

Predictor	Units
Type	categorical
Aperture & Aperture2	Å
Apertureatom_σ	Å
ApertureAtoms_e	kJ/mol
ionicRad	Å
Linker_length & func_length	Å
Linker_mass & func_mass	Standard atomic weight (g/mol)
Diameter	Å
Mass	Standard atomic weight (g/mol)
acentricF	Unitless
Kdiameter	Å
ionicRad	Å
logD	Unitless

type	aperture	aperture 2	aperture Atom_σ	aperture Atom_e	ionicRad	linker_le ngth1	linker_le ngth2	linker_le ngth3	linker_m ass1	linker_m ass2	linker_m ass3	func1_len gth	func2_len gth	func3_len gth	func1_m ass	func2_m ass	func3_m ass	gas	diameter	mass	acentricF	kdiamete r	logD
CdIF-1	3.92	3.93	0.25	0.0627	92	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-7.22185
CdIF-1	3.92	3.99	0.25	0.0627	92	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-7.30103
CdIF-1	3.92	4.02	0.25	0.0627	92	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	O2	2.94	31.999	0.022	3.46	-8
CdIF-1	3.92	3.97	0.25	0.0627	92	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-8.39794
CdIF-1	3.92	4.0415	0.25	0.0627	92	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-8.30103
CdIF-1	3.92	4.08	0.25	0.0627	92	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-8.58503

CdIF-1	3.92	4.11	0.25	0.0627	92	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-9.23657
CdIF-1	3.92	4.11	0.25	0.0627	92	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-9.19723
CdIF-1	3.92	4.16	0.25	0.0627	92	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	propylene	4.03	42.08	0.142	4.5	-9.66756
CdIF-1	3.92	4.22	0.25	0.0627	92	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	propane	4.16	44.1	0.152	4.3	-10.6778
CdIF-1	3.92	4.23	0.25	0.0627	92	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	butane	4.52	58.12	0.2	4.5	-10.9747
ZIF-8	3.46	3.47	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-7.65561
ZIF-8	3.46	3.48	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-7.79588
ZIF-8	3.46	3.5	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	O2	2.94	31.999	0.022	3.46	-9
ZIF-8	3.46	3.5	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-9.30103
ZIF-8	3.46	3.55	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-9.56864
ZIF-8	3.46	3.63	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-10.2441
ZIF-8	3.46	3.64	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-10.7959
ZIF-8	3.46	3.65	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-11.0804
ZIF-8	3.46	3.75	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	propylene	4.03	42.08	0.142	4.5	-12.327
ZIF-8	3.46	3.78	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	propane	4.16	44.1	0.152	4.3	-14.2147
ZIF-8	3.46	3.8	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	butane	4.52	58.12	0.2	4.5	-14.3468
ZIF-8	3.46	4.37	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	iso-butane	4.8	58.12	0.183	4.42	-27.2916
ZIF-Cu	3.2	3.26	0.25	0.0627	71	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-7.79588
ZIF-Cu	3.2	3.28	0.25	0.0627	71	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-7.88606
ZIF-Cu	3.2	3.31	0.25	0.0627	71	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	O2	2.94	31.999	0.022	3.46	-9.29243
ZIF-Cu	3.2	3.3	0.25	0.0627	71	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-9.50864
ZIF-Cu	3.2	3.356	0.25	0.0627	71	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-9.36653
ZIF-Cu	3.2	3.47	0.25	0.0627	71	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-11.8239
