Supporting Information

Understanding the adsorption mechanism of noble gases Kr and Xe in CPO-27-Ni, CPO-27-Mg, and ZIF-8

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Gas-sorption measurements

Low-pressure Kr and Xe sorption isotherms up to 1 bar and different temperatures (180K, 200K and 220K for Kr and 240K, 260K and 280K for Xe) were recorder on an Autosorb 1-MP instrument from Quantachrome equipped with a cryocooler system. High purity grade Kr (99.99%) and Xe (99.99%) were used for all measurements. The CPO-27-Mg and CPO-27-Ni samples were activated by heating at 170 ^{o}C and 150 ^{o}C respectively, for at least 12 hours overnight under dynamic vacuum (turbo pump system) and until the outgas rate was less than 2 mTorr/min. Between different measurements the sample was evacuated at room temperature for 2 hours under dynamic vacuum in order to remove all adsorbed gas molecules. The equilibrium time for each adsorption/desorption point was set to 10 minutes.

The corresponding adsorption/desorption isotherms as shown below.

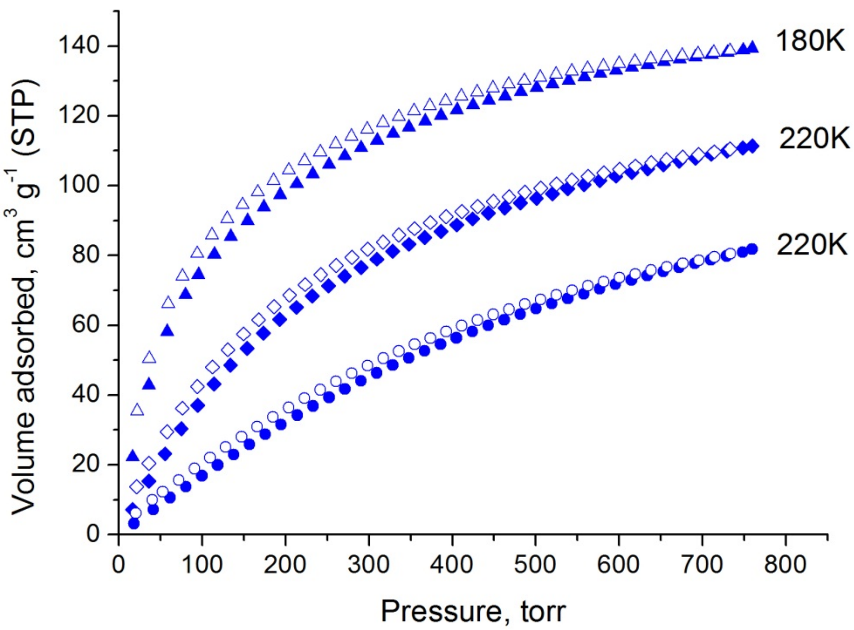

Figure S1. Low pressure Kr adsorption (closed symbols) and desorption (open symbols) isotherms of CPO-27-Mg at the indicated temperatures.

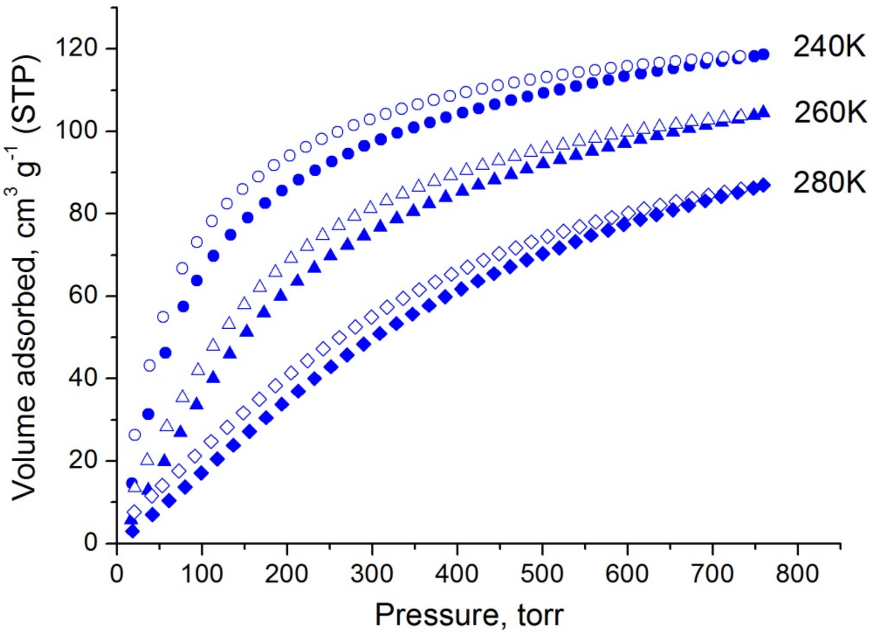

Figure S2. Low pressure Xe adsorption (closed symbols) and desorption (open symbols) isotherms of CPO-27-Mg at the indicated temperatures.

