



Journal Name

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<Table 2, to be inserted on page 6>

MOF Gas Temp	Side-on Bonding			Bent Bonding			Linear Bonding		
	%	Bond length (Å)	Angle (°)	%	Bond length (Å)	Angle (°)	%	Bond length (Å)	Angle (°)
Cr ₂ (dobdc)									
N ₂									
201 K				52.4	2.30 ± 0.17	135 ± 13	47.6	1.90 ± 0.04	172 ± 4
258 K				51.4	2.27 ± 0.18	136 ± 13	48.6	1.90 ± 0.04	172 ± 4
298 K				98.1	2.35 ± 0.11	133 ± 11	1.9	2.08 ± 0.25	170 ± 4
O ₂									
201 K	70.7	1.83 ± 0.03	70 ± 2	29.3	1.84 ± 0.06	122 ± 5			
258 K	40.3	1.83 ± 0.03	70 ± 2	59.7	1.84 ± 0.06	121 ± 6			
298 K	40.4	1.83 ± 0.04	70 ± 2	59.6	1.84 ± 0.05	121 ± 6			
Mn ₂ (dobdc)									
N ₂									
201 K				48.1	2.36 ± 0.11	140 ± 11	51.9	1.81 ± 0.10	174 ± 3
258 K				49.1	2.35 ± 0.14	141 ± 11	50.9	1.81 ± 0.10	173 ± 3
298 K				37.6	2.32 ± 0.19	142 ± 12	62.4	1.80 ± 0.09	173 ± 4
O ₂									
201 K	20.2	1.84 ± 0.04	70 ± 2	79.9	1.91 ± 0.05	120 ± 6			
258 K	52.3	1.84 ± 0.04	71 ± 2	47.7	1.92 ± 0.09	120 ± 7			
298 K	61.0	1.85 ± 0.04	71 ± 2	39.0	1.93 ± 0.09	119 ± 9			
Fe ₂ (dobdc)									
N ₂									
201 K				73.5	2.17 ± 0.14	153 ± 9	26.5	2.10 ± 0.12	170 ± 4
258 K				70.0	2.15 ± 0.14	153 ± 9	30.0	2.08 ± 0.14	170 ± 4
298 K				71.5	2.14 ± 0.15	153 ± 9	28.5	2.05 ± 0.12	170 ± 4
O ₂									
201 K	40.2	1.87 ± 0.11	71 ± 3	59.8	1.87 ± 0.06	125 ± 8			
258 K	21.6	1.97 ± 0.14	73 ± 3	78.4	1.89 ± 0.08	123 ± 12			
298 K	59.5	1.89 ± 0.13	72 ± 3	40.5	1.89 ± 0.08	121 ± 14			