	1.479886e+00	1.470725e+00	1.103203e+01
N	6.482187e+00	3.503351e+00	1.103934e+01
N	3.533512e+00	6.455976e+00	1.103974e+01
Cr	1.001548e+01	-1.399735e-03	1.112622e+01
Cr	5.007750e+00	4.979580e+00	1.113670e+01
C	1.535971e+00	7.465908e+00	1.194989e+01
C	8.479228e+00	2.492897e+00	1.195028e+01
C	7.523865e+00	8.441780e+00	1.195028e+01
C	2.491631e+00	1.517385e+00	1.195041e+01
C	6.543511e+00	7.475731e+00	1.195062e+01
C	3.472018e+00	2.483307e+00	1.195071e+01
C	2.522132e+00	6.505409e+00	1.195818e+01
C	7.493100e+00	3.453608e+00	1.195835e+01
F	5.823881e-01	7.475713e+00	1.289128e+01
F	9.432426e+00	2.482643e+00	1.289196e+01
F	7.549693e+00	9.398964e+00	1.289286e+01
F	2.465731e+00	5.601788e-01	1.289303e+01
F	5.592038e+00	7.468640e+00	1.289399e+01
F	4.423536e+00	2.490316e+00	1.289410e+01
F	2.555730e+00	5.556514e+00	1.290893e+01
F	7.459074e+00	4.402236e+00	1.290927e+01
Au	9.842065e+00	2.428242e-01	1.519927e+01
Au	7.338185e+00	2.433168e-01	1.519927e+01
Au	4.834305e+00	2.438094e-01	1.519927e+01
Au	2.330425e+00	2.443021e-01	1.519927e+01
Au	9.842065e+00	2.732851e+00	1.519927e+01
Au	7.338185e+00	2.733344e+00	1.519927e+01
Au	4.834305e+00	2.733836e+00	1.519927e+01

Au	2.330425e+00	2.734329e+00	1.519927e+01
Au	9.842065e+00	5.222879e+00	1.519927e+01
Au	7.338185e+00	5.223372e+00	1.519927e+01
Au	4.834305e+00	5.223865e+00	1.519927e+01
Au	2.330425e+00	5.224357e+00	1.519927e+01
Au	9.842065e+00	7.712908e+00	1.519927e+01
Au	7.338185e+00	7.713400e+00	1.519927e+01
Au	4.834305e+00	7.713893e+00	1.519927e+01
Au	2.330425e+00	7.714386e+00	1.519927e+01
Au	8.590125e+00	1.488083e+00	1.723840e+01
Au	6.086245e+00	1.488576e+00	1.723840e+01
Au	3.582365e+00	1.489068e+00	1.723840e+01
Au	1.078485e+00	1.489561e+00	1.723840e+01
Au	8.590125e+00	3.978112e+00	1.723840e+01
Au	6.086245e+00	3.978604e+00	1.723840e+01
Au	3.582365e+00	3.979097e+00	1.723840e+01
Au	1.078485e+00	3.979589e+00	1.723840e+01
Au	8.590125e+00	6.468140e+00	1.723840e+01
Au	6.086245e+00	6.468632e+00	1.723840e+01
Au	3.582365e+00	6.469125e+00	1.723840e+01
Au	1.078485e+00	6.469618e+00	1.723840e+01
Au	8.590125e+00	8.958168e+00	1.723840e+01
Au	6.086245e+00	8.958661e+00	1.723840e+01
Au	3.582365e+00	8.959153e+00	1.723840e+01
Au	1.078485e+00	8.959646e+00	1.723840e+01
Au	9.842065e+00	2.428242e-01	1.927752e+01
Au	7.338185e+00	2.433168e-01	1.927752e+01
Au	4.834305e+00	2.438094e-01	1.927752e+01
Au	2.330425e+00	2.443021e-01	1.927752e+01
Au	9.842065e+00	2.732851e+00	1.927752e+01
Au	7.338185e+00	2.733344e+00	1.927752e+01
Au	4.834305e+00	2.733836e+00	1.927752e+01
Au	2.330425e+00	2.734329e+00	1.927752e+01
Au	9.842065e+00	5.222879e+00	1.927752e+01
Au	7.338185e+00	5.223372e+00	1.927752e+01
Au	4.834305e+00	5.223865e+00	1.927752e+01
Au	2.330425e+00	5.224357e+00	1.927752e+01
Au	9.842065e+00	7.712908e+00	1.927752e+01
Au	7.338185e+00	7.713400e+00	1.927752e+01
Au	4.834305e+00	7.713893e+00	1.927752e+01
Au	2.330425e+00	7.714386e+00	1.927752e+01
Au	8.590125e+00	1.488083e+00	2.131665e+01
Au	6.086245e+00	1.488576e+00	2.131665e+01
Au	3.582365e+00	1.489068e+00	2.131665e+01