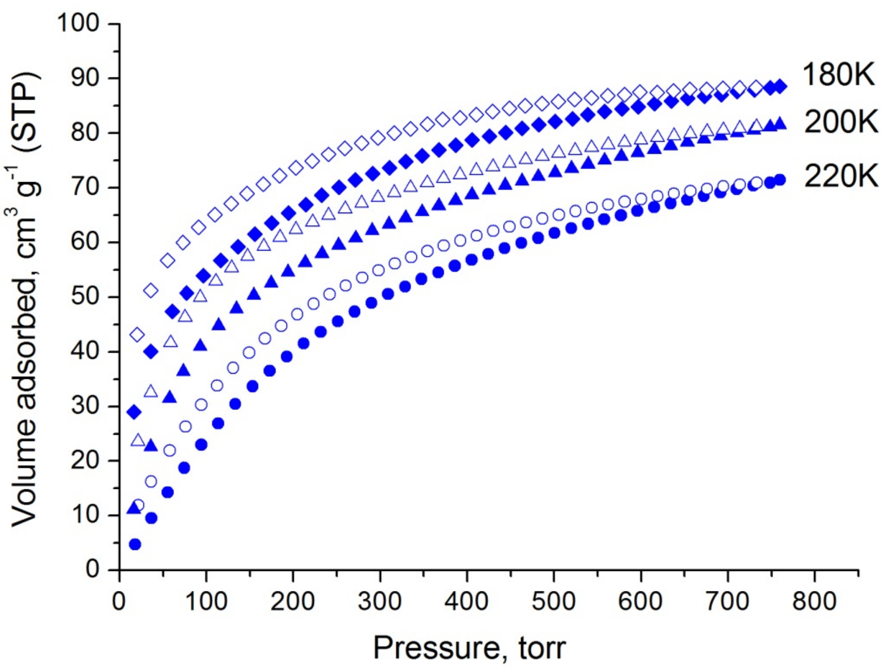

Figure S3. Low pressure Kr adsorption (closed symbols) and desorption (open symbols) isotherms of CPO-27-Ni at the indicated temperatures.

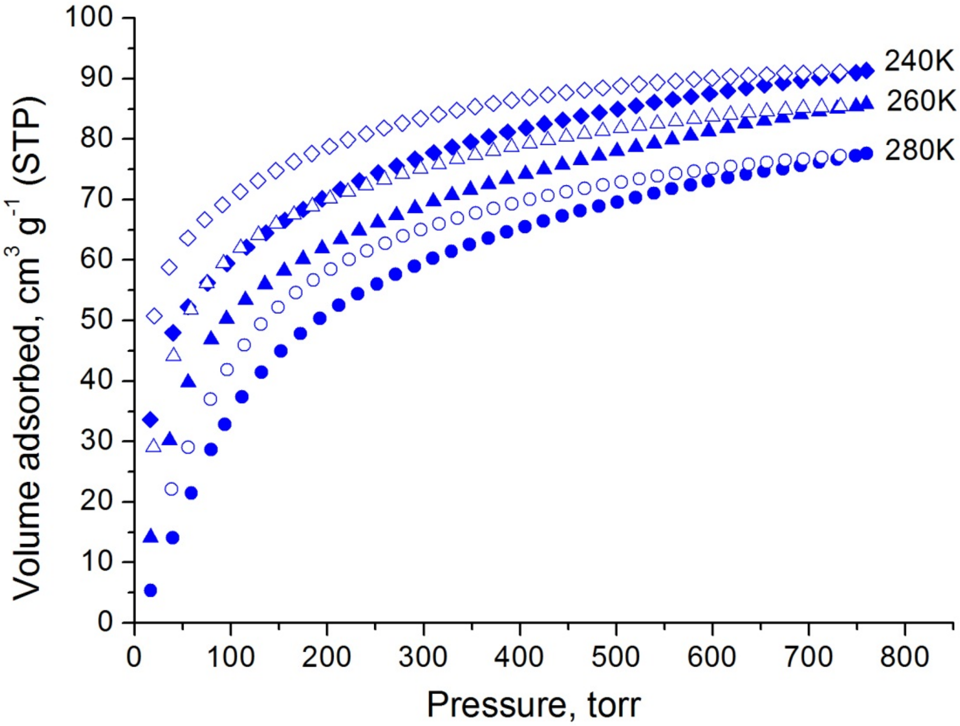

Figure S4. Low pressure Xe adsorption (closed symbols) and desorption (open symbols) isotherms of CPO-27-Ni at the indicated temperatures.