ZIF-Cu	3.2	3.47	0.25	0.0627	71	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-12.4089
ZIF-Cu	3.2	3.482	0.25	0.0627	71	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-13.1805
ZIF-Cu	3.2	3.56	0.25	0.0627	71	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	propylene	4.03	42.08	0.142	4.5	-14.2441
ZIF-Cu	3.2	3.63	0.25	0.0627	71	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	propane	4.16	44.1	0.152	4.3	-16.7696
ZIF-67	3.32	3.36	0.25	0.0627	72	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-7.8729
ZIF-67	3.32	3.3865	0.25	0.0627	72	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-8.06048
ZIF-67	3.32	3.418	0.25	0.0627	72	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	O2	2.94	31.999	0.022	3.46	-9.01011
ZIF-67	3.32	3.4	0.25	0.0627	72	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-9.35262
ZIF-67	3.32	3.45	0.25	0.0627	72	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-9.60206
ZIF-67	3.32	3.53	0.25	0.0627	72	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-11.3645
ZIF-67	3.32	3.5	0.25	0.0627	72	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-10.699
ZIF-67	3.32	3.52	0.25	0.0627	72	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-11.3979

ZIF-67	3.32	3.65	0.25	0.0627	72	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	propylene	4.03	42.08	0.142	4.5	-12.5229
ZIF-67	3.32	3.7	0.25	0.0627	72	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	propane	4.16	44.1	0.152	4.3	-14.8239
ZIF-67	3.32	3.7	0.25	0.0627	72	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	butane	4.52	58.12	0.2	4.5	-16.2518
BeIF-1	2.88	2.88	0.25	0.0627	41	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-8.19382
BeIF-1	2.88	2.9	0.25	0.0627	41	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-9.02687
BeIF-1	2.88	2.96	0.25	0.0627	41	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	O2	2.94	31.999	0.022	3.46	-10.6757
BeIF-1	2.88	2.93	0.25	0.0627	41	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-10.5058
BeIF-1	2.88	3.02	0.25	0.0627	41	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-12.4949
BeIF-1	2.88	3.2	0.25	0.0627	41	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-16.0969
BeIF-1	2.88	3.17	0.25	0.0627	41	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-18.2218
BeIF-1	2.88	3.2	0.25	0.0627	41	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-19
BeIF-1	2.88	3.29	0.25	0.0627	41	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	propylene	4.03	42.08	0.142	4.5	-23.301
BeIF-1	2.88	3.34	0.25	0.0627	41	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	propane	4.16	44.1	0.152	4.3	-26.5229
BeIF-1	2.88	3.35	0.25	0.0627	41	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	butane	4.52	58.12	0.2	4.5	-27.0969
ZIF-7-8	2.32	2.67	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	He	2.66	4.002	-0.39	2.6	-8.48149
ZIF-7-8	2.32	2.9	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	H2	2.76	2.01	-0.217	2.89	-9.61979
ZIF-7-8	2.32	3.17	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	O2	2.94	31.999	0.022	3.46	-12
ZIF-7-8	2.32	3.18	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	CO2	3.24	44.01	0.225	3.3	-11.8013
ZIF-7-8	2.32	3.37	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	N2	3.13	28	0.037	3.64	-13.0969
ZIF-7-8	2.32	3.59	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	CH4	3.25	16.04	0.011	3.8	-15.301
ZIF-7-8	2.32	3.58	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	ethylene	3.59	28.05	0.087	3.9	-16.9586