Au	1.078485e+00	1.489561e+00	2.131665e+01
Au	8.590125e+00	3.978112e+00	2.131665e+01
Au	6.086245e+00	3.978604e+00	2.131665e+01
Au	3.582365e+00	3.979097e+00	2.131665e+01
Au	1.078485e+00	3.979589e+00	2.131665e+01
Au	8.590125e+00	6.468140e+00	2.131665e+01
Au	6.086245e+00	6.468632e+00	2.131665e+01
Au	3.582365e+00	6.469125e+00	2.131665e+01
Au	1.078485e+00	6.469618e+00	2.131665e+01
Au	8.590125e+00	8.958168e+00	2.131665e+01
Au	6.086245e+00	8.958661e+00	2.131665e+01
Au	3.582365e+00	8.959153e+00	2.131665e+01
Au	1.078485e+00	8.959646e+00	2.131665e+01

2L-Cr(h-pyz)₂ molecular junction

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Device

Au	7.872994e-01	1.769849e+00	1.019562e+00
Au	3.291179e+00	1.769356e+00	1.019562e+00
Au	5.795059e+00	1.768864e+00	1.019562e+00
Au	8.298939e+00	1.768371e+00	1.019562e+00
Au	7.872994e-01	4.259877e+00	1.019562e+00
Au	3.291179e+00	4.259385e+00	1.019562e+00
Au	5.795059e+00	4.258892e+00	1.019562e+00
Au	8.298939e+00	4.258399e+00	1.019562e+00
Au	7.872994e-01	6.749906e+00	1.019562e+00
Au	3.291179e+00	6.749413e+00	1.019562e+00
Au	5.795059e+00	6.748920e+00	1.019562e+00
Au	8.298939e+00	6.748428e+00	1.019562e+00
Au	7.872994e-01	9.239934e+00	1.019562e+00
Au	3.291179e+00	9.239441e+00	1.019562e+00
Au	5.795059e+00	9.238949e+00	1.019562e+00
Au	8.298939e+00	9.238456e+00	1.019562e+00
Au	2.039239e+00	5.245899e-01	3.058688e+00
Au	4.543119e+00	5.240973e-01	3.058688e+00