Heat of adsorption calculations

To calculate heats of adsorptions, the corresponding adsorption isotherms at the three different temperatures were simultaneously fitted using the virial type equation 1 :

$$\ln P = \ln N + \frac{1}{T}\sum_{i=0}^{m} a_i N^i + \sum_{i=0}^{n} b_i N^i \qquad \textbf{(1)}$$

The isosteric heat of adsorption, Q_{st}, as a function of surface coverage was calculated from equation 2 :

$$Q_{st}(N) = -R\sum_{i=0}^{m} a_i N^i \qquad \textbf{(2)}$$

We note that very similar results were obtained using the Clausius–Clayperon equation.

The corresponding virial type fittings are provided below.

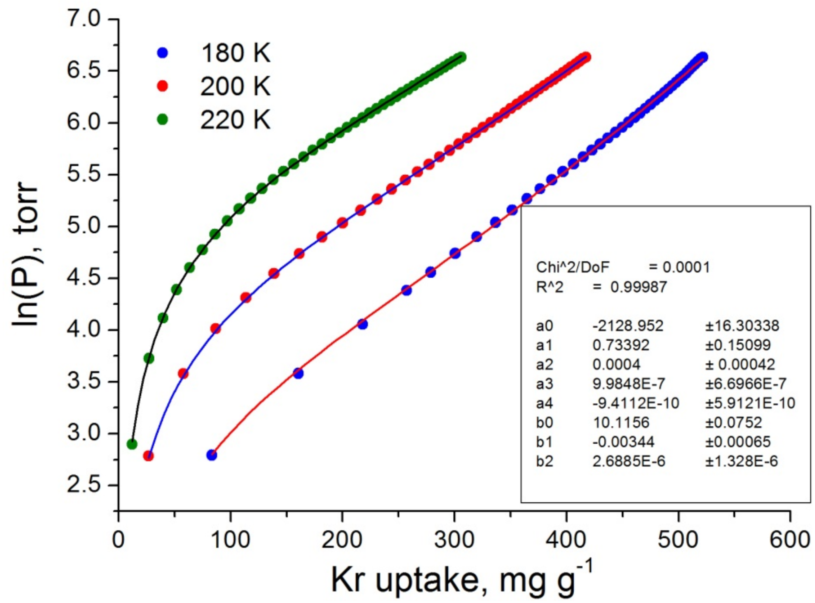

Figure S5. Virial type fitting of Kr adsorption isotherms of CPO-27-Mg at 180K, 200K and 220K according to equation 1.

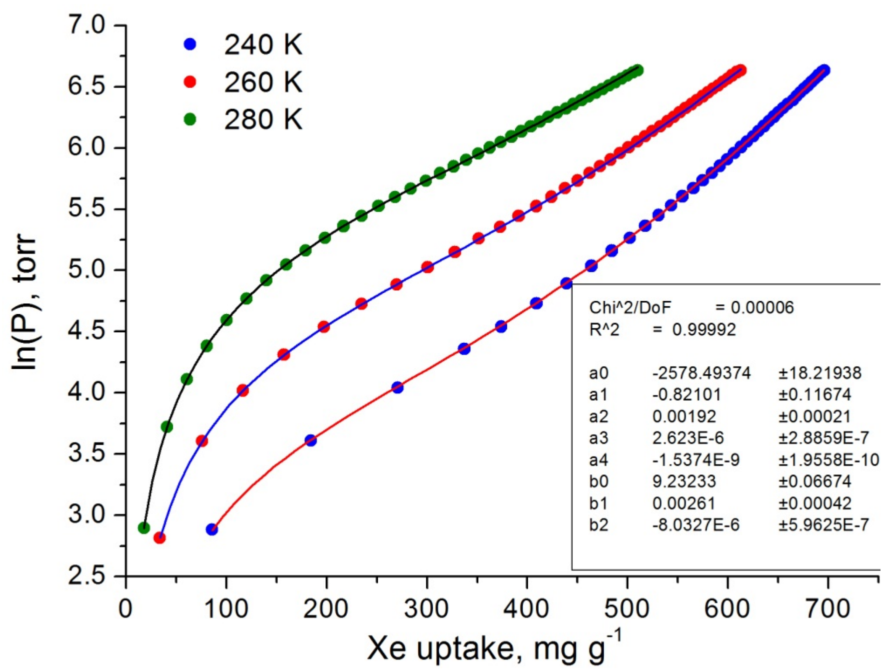

Figure S6. Virial type fitting of Xe adsorption isotherms of CPO-27-Mg at 240K, 260K and 280K according to equation 1.