ZIF-7-8	2.32	3.58	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	ethane	3.72	30.07	0.099	4	-17.466
ZIF-7-8	2.32	3.59	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	propylene	4.03	42.08	0.142	4.5	-18.2403
ZIF-7-8	2.32	3.64	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	propane	4.16	44.1	0.152	4.3	-19.7696
ZIF-7-8	2.32	4	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	butane	4.52	58.12	0.2	4.5	-20.0013
Co-ZIF-7-8	2.31	2.6393	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	He	2.66	4.002	-0.39	2.6	-8.82391
Co-ZIF-7-8	2.31	2.8869	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	H2	2.76	2.01	-0.217	2.89	-9.76955
Co-ZIF-7-8	2.31	3.1288	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	O2	2.94	31.999	0.022	3.46	-11.7447
Co-ZIF-7-8	2.31	3.1507	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	CO2	3.24	44.01	0.225	3.3	-12
Co-ZIF-7-8	2.31	3.3298	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	N2	3.13	28	0.037	3.64	-13.2441
Co-ZIF-7-8	2.31	3.5587	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	CH4	3.25	16.04	0.011	3.8	-15.7447

Co-ZIF-7-8	2.31	3.55	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	ethylene	3.59	28.05	0.087	3.9	-17.4737
Co-ZIF-7-8	2.31	3.55	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	ethane	3.72	30.07	0.099	4	-17.3487
Co-ZIF-7-8	2.31	3.52	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	propylene	4.03	42.08	0.142	4.5	-18.8013
Co-ZIF-7-8	2.31	3.48	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	propane	4.16	44.1	0.152	4.3	-20.4868
Co-ZIF-7-8	2.31	3.58	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	butane	4.52	58.12	0.2	4.5	-20.8633
Cl-ZIF-7-8	2.1052	2.4059	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	3.54	15	15	35.45	He	2.66	4.002	-0.39	2.6	-9.60906
Cl-ZIF-7-8	2.1052	2.6504	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	3.54	15	15	35.45	H2	2.76	2.01	-0.217	2.89	-10.7212
Cl-ZIF-7-8	2.1052	2.8742	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	3.54	15	15	35.45	O2	2.94	31.999	0.022	3.46	-14
Cl-ZIF-7-8	2.1052	2.8966	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	3.54	15	15	35.45	CO2	3.24	44.01	0.225	3.3	-14.284
Cl-ZIF-7-8	2.1052	3.0551	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	3.54	15	15	35.45	N2	3.13	28	0.037	3.64	-15.6778
Cl-ZIF-7-8	2.1052	3.3155	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	3.54	15	15	35.45	CH4	3.25	16.04	0.011	3.8	-19.8861
Cl-ZIF-7-8	2.1052	3.36	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	3.54	15	15	35.45	ethylene	3.59	28.05	0.087	3.9	-19.1824
Cl-ZIF-7-8	2.1052	3.41	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	3.54	15	15	35.45	ethane	3.72	30.07	0.099	4	-21.0035
Cl-ZIF-7-8	2.1052	3.51	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	3.54	15	15	35.45	propylene	4.03	42.08	0.142	4.5	-23.1255
Cl-ZIF-7-8	2.1052	3.61	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	3.54	15	15	35.45	propane	4.16	44.1	0.152	4.3	-26.8894
Cl-ZIF-7-8	2.1052	3.62	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	3.54	15	15	35.45	butane	4.52	58.12	0.2	4.5	-26.4881
Br-ZIF-7-8	2.1021	2.3821	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	He	2.66	4.002	-0.39	2.6	-9.20831
Br-ZIF-7-8	2.1021	2.6237	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	H2	2.76	2.01	-0.217	2.89	-10.5969
Br-ZIF-7-8	2.1021	2.847	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	O2	2.94	31.999	0.022	3.46	-13.9469