Au	7.046999e+00	5.236046e-01	3.058688e+00
Au	9.550879e+00	5.231120e-01	3.058688e+00
Au	2.039239e+00	3.014617e+00	3.058688e+00
Au	4.543119e+00	3.014124e+00	3.058688e+00
Au	7.046999e+00	3.013632e+00	3.058688e+00
Au	9.550879e+00	3.013139e+00	3.058688e+00
Au	2.039239e+00	5.504645e+00	3.058688e+00
Au	4.543119e+00	5.504152e+00	3.058688e+00
Au	7.046999e+00	5.503660e+00	3.058688e+00
Au	9.550879e+00	5.503167e+00	3.058688e+00
Au	2.039239e+00	7.994673e+00	3.058688e+00
Au	4.543119e+00	7.994181e+00	3.058688e+00
Au	7.046999e+00	7.993688e+00	3.058688e+00
Au	9.550879e+00	7.993196e+00	3.058688e+00
Au	7.872994e-01	1.769849e+00	5.097813e+00
Au	3.291179e+00	1.769356e+00	5.097813e+00
Au	5.795059e+00	1.768864e+00	5.097813e+00
Au	8.298939e+00	1.768371e+00	5.097813e+00
Au	7.872994e-01	4.259877e+00	5.097813e+00
Au	3.291179e+00	4.259385e+00	5.097813e+00
Au	5.795059e+00	4.258892e+00	5.097813e+00
Au	8.298939e+00	4.258399e+00	5.097813e+00
Au	7.872994e-01	6.749906e+00	5.097813e+00
Au	3.291179e+00	6.749413e+00	5.097813e+00
Au	5.795059e+00	6.748920e+00	5.097813e+00
Au	8.298939e+00	6.748428e+00	5.097813e+00
Au	7.872994e-01	9.239934e+00	5.097813e+00
Au	3.291179e+00	9.239441e+00	5.097813e+00
Au	5.795059e+00	9.238949e+00	5.097813e+00
Au	8.298939e+00	9.238456e+00	5.097813e+00

Au	2.039239e+00	5.245899e-01	7.136938e+00
Au	4.543119e+00	5.240973e-01	7.136938e+00
Au	7.046999e+00	5.236046e-01	7.136938e+00
Au	9.550879e+00	5.231120e-01	7.136938e+00
Au	2.039239e+00	3.014617e+00	7.136938e+00
Au	4.543119e+00	3.014124e+00	7.136938e+00
Au	7.046999e+00	3.013632e+00	7.136938e+00
Au	9.550879e+00	3.013139e+00	7.136938e+00
Au	2.039239e+00	5.504645e+00	7.136938e+00
Au	4.543119e+00	5.504152e+00	7.136938e+00
Au	7.046999e+00	5.503660e+00	7.136938e+00
Au	9.550879e+00	5.503167e+00	7.136938e+00
Au	2.039239e+00	7.994673e+00	7.136938e+00
Au	4.543119e+00	7.994181e+00	7.136938e+00
Au	7.046999e+00	7.993688e+00	7.136938e+00
Au	9.550879e+00	7.993196e+00	7.136938e+00
H	7.153660e+00	9.238162e-01	9.423095e+00
H	2.279939e+00	9.596230e+00	9.423628e+00
H	7.288680e+00	5.898519e+00	9.430198e+00
H	2.144705e+00	4.621119e+00	9.430208e+00
H	3.699553e-01	2.876354e+00	9.432343e+00
H	9.063388e+00	7.643381e+00	9.432358e+00
H	5.370042e+00	2.660080e+00	9.440139e+00
H	4.063439e+00	7.859911e+00	9.440771e+00
C	7.190900e+00	1.759047e+00	1.013890e+01
C	2.242425e+00	8.760894e+00	1.013924e+01
C	7.250143e+00	6.736566e+00	1.014251e+01
C	2.183180e+00	3.783107e+00	1.014253e+01
C	8.229216e+00	7.699582e+00	1.014333e+01
C	1.203989e+00	2.820125e+00	1.014341e+01