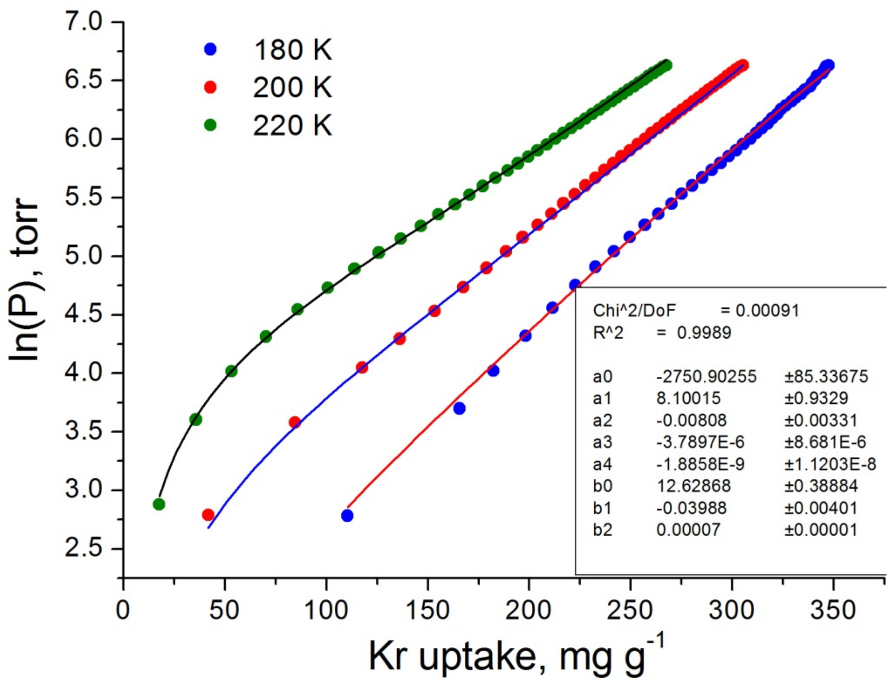

Figure S7. Virial type fitting of Kr adsorption isotherms of CPO-27-Ni at 180K, 200K and 220K according to equation 1.

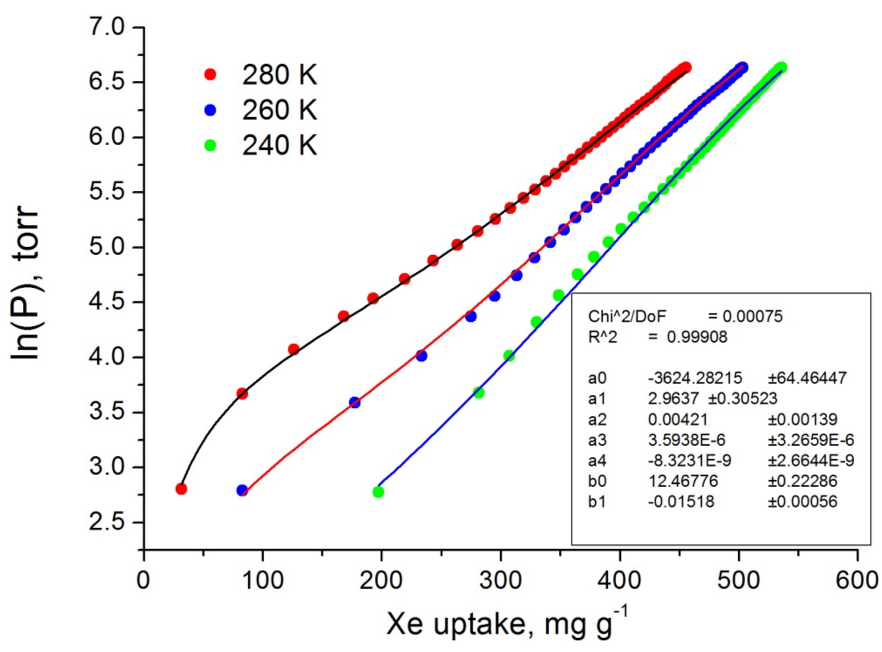

Figure S8. Virial type fitting of Xe adsorption isotherms of CPO-27-Ni at 240K, 260K and 280K according to equation 1.