Br-ZIF-7-8	2.1021	2.8571	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	CO2	3.24	44.01	0.225	3.3	-13.8962
Br-ZIF-7-8	2.1021	3.0268	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	N2	3.13	28	0.037	3.64	-15.4353

Br-ZIF-7-8	2.1021	3.275	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	CH4	3.25	16.04	0.011	3.8	-18.9788
Br-ZIF-7-8	2.1021	3.3414	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	ethylene	3.59	28.05	0.087	3.9	-19.9957
Br-ZIF-7-8	2.1021	3.3516	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	ethane	3.72	30.07	0.099	4	-20.1599
Br-ZIF-7-8	2.1021	3.47	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	propylene	4.03	42.08	0.142	4.5	-22.699
Br-ZIF-7-8	2.1021	3.57	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	propane	4.16	44.1	0.152	4.3	-25.699
Be-ZIF-7-8	1.99	2.335	0.25	0.0627	41	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	He	2.66	4.002	-0.39	2.6	-11.1512
Be-ZIF-7-8	1.99	2.607	0.25	0.0627	41	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	H2	2.76	2.01	-0.217	2.89	-14.4976
Be-ZIF-7-8	1.99	2.8099	0.25	0.0627	41	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	O2	2.94	31.999	0.022	3.46	-19.0883
Be-ZIF-7-8	1.99	2.82	0.25	0.0627	41	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	CO2	3.24	44.01	0.225	3.3	-19.451
Be-ZIF-7-8	1.99	2.979	0.25	0.0627	41	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	N2	3.13	28	0.037	3.64	-22.3401
Be-ZIF-7-8	1.99	3.2047	0.25	0.0627	41	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	CH4	3.25	16.04	0.011	3.8	-29.2588
Be-ZIF-7-8	1.99	3.2133	0.25	0.0627	41	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	ethylene	3.59	28.05	0.087	3.9	-31.4815
Be-ZIF-7-8	1.99	3.2093	0.25	0.0627	41	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	ethane	3.72	30.07	0.099	4	-32.8794
Be-ZIF-7-8	1.99	3.27	0.25	0.0627	41	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	propylene	4.03	42.08	0.142	4.5	-36.8861
Be-ZIF-7-8	1.99	3.63	0.25	0.0627	41	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	propane	4.16	44.1	0.152	4.3	-39.3526
Br-ZIF-8	3.66	3.60863	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.85	3.85	3.85	79.9	79.9	79.9	He	2.66	4.002	-0.39	2.6	-7.46852
Br-ZIF-8	3.66	3.61345	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.85	3.85	3.85	79.9	79.9	79.9	H2	2.76	2.01	-0.217	2.89	-7.52288
Br-ZIF-8	3.66	3.7624	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.85	3.85	3.85	79.9	79.9	79.9	O2	2.94	31.999	0.022	3.46	-8.48149
Br-ZIF-8	3.66	3.77	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.85	3.85	3.85	79.9	79.9	79.9	CO2	3.24	44.01	0.225	3.3	-9.35655
Br-ZIF-8	3.66	3.8	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.85	3.85	3.85	79.9	79.9	79.9	N2	3.13	28	0.037	3.64	-9.14448
Br-ZIF-8	3.66	3.66	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.85	3.85	3.85	79.9	79.9	79.9	CH4	3.25	16.04	0.011	3.8	-8.83863
Br-ZIF-8	3.66	3.88	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.85	3.85	3.85	79.9	79.9	79.9	ethylene	3.59	28.05	0.087	3.9	-9.39577
Br-ZIF-8	3.66	3.88	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.85	3.85	3.85	79.9	79.9	79.9	ethane	3.72	30.07	0.099	4	-9.86646
Br-ZIF-8	3.66	3.91	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.85	3.85	3.85	79.9	79.9	79.9	propylene	4.03	42.08	0.142	4.5	-10.7595
Br-ZIF-8	3.66	3.99	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.85	3.85	3.85	79.9	79.9	79.9	propane	4.16	44.1	0.152	4.3	-12.1487