C	6.207358e+00	2.717701e+00	1.014715e+01
C	3.225983e+00	7.802141e+00	1.014751e+01
N	8.258376e+00	1.765171e+00	1.102334e+01
N	1.174920e+00	8.754814e+00	1.102363e+01
N	6.185973e+00	6.741158e+00	1.103097e+01
N	3.247276e+00	3.778466e+00	1.103106e+01
N	8.244375e+00	8.768797e+00	1.103186e+01
N	1.188701e+00	1.751013e+00	1.103203e+01
N	6.191001e+00	3.783639e+00	1.103934e+01
N	3.242326e+00	6.736264e+00	1.103974e+01
Cr	9.724297e+00	2.788881e-01	1.112622e+01
Cr	4.716565e+00	5.259868e+00	1.113670e+01
C	1.244786e+00	7.746195e+00	1.194989e+01
C	8.188043e+00	2.773185e+00	1.195028e+01
C	7.232680e+00	8.722068e+00	1.195028e+01
C	2.200446e+00	1.797673e+00	1.195041e+01
C	6.252326e+00	7.756019e+00	1.195062e+01
C	3.180832e+00	2.763595e+00	1.195071e+01
C	2.230947e+00	6.785697e+00	1.195818e+01
C	7.201914e+00	3.733896e+00	1.195835e+01
F	2.912029e-01	7.756001e+00	1.289128e+01
F	9.141241e+00	2.762931e+00	1.289196e+01
F	7.258507e+00	9.679252e+00	1.289286e+01
F	2.174546e+00	8.404667e-01	1.289303e+01
F	5.300852e+00	7.748928e+00	1.289399e+01
F	4.132351e+00	2.770604e+00	1.289410e+01
F	2.264545e+00	5.836802e+00	1.290893e+01
F	7.167889e+00	4.682524e+00	1.290927e+01
H	7.153660e+00	9.238162e-01	1.452310e+01
H	2.279939e+00	9.596230e+00	1.452363e+01

H	7.288680e+00	5.898519e+00	1.453020e+01
H	2.144705e+00	4.621119e+00	1.453021e+01
H	3.699553e-01	2.876354e+00	1.453234e+01
H	9.063388e+00	7.643381e+00	1.453236e+01
H	5.370042e+00	2.660080e+00	1.454014e+01
H	4.063439e+00	7.859911e+00	1.454077e+01
C	7.190900e+00	1.759047e+00	1.523890e+01
C	2.242425e+00	8.760894e+00	1.523924e+01
C	7.250143e+00	6.736566e+00	1.524251e+01
C	2.183180e+00	3.783107e+00	1.524253e+01
C	8.229216e+00	7.699582e+00	1.524333e+01
C	1.203989e+00	2.820125e+00	1.524341e+01
C	6.207358e+00	2.717701e+00	1.524715e+01
C	3.225983e+00	7.802141e+00	1.524751e+01
N	8.258376e+00	1.765171e+00	1.612334e+01
N	1.174920e+00	8.754814e+00	1.612363e+01
N	6.185973e+00	6.741158e+00	1.613097e+01
N	3.247276e+00	3.778466e+00	1.613106e+01
N	8.244375e+00	8.768797e+00	1.613186e+01
N	1.188701e+00	1.751013e+00	1.613203e+01
N	6.191001e+00	3.783639e+00	1.613934e+01
N	3.242326e+00	6.736264e+00	1.613974e+01
Cr	9.724297e+00	2.788881e-01	1.622622e+01
Cr	4.716565e+00	5.259868e+00	1.623670e+01
C	1.244786e+00	7.746195e+00	1.704989e+01
C	8.188043e+00	2.773185e+00	1.705028e+01
C	7.232680e+00	8.722068e+00	1.705028e+01
C	2.200446e+00	1.797673e+00	1.705041e+01
C	6.252326e+00	7.756019e+00	1.705062e+01
C	3.180832e+00	2.763595e+00	1.705071e+01