Atomic positions of Xe and Kr in CPO-27-Ni:

Atom	Wp	x	y	z	Occ	B_{iso}
Ni	18	0.65048	0.61512	0.64538	1	2
C1	18	0.59887	0.58042	0.2532	1	2
C2	18	0.54667	0.54219	0.1138	1	2
C3	18	0.5038	0.48402	0.2109	1	2
C4	18	0.54217	0.55212	-0.0742	1	2
O1	18	0.59584	0.56041	0.4326	1	2
O2	18	0.6382	0.6288	0.1891	1	2
O3	18	0.58373	0.60612	-0.1574	1	2
250K, 50 mbar						
Xe1	18	-0.4814(8)	0.6812(8)	0.151(3)	0.268(8)	8(1)
Xe2	18	-0.013(4)	0.834(4)	0.240(3)	0.05(1)	8(1)
Xe3	3	0	0	0.5	0.072(9)	8(1)
250K, 100 mbar						
Xe1	18	-0.4806(9)	0.6810(7)	0.153(2)	0.344(7)	8(1)
Xe2	18	-0.012(3)	0.841(2)	0.175(1)	0.08(1)	8(1)
Xe3	3	0	0	0.5	0.114(9)	8(1)
250K, 250 mbar						
Xe1	18	-0.4802(8)	0.6816(7)	0.152(2)	0.391(7)	8(1)
Xe2	18	-0.013(2)	0.849(2)	0.109(2)	0.15(1)	8(1)
Xe3	3	0	0	0.5	0.19(1)	8(1)
250K, 500 mbar						
Xe1	18	-0.4798(9)	0.6812(7)	0.150(2)	0.412(8)	8(1)
Xe2	18	-0.015(2)	0.855(2)	0.087(2)	0.19(1)	8(1)
Xe3	3	0	0	0.5	0.28(2)	8(1)
250K, 1000 mbar						
Xe1	18	-0.4795(9)	0.6812(8)	0.149(2)	0.416(8)	8(1)
Xe2	18	-0.016(2)	0.857(2)	0.076(2)	0.21(1)	8(1)
Xe3	3	0	0	0.5	0.36(2)	8(1)
170K, 50 mbar						
Xe1	18	-0.4778(8)	0.6815(7)	0.154(2)	0.459(8)	8(1)
Xe2	18	-0.019(2)	0.856(2)	0.054(2)	0.23(1)	8(1)
Xe3	3	0	0	0.5	0.38(2)	8(1)
170K, 100 mbar						
Xe1	18	-0.4766(8)	0.6813(8)	0.155(2)	0.419(8)	8(1)
Xe2	18	-0.019(2)	0.859(2)	0.047(2)	0.22(1)	8(1)
Xe3	3	0	0	0.5	0.38(2)	8(1)
170K, 250 mbar						
Xe1	18	-0.4768(8)	0.6817(8)	0.155(2)	0.432(8)	8(1)
Xe2	18	-0.020(2)	0.859(2)	0.043(2)	0.23(1)	8(1)
Xe3	3	0	0	0.5	0.40(2)	8(1)
170K, 500 mbar						

Xe1	18	-0.4766(8)	0.6816(8)	0.155(2)	0.436(8)	8(1)
Xe2	18	-0.021(2)	0.858(2)	0.043(2)	0.24(1)	8(1)
Xe3	3	0	0	0.5	0.41(2)	8(1)
170K, 1000 mbar						
Xe1	18	-0.4795(9)	0.6812(8)	0.149(2)	0.416(8)	8(1)
Xe2	18	-0.016(2)	0.857(2)	0.076(2)	0.21(1)	8(1)
Xe3	3	0	0	0.5	0.36(2)	8(1)
250K, 100 mbar						
Kr1	18	-0.024(7)	0.162(7)	0.506(3)	0.05(2)	8(1)
250K, 250 mbar						
Kr1	18	-0.027(7)	0.169(6)	0.528(6)	0.14(4)	8(1)
Kr2	18	0.009(2)	0.858(8)	0.008(3)	0.09(3)	8(1)
Kr3	3	0	0	0.5	0.06(3)	8(1)
250K, 500 mbar						
Kr1	18	-0.021(3)	0.170(3)	0.513(6)	0.22(3)	8(1)
Kr2	18	0.007(2)	0.853(6)	0.049(4)	0.10(4)	8(1)
Kr3	3	0	0	0.5	0.07(3)	8(1)
250K, 1000 mbar						
Kr1	18	-0.019(3)	0.169(3)	0.503(6)	0.31(3)	8(1)
Kr2	18	0.006(1)	0.841(7)	0.116(4)	0.10(3)	8(1)
Kr3	3	0	0	0.5	0.09(3)	8(1)
170K, 50 mbar						
Kr1	18	-0.017(1)	0.173(2)	0.493(4)	0.48(2)	8(1)
Kr2	18	-0.005(4)	0.839(4)	0.113(6)	0.15(3)	8(1)
Kr3	3	0	0	0.5	0.14(3)	8(1)
170K, 100 mbar						
Kr1	18	-0.017(1)	0.173(2)	0.491(4)	0.51(2)	8(1)
Kr2	18	-0.011(3)	0.843(3)	0.089(6)	0.19(3)	8(1)
Kr3	3	0	0	0.5	0.19(3)	8(1)
170K, 250 mbar						
Kr1	18	-0.018(1)	0.172(1)	0.487(3)	0.53(2)	8(1)
Kr2	18	-0.017(2)	0.847(2)	0.079(4)	0.25(3)	8(1)
Kr3	3	0	0	0.5	0.36(3)	8(1)
170K, 500 mbar						
Kr1	18	-0.018(1)	0.173(1)	0.484(3)	0.55(2)	8(1)
Kr2	18	-0.021(2)	0.849(2)	0.076(4)	0.28(3)	8(1)
Kr3	3	0	0	0.5	0.49(3)	8(1)
170K, 1000 mbar						
Kr1	18	-0.0182(9)	0.1724(9)	0.482(3)	0.54(2)	8(1)
Kr2	18	-0.026(2)	0.848(2)	0.074(4)	0.30(2)	8(1)
Kr3	3	0	0	0.5	0.57(3)	8(1)
130K, 50 mbar						
Kr1	18	-0.0180(9)	0.1736(9)	0.481(3)	0.58(2)	8(1)
Kr2	18	-0.029(2)	0.844(2)	0.067(4)	0.35(2)	8(1)
Kr3	3	0	0	0.5	0.54(3)	8(1)
130K, 100 mbar						