Br-ZIF-8	3.66	3.97	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.85	3.85	3.85	79.9	79.9	79.9	butane	4.52	58.12	0.2	4.5	-12.4342
Br-ZIF-8	3.66	4.49	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.85	3.85	3.85	79.9	79.9	79.9	iso-butane	4.8	58.12	0.183	4.42	-22.2218
Im-ZIF-8 (1)	3.5139	3.54391	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	3.78	2.278	15	15	1	He	2.66	4.002	-0.39	2.6	-7.5376
Im-ZIF-8 (1)	3.5139	3.55867	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	3.78	2.278	15	15	1	H2	2.76	2.01	-0.217	2.89	-7.55284
Im-ZIF-8 (1)	3.5139	3.61	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	3.78	2.278	15	15	1	O2	2.94	31.999	0.022	3.46	-8.77728
Im-ZIF-8 (1)	3.5139	3.59	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	3.78	2.278	15	15	1	CO2	3.24	44.01	0.225	3.3	-9.16749
Im-ZIF-8 (1)	3.5139	3.66	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	3.78	2.278	15	15	1	N2	3.13	28	0.037	3.64	-9.55284
Im-ZIF-8 (1)	3.5139	3.75	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	3.78	2.278	15	15	1	CH4	3.25	16.04	0.011	3.8	-9.95861
Im-ZIF-8 (1)	3.5139	3.76	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	3.78	2.278	15	15	1	ethylene	3.59	28.05	0.087	3.9	-10.6198
Im-ZIF-8 (1)	3.5139	3.78	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	3.78	2.278	15	15	1	ethane	3.72	30.07	0.099	4	-10.699
Im-ZIF-8 (1)	3.5139	3.84	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	3.78	2.278	15	15	1	propylene	4.03	42.08	0.142	4.5	-11.5229
Im-ZIF-8 (1)	3.5139	3.94	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	3.78	2.278	15	15	1	propane	4.16	44.1	0.152	4.3	-13.1739
Im-ZIF-8 (1)	3.5139	3.92	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	3.78	2.278	15	15	1	butane	4.52	58.12	0.2	4.5	-13.5654
Im-ZIF-8 (1)	3.5139	4.8	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	3.78	2.278	15	15	1	iso-butane	4.8	58.12	0.183	4.42	-22.8356
Im-ZIF-8 (2)	3.56	3.59781	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	2.278	2.278	15	1	1	He	2.66	4.002	-0.39	2.6	-7.4437
Im-ZIF-8 (2)	3.56	3.61555	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	2.278	2.278	15	1	1	H2	2.76	2.01	-0.217	2.89	-7.49485
Im-ZIF-8 (2)	3.56	3.66	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	2.278	2.278	15	1	1	O2	2.94	31.999	0.022	3.46	-8.76955
Im-ZIF-8 (2)	3.56	3.64	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	2.278	2.278	15	1	1	CO2	3.24	44.01	0.225	3.3	-9.1986
Im-ZIF-8 (2)	3.56	3.73	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	2.278	2.278	15	1	1	N2	3.13	28	0.037	3.64	-9.3851
Im-ZIF-8 (2)	3.56	3.8	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	2.278	2.278	15	1	1	CH4	3.25	16.04	0.011	3.8	-9.83565
Im-ZIF-8 (2)	3.56	3.82	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	2.278	2.278	15	1	1	ethylene	3.59	28.05	0.087	3.9	-10.2857

Im-ZIF-8 (2)	3.56	3.84	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	2.278	2.278	15	1	1	ethane	3.72	30.07	0.099	4	-10.5575
Im-ZIF-8 (2)	3.56	3.9	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	2.278	2.278	15	1	1	propylene	4.03	42.08	0.142	4.5	-11.2676
Im-ZIF-8 (2)	3.56	4.01	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	2.278	2.278	15	1	1	propane	4.16	44.1	0.152	4.3	-12.4815
Im-ZIF-8 (2)	3.56	3.99	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	2.278	2.278	15	1	1	butane	4.52	58.12	0.2	4.5	-12.9508