C	2.230947e+00	6.785697e+00	1.705818e+01
C	7.201914e+00	3.733896e+00	1.705835e+01
F	2.912029e-01	7.756001e+00	1.799128e+01
F	9.141241e+00	2.762931e+00	1.799196e+01
F	7.258507e+00	9.679252e+00	1.799286e+01
F	2.174546e+00	8.404667e-01	1.799303e+01
F	5.300852e+00	7.748928e+00	1.799399e+01
F	4.132351e+00	2.770604e+00	1.799410e+01
F	2.264545e+00	5.836802e+00	1.800893e+01
F	7.167889e+00	4.682524e+00	1.800927e+01
Au	2.039240e+00	5.245948e-01	2.080890e+01
Au	4.543120e+00	5.241022e-01	2.080890e+01
Au	7.047000e+00	5.236095e-01	2.080890e+01
Au	9.550880e+00	5.231169e-01	2.080890e+01
Au	2.039240e+00	3.014622e+00	2.080890e+01
Au	4.543120e+00	3.014129e+00	2.080890e+01
Au	7.047000e+00	3.013636e+00	2.080890e+01
Au	9.550880e+00	3.013144e+00	2.080890e+01
Au	2.039240e+00	5.504650e+00	2.080890e+01
Au	4.543120e+00	5.504157e+00	2.080890e+01
Au	7.047000e+00	5.503665e+00	2.080890e+01
Au	9.550880e+00	5.503172e+00	2.080890e+01
Au	2.039240e+00	7.994678e+00	2.080890e+01
Au	4.543120e+00	7.994186e+00	2.080890e+01
Au	7.047000e+00	7.993693e+00	2.080890e+01
Au	9.550880e+00	7.993200e+00	2.080890e+01
Au	7.873000e-01	1.769854e+00	2.284803e+01
Au	3.291180e+00	1.769361e+00	2.284803e+01
Au	5.795060e+00	1.768869e+00	2.284803e+01
Au	8.298940e+00	1.768376e+00	2.284803e+01

Au	7.873000e-01	4.259882e+00	2.284803e+01
Au	3.291180e+00	4.259390e+00	2.284803e+01
Au	5.795060e+00	4.258897e+00	2.284803e+01
Au	8.298940e+00	4.258404e+00	2.284803e+01
Au	7.873000e-01	6.749910e+00	2.284803e+01
Au	3.291180e+00	6.749418e+00	2.284803e+01
Au	5.795060e+00	6.748925e+00	2.284803e+01
Au	8.298940e+00	6.748433e+00	2.284803e+01
Au	7.873000e-01	9.239939e+00	2.284803e+01
Au	3.291180e+00	9.239446e+00	2.284803e+01
Au	5.795060e+00	9.238954e+00	2.284803e+01
Au	8.298940e+00	9.238461e+00	2.284803e+01
Au	2.039240e+00	5.245948e-01	2.488715e+01
Au	4.543120e+00	5.241022e-01	2.488715e+01
Au	7.047000e+00	5.236095e-01	2.488715e+01
Au	9.550880e+00	5.231169e-01	2.488715e+01
Au	2.039240e+00	3.014622e+00	2.488715e+01
Au	4.543120e+00	3.014129e+00	2.488715e+01
Au	7.047000e+00	3.013636e+00	2.488715e+01
Au	9.550880e+00	3.013144e+00	2.488715e+01
Au	2.039240e+00	5.504650e+00	2.488715e+01
Au	4.543120e+00	5.504157e+00	2.488715e+01
Au	7.047000e+00	5.503665e+00	2.488715e+01
Au	9.550880e+00	5.503172e+00	2.488715e+01
Au	2.039240e+00	7.994678e+00	2.488715e+01
Au	4.543120e+00	7.994186e+00	2.488715e+01
Au	7.047000e+00	7.993693e+00	2.488715e+01
Au	9.550880e+00	7.993200e+00	2.488715e+01
Au	7.873000e-01	1.769854e+00	2.692628e+01
Au	3.291180e+00	1.769361e+00	2.692628e+01

Au	5.795060e+00	1.768869e+00	2.692628e+01
Au	8.298940e+00	1.768376e+00	2.692628e+01
Au	7.873000e-01	4.259882e+00	2.692628e+01
Au	3.291180e+00	4.259390e+00	2.692628e+01
Au	5.795060e+00	4.258897e+00	2.692628e+01
Au	8.298940e+00	4.258404e+00	2.692628e+01
Au	7.873000e-01	6.749910e+00	2.692628e+01
Au	3.291180e+00	6.749418e+00	2.692628e+01
Au	5.795060e+00	6.748925e+00	2.692628e+01
Au	8.298940e+00	6.748433e+00	2.692628e+01
Au	7.873000e-01	9.239939e+00	2.692628e+01
Au	3.291180e+00	9.239446e+00	2.692628e+01
Au	5.795060e+00	9.238954e+00	2.692628e+01
Au	8.298940e+00	9.238461e+00	2.692628e+01