Kr1	18	-0.018(1)	0.173(1)	0.481(3)	0.55(2)	8(1)
Kr2	18	-0.029(2)	0.845(2)	0.070(4)	0.33(3)	8(1)
Kr3	3	0	0	0.5	0.54(3)	8(1)
130K, 250 mbar						
Kr1	18	-0.019(1)	0.173(1)	0.478(3)	0.55(2)	8(1)
Kr2	18	-0.034(2)	0.842(2)	0.069(4)	0.35(2)	8(1)
Kr3	3	0	0	0.5	0.62(3)	8(1)
130K, 500 mbar						
Kr1	18	-0.019(1)	0.172(1)	0.475(3)	0.55(2)	8(1)
Kr2	18	-0.036(2)	0.840(2)	0.068(4)	0.38(2)	8(1)
Kr3	3	0	0	0.5	0.67(3)	8(1)
130K, 1000 mbar						
Kr1	18	-0.020(1)	0.171(1)	0.473(3)	0.55(2)	8(1)
Kr2	18	-0.038(2)	0.839(1)	0.067(4)	0.39(2)	8(1)
Kr3	3	0	0	0.5	0.70(3)	8(1)

Atomic positions of Xe and Kr in CPO-27-Ni:

Atom	Wp	x	y	z	Occ	B_{iso}
Ni	18	0.65048	0.61512	0.64538	1	2
C1	18	0.59887	0.58042	0.2532	1	2
C2	18	0.54667	0.54219	0.1138	1	2
C3	18	0.5038	0.48402	0.2109	1	2
C4	18	0.54217	0.55212	-0.0742	1	2
O1	18	0.59584	0.56041	0.4326	1	2
O2	18	0.6382	0.6288	0.1891	1	2
O3	18	0.58373	0.60612	-0.1574	1	2
250K, 250 mbar						
Xe1	18	0.658(2)	0.509(2)	0.845(7)	0.23(1)	8(1)
Xe2	18	-0.122(2)	0.036(2)	0.126(5)	0.18(2)	8(1)
250K, 500 mbar						
Xe1	18	0.658(2)	0.508(2)	0.855(6)	0.28(1)	8(1)
Xe2	18	-0.120(2)	0.035(2)	0.120(4)	0.27(2)	8(1)
170K, 50 mbar						
Xe1	18	0.655(1)	0.505(1)	0.824(4)	0.34(1)	8(1)
Xe2	18	-0.1275(9)	0.0340(8)	0.107(3)	0.342(9)	8(1)
Xe3	3	0	0	0.5	0.38(2)	8(1)
170K, 100 mbar						
Xe1	18	0.655(1)	0.505(1)	0.814(4)	0.35(1)	8(1)
Xe2	18	-0.1274(8)	0.0340(8)	0.105(3)	0.35(1)	8(1)
Xe3	3	0	0	0.5	0.39(2)	8(1)
170K, 250 mbar						
Xe1	18	0.655(1)	0.504(1)	0.805(4)	0.34(2)	8(1)
Xe2	18	-0.1271(9)	0.0344(9)	0.103(3)	0.35(1)	8(1)
Xe3	3	0	0	0.5	0.39(2)	8(1)