Im-ZIF-8 (2)	3.56	4.63	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.78	2.278	2.278	15	1	1	iso-butane	4.8		0.183	4.42	-21.6162
Cd-Cl- ZIF-7-8	2.27	2.6	0.25	0.0627	92	4.438	4.438	5.996	81	81	117	3.78	3.78	3.54	15	15	35.45	He	2.66	4.002	-0.39	2.6	-8.56864
Cd-Cl- ZIF-7-8	2.27	2.83	0.25	0.0627	92	4.438	4.438	5.996	81	81	117	3.78	3.78	3.54	15	15	35.45	H2	2.76	2.01	-0.217	2.89	-8.52288
Cd-Cl- ZIF-7-8	2.27	3.08	0.25	0.0627	92	4.438	4.438	5.996	81	81	117	3.78	3.78	3.54	15	15	35.45	O2	2.94	31.999	0.022	3.46	-11.9586
Cd-Cl- ZIF-7-8	2.27	3.1	0.25	0.0627	92	4.438	4.438	5.996	81	81	117	3.78	3.78	3.54	15	15	35.45	CO2	3.24	44.01	0.225	3.3	-12.1824
Cd-Cl- ZIF-7-8	2.27	3.25	0.25	0.0627	92	4.438	4.438	5.996	81	81	117	3.78	3.78	3.54	15	15	35.45	N2	3.13	28	0.037	3.64	-13.699
Cd-Cl- ZIF-7-8	2.27	3.5	0.25	0.0627	92	4.438	4.438	5.996	81	81	117	3.78	3.78	3.54	15	15	35.45	CH4	3.25	16.04	0.011	3.8	-15.8013
Cd-Cl- ZIF-7-8	2.27	3.73	0.25	0.0627	92	4.438	4.438	5.996	81	81	117	3.78	3.78	3.54	15	15	35.45	ethylene	3.59	28.05	0.087	3.9	-16.8539
Cd-Cl- ZIF-7-8	2.27	3.73	0.25	0.0627	92	4.438	4.438	5.996	81	81	117	3.78	3.78	3.54	15	15	35.45	ethane	3.72	30.07	0.099	4	-17.1367
Cd-Cl- ZIF-7-8	2.27	3.87	0.25	0.0627	92	4.438	4.438	5.996	81	81	117	3.78	3.78	3.54	15	15	35.45	propylene	4.03	42.08	0.142	4.5	-18.4318
Cd-Cl- ZIF-7-8	2.27	3.85	0.25	0.0627	92	4.438	4.438	5.996	81	81	117	3.78	3.78	3.54	15	15	35.45	propane	4.16	44.1	0.152	4.3	-20.3979
ZIF8_Mg	3.56	3.6	0.25	0.0627	71	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-7.38091
ZIF8_Mg	3.56	3.62	0.25	0.0627	71	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-7.52288
ZIF8_Mg	3.56	3.65	0.25	0.0627	71	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-8.74473
ZIF8_Mg	3.56	3.73	0.25	0.0627	71	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-8.92082
ZIF8_Mg	3.56	3.82	0.25	0.0627	71	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-9.23657
ZIF8_Mg	3.56	3.84	0.25	0.0627	71	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-10.9208
ZIF8_Mg	3.56	3.85	0.25	0.0627	71	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-10.6478
ZIF8_Mg	3.56	3.92	0.25	0.0627	71	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	propylene	4.03	42.08	0.142	4.5	-11.5229
ZIF8_Mg	3.56	4.02	0.25	0.0627	71	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	propane	4.16	44.1	0.152	4.3	-12.1391
ZIF8_Mn	3.77	3.79	0.25	0.0627	80	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-7.52288

ZIF8_Mn	3.77	3.81	0.25	0.0627	80	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-7.52288
ZIF8_Mn	3.77	3.84	0.25	0.0627	80	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-8.55284
ZIF8_Mn	3.77	3.91	0.25	0.0627	80	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-8.55284
ZIF8_Mn	3.77	3.95	0.25	0.0627	80	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-8.55284
ZIF8_Mn	3.77	3.97	0.25	0.0627	80	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-9.12494
ZIF8_Mn	3.77	3.99	0.25	0.0627	80	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-9.16749
ZIF8_Mn	3.77	3.99	0.25	0.0627	80	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	propylene	4.03	42.08	0.142	4.5	-9.79588
ZIF8_Mn	3.77	4.1	0.25	0.0627	80	4.438	4.438	4.438	81	81	81	3.78	3.78	3.78	15	15	15	propane	4.16	44.1	0.152	4.3	-11.585
Cd-Br-ZIF-7-8	2.2517	2.53	0.25	0.0627	92	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	He	2.66	4.002	-0.39	2.6	-8.69897
Cd-Br-ZIF-7-8	2.2517	2.77	0.25	0.0627	92	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	H2	2.76	2.01	-0.217	2.89	-8.69897
Cd-Br-ZIF-7-8	2.2517	3.01	0.25	0.0627	92	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	O2	2.94	31.999	0.022	3.46	-11.5229
Cd-Br-ZIF-7-8	2.2517	3.025	0.25	0.0627	92	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	CO2	3.24	44.01	0.225	3.3	-11.6144
Cd-Br-ZIF-7-8	2.2517	3.19	0.25	0.0627	92	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	N2	3.13	28	0.037	3.64	-12.9281
Cd-Br-ZIF-7-8	2.2517	3.478	0.25	0.0627	92	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	CH4	3.25	16.04	0.011	3.8	-15.1831
Cd-Br-ZIF-7-8	2.2517	3.515	0.25	0.0627	92	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	ethylene	3.59	28.05	0.087	3.9	-16
Cd-Br-ZIF-7-8	2.2517	3.55	0.25	0.0627	92	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	ethane	3.72	30.07	0.099	4	-16.4089
Cd-Br-ZIF-7-8	2.2517	3.65	0.25	0.0627	92	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	propylene	4.03	42.08	0.142	4.5	-18.158
Cd-Br-ZIF-7-8	2.2517	3.77	0.25	0.0627	92	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	propane	4.16	44.1	0.152	4.3	-19.7747
Cl-ZIF-8	3.58	3.6	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.54	3.54	3.54	35.45	35.45	35.45	He	2.66	4.002	-0.39	2.6	-7.52288
Cl-ZIF-8	3.58	3.6	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.54	3.54	3.54	35.45	35.45	35.45	H2	2.76	2.01	-0.217	2.89	-7.65758
Cl-ZIF-8	3.58	3.67	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.54	3.54	3.54	35.45	35.45	35.45	O2	2.94	31.999	0.022	3.46	-8.63827
Cl-ZIF-8	3.58	3.71	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.54	3.54	3.54	35.45	35.45	35.45	CO2	3.24	44.01	0.225	3.3	-9.5157
Cl-ZIF-8	3.58	3.76	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.54	3.54	3.54	35.45	35.45	35.45	N2	3.13	28	0.037	3.64	-9.5784
Cl-ZIF-8	3.58	3.85	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.54	3.54	3.54	35.45	35.45	35.45	CH4	3.25	16.04	0.011	3.8	-9.79317
Cl-ZIF-8	3.58	3.92	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.54	3.54	3.54	35.45	35.45	35.45	ethylene	3.59	28.05	0.087	3.9	-10.6799
Cl-ZIF-8	3.58	3.9	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.54	3.54	3.54	35.45	35.45	35.45	ethane	3.72	30.07	0.099	4	-10.4881
Cl-ZIF-8	3.58	4.01	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.54	3.54	3.54	35.45	35.45	35.45	propylene	4.03	42.08	0.142	4.5	-11.5331
Cl-ZIF-8	3.58	4.19	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.54	3.54	3.54	35.45	35.45	35.45	propane	4.16	44.1	0.152	4.3	-12.2321

Cl-ZIF-8	3.58	4.2	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.54	3.54	3.54	35.45	35.45	35.45	butane	4.52	58.12	0.2	4.5	-12.2676
Cl-ZIF-8	3.58	4.96	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	3.54	3.54	3.54	35.45	35.45	35.45	isobutane	4.8	58.12	0.183	4.42	-17.1871
Im-ZIF-8 (3)	3.6	3.63729	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	2.278	2.278	2.278	1	1	1	He	2.66	4.002	-0.39	2.6	-7.49485
Im-ZIF-8 (3)	3.6	3.65448	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	2.278	2.278	2.278	1	1	1	H2	2.76	2.01	-0.217	2.89	-7.58503
Im-ZIF-8 (3)	3.6	3.81	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	2.278	2.278	2.278	1	1	1	O2	2.94	31.999	0.022	3.46	-8.36653
Im-ZIF-8 (3)	3.6	3.8	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	2.278	2.278	2.278	1	1	1	CO2	3.24	44.01	0.225	3.3	-8.82391
Im-ZIF-8 (3)	3.6	3.86	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	2.278	2.278	2.278	1	1	1	N2	3.13	28	0.037	3.64	-8.85387