170K, 500 mbar						
Xe1	18	0.656(1)	0.503(1)	0.797(4)	0.35(2)	8(1)
Xe2	18	-0.1282(9)	0.0350(8)	0.107(3)	0.35(1)	8(1)
Xe3	3	0	0	0.5	0.40(2)	8(1)
250K, 250 mbar						
Kr1	18	0.659(2)	0.5014(8)	0.696(3)	0.05(2)	8(1)
Kr2	18	-0.162(3)	0.016(4)	0.338(2)	0.08(2)	8(1)
250K, 500 mbar						
Kr1	18	0.659(2)	0.5014(8)	0.816(3)	0.15(2)	8(1)
Kr2	18	-0.226(3)	-0.034(3)	0.111(4)	0.10(2)	8(1)
250K, 1000 mbar						
Kr1	18	0.659(2)	0.5014(8)	0.816(3)	0.12(3)	8(1)
Kr2	18	-0.154(3)	0.022(4)	0.362(4)	0.16(2)	8(1)
170K, 50 mbar						
Kr1	18	0.659(2)	0.5014(8)	0.816(3)	0.21(2)	8(1)
Kr2	18	0.681(2)	0.499(1)	0.064(4)	0.27(2)	8(1)
170K, 100 mbar						
Kr1	18	0.659(2)	0.5014(8)	0.816(3)	0.28(2)	8(1)
Kr2	18	0.686(2)	0.503(1)	0.071(4)	0.22(2)	8(1)
Kr3	3	0	0	0.5	0.06(1)	8(1)
170K, 250 mbar						
Kr1	18	-0.181(2)	-0.004(2)	0.526(3)	0.39(1)	8(1)
Kr2	18	0.691(1)	0.4893(7)	0.146(5)	0.39(2)	8(1)
Kr3	3	0	0	0.5	0.18(1)	8(1)
170K, 500 mbar						
Kr1	18	0.6671(7)	0.5070(7)	0.899(3)	0.52(1)	8(1)
Kr2	18	-0.112(2)	0.041(2)	0.122(3)	0.35(1)	8(1)
Kr3	3	0	0	0.5	0.34(2)	8(1)
170K, 1000 mbar						
Kr1	18	0.660(1)	0.5054(6)	0.819(3)	0.51(1)	8(1)
Kr2	18	-0.1287(9)	0.024(1)	0.128(3)	0.46(1)	8(1)
Kr3	3	0	0	0.5	0.60(2)	8(1)
130K, 50 mbar						
Kr1	18	0.641(2)	0.532(2)	0.741(5)	0.24(1)	8(1)
Kr2	18	-0.101(4)	0.033(4)	-0.114(2)	0.12(2)	8(1)
130K, 100 mbar						
Kr1	18	0.6597(9)	0.5088(6)	0.806(2)	0.54(1)	8(1)
Kr2	18	-0.115(1)	0.041(1)	0.106(2)	0.42(1)	8(1)
Kr3	3	0	0	0.5	0.51(2)	8(1)
130K, 250 mbar						
Kr1	18	0.6648(7)	0.5072(6)	0.886(2)	0.61(1)	8(1)
Kr2	18	-0.106(1)	0.049(1)	0.078(3)	0.40(1)	8(1)
Kr3	3	0	0	0.5	0.62(2)	8(1)
130K, 500 mbar						
Kr1	18	0.659(1)	0.5014(8)	0.816(3)	0.53(1)	8(1)
Kr2	18	-0.1303(8)	0.0285(8)	0.081(3)	0.49(2)	8(1)

Kr3	3	0	0	0.5	0.69(2)	8(1)
130K, 1000 mbar						
Kr1	18	0.652(1)	0.4972(8)	0.801(3)	0.53(2)	8(1)
Kr2	18	-0.1317(8)	0.0277(8)	0.079(3)	0.51(2)	8(1)
Kr3	3	0	0	0.5	0.78(2)	8(1)

Atomic positions of Xe and Kr in ZIF-8:

Atom	Wp	x	y	z	Occ	B_{iso}
Zn1	12	0.5	0	0.75	1	8
N1	48	0.40973	0.96832	0.68278	1	8
C1	24	0.37705	1.0079	0.62295	1	8
C2	48	0.36851	0.89914	0.6875	1	8
H1	48	0.3777	0.8589	0.7234	1	8
C3	24	0.4061	1.0855	0.5939	1	8
H2	48	0.4587	1.0798	0.5743	1	8
H3	48	0.4058	1.1228	0.6364	1	8
H4	48	0.3724	1.1039	0.5525	1	8
180K, 9 mbar						
Xe1	24	0.181(1)	0.181(1)	0.041(2)	0.09(1)	10(1)
Xe2	12	0.180(3)	0	0	0.05(1)	10(1)
Xe3	8	0.207(2)	0.207(2)	0.207(2)	0.09(1)	10(1)
180K, 17 mbar						
Xe1	24	0.1807(9)	0.1807(9)	0.045(2)	0.13(1)	10(1)
Xe2	12	0.203(3)	0	0	0.05(1)	10(1)
Xe3	8	0.201(2)	0.201(2)	0.201(2)	0.09(1)	10(1)
180K, 36 mbar						
Xe1	24	0.1823(5)	0.1823(5)	0.034(1)	0.19(1)	10(1)
Xe2	12	0.212(3)	0	0	0.06(1)	10(1)
Xe3	8	0.185(1)	0.185(1)	0.185(1)	0.13(1)	10(1)
180K, 53 mbar						
Xe1	24	0.1831(5)	0.1831(5)	0.0339(9)	0.27(1)	10(1)
Xe2	12	0.228(3)	0	0	0.09(1)	10(1)
Xe3	8	0.187(1)	0.187(1)	0.187(1)	0.14(1)	10(1)
180K, 93 mbar						
Xe1	24	0.1844(3)	0.1844(3)	0.0176(7)	0.44(1)	10(1)
Xe2	12	0.207(2)	0	0	0.12(1)	10(1)
Xe3	8	0.150(1)	0.150(1)	0.150(1)	0.25(1)	10(1)
180K, 394 mbar						
Xe1	24	0.1909(1)	0.1909(1)	0.0037(5)	0.73(1)	10(1)
Xe3	8	0.224(4)	0.224(4)	0.224(4)	0.04(1)	10(1)
Xe4	2	0	0	0	0.63(1)	10(1)
180K, 500 mbar						
Xe1	24	0.19138(8)	0.19138(8)	0.0034(4)	0.84(1)	10(1)
Xe3	8	0.232(3)	0.232(3)	0.232(3)	0.09(1)	10(1)

Xe4	2	0	0	0	0.86(1)	10(1)
180K, 1000 mbar						
Xe1	24	0.19146(9)	0.19146(9)	0.0029(4)	0.88(1)	10(1)
Xe3	8	0.227(3)	0.227(3)	0.227(3)	0.10(1)	10(1)
Xe4	2	0	0	0	0.92(1)	10(1)
180K, 50 mbar						
Kr1	24	0.174(2)	0.174(2)	0.057(3)	0.08(1)	10(1)
Kr2	8	0.209(3)	0.209(3)	0.209(3)	0.08(1)	10(1)
Kr4	2	0	0	0	0.08(1)	10(1)
180K, 100 mbar						
Kr1	24	0.175(2)	0.175(2)	0.062(3)	0.10(1)	10(1)
Kr2	8	0.210(3)	0.210(3)	0.210(3)	0.06(1)	10(1)
Kr4	2	0	0	0	0.05(1)	10(1)
180K, 250 mbar						
Kr1	24	0.1930(1)	0.1930(1)	0.043(2)	0.23(1)	10(1)
Kr2	8	0.204(3)	0.204(3)	0.204(3)	0.20(1)	10(1)
Kr4	2	0	0	0	0.09(1)	10(1)
Kr3	24	-0.777(2)	0.038(2)	-0.038(2)	0.10(1)	10(1)
180K, 500 mbar						
Kr1	24	0.1878(6)	0.1878(6)	0.034(2)	0.36(1)	10(1)
Kr2	8	0.193(1)	0.193(1)	0.193(1)	0.36(1)	10(1)
Kr4	2	0	0	0	0.09(1)	10(1)
Kr3	24	-0.771(2)	0.043(1)	-0.043(1)	0.18(1)	10(1)
180K, 750 mbar						
Kr1	24	0.1884(4)	0.1884(4)	0.0222(8)	0.42(1)	10(1)
Kr2	8	0.1858(5)	0.1858(5)	0.1858(5)	0.43(1)	10(1)
Kr4	2	0	0	0	0.12(1)	10(1)
Kr3	24	-0.772(1)	0.0441(7)	-0.0441(7)	0.19(1)	10(1)
180K, 1000 mbar						
Kr1	24	0.1887(3)	0.1887(3)	0.0199(7)	0.46(1)	10(1)
Kr2	8	0.1879(5)	0.1879(5)	0.1879(5)	0.47(1)	10(1)
Kr4	2	0	0	0	0.16(1)	10(1)
Kr3	24	-0.7739(1)	0.0442(6)	-0.0442(6)	0.20(1)	10(1)