Im-ZIF-8 (3)	3.6	3.92	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	2.278	2.278	2.278	1	1	1	CH4	3.25	16.04	0.011	3.8	-9.10846
Im-ZIF-8 (3)	3.6	3.94	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	2.278	2.278	2.278	1	1	1	ethylene	3.59	28.05	0.087	3.9	-9.60555
Im-ZIF-8 (3)	3.6	3.95	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	2.278	2.278	2.278	1	1	1	ethane	3.72	30.07	0.099	4	-10.0044
Im-ZIF-8 (3)	3.6	4.02	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	2.278	2.278	2.278	1	1	1	propylene	4.03	42.08	0.142	4.5	-10.3279
Im-ZIF-8 (3)	3.6	4.1	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	2.278	2.278	2.278	1	1	1	propane	4.16	44.1	0.152	4.3	-11.8539
Im-ZIF-8 (3)	3.6	4.11	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	2.278	2.278	2.278	1	1	1	butane	4.52	58.12	0.2	4.5	-11.2218
Im-ZIF-8 (3)	3.6	4.57	0.25	0.0627	74	4.438	4.438	4.438	81	81	81	2.278	2.278	2.278	1	1	1	iso-butane	4.8	58.12	0.183	4.42	-19.6364
Br-ZIF8-Co	3.76	3.8	0.25	0.0627	72	4.438	4.438	4.438	81	81	81	3.85	3.85	3.85	79.9	79.9	79.9	CO2	3.24	44.01	0.225	3.3	-9
Br-ZIF8-Co	3.76	3.82	0.25	0.0627	72	4.438	4.438	4.438	81	81	81	3.85	3.85	3.85	79.9	79.9	79.9	N2	3.13	28	0.037	3.64	-8.95468
Br-ZIF8-Co	3.76	3.89	0.25	0.0627	72	4.438	4.438	4.438	81	81	81	3.85	3.85	3.85	79.9	79.9	79.9	CH4	3.25	16.04	0.011	3.8	-9
Br-ZIF8-Co	3.76	3.87	0.25	0.0627	72	4.438	4.438	4.438	81	81	81	3.85	3.85	3.85	79.9	79.9	79.9	ethylene	3.59	28.05	0.087	3.9	-9.19791
Br-ZIF8-Co	3.76	3.88	0.25	0.0627	72	4.438	4.438	4.438	81	81	81	3.85	3.85	3.85	79.9	79.9	79.9	ethane	3.72	30.07	0.099	4	-9.42022
Br-ZIF8-Co	3.76	3.93	0.25	0.0627	72	4.438	4.438	4.438	81	81	81	3.85	3.85	3.85	79.9	79.9	79.9	propylene	4.03	42.08	0.142	4.5	-10.2725
Br-ZIF8-Co	3.76	3.99	0.25	0.0627	72	4.438	4.438	4.438	81	81	81	3.85	3.85	3.85	79.9	79.9	79.9	propane	4.16	44.1	0.152	4.3	-11.5086

Br-ZIF8-Co	3.76	3.99	0.25	0.0627	72	4.438	4.438	4.438	81	81	81	3.85	3.85	3.85	79.9	79.9	79.9	butane	4.52	58.12	0.2	4.5	-11.4895
Br-ZIF8-Co	3.76	4.48	0.25	0.0627	72	4.438	4.438	4.438	81	81	81	3.85	3.85	3.85	79.9	79.9	79.9	isobutane	4.8	58.12	0.183	4.42	-22.0809
Co-Br-ZIF-7-8	2.156	2.42	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	He	2.66	4.002	-0.39	2.6	-8.90658
Co-Br-ZIF-7-8	2.156	2.66	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	H2	2.76	2.01	-0.217	2.89	-9.98297
Co-Br-ZIF-7-8	2.156	2.87	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	O2	2.94	31.999	0.022	3.46	-12.6108
Co-Br-ZIF-7-8	2.156	2.88	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	CO2	3.24	44.01	0.225	3.3	-13
Co-Br-ZIF-7-8	2.156	3.06	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	N2	3.13	28	0.037	3.64	-13.8729
Co-Br-ZIF-7-8	2.156	3.36	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	CH4	3.25	16.04	0.011	3.8	-18.27
Co-Br-ZIF-7-8	2.156	3.38	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	ethylene	3.59	28.05	0.087	3.9	-18.752
Co-Br-ZIF-7-8	2.156	3.43	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	ethane	3.72	30.07	0.099	4	-19.3675
Co-Br-ZIF-7-8	2.156	3.53	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	propylene	4.03	42.08	0.142	4.5	-21.0487
Co-Br-ZIF-7-8	2.156	3.64	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	propane	4.16	44.1	0.152	4.3	-23.8928
Co-Cl-ZIF-7-8	2.120758 278	2.42	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	3.54	15	15	35.45	He	2.66	4.002	-0.39	2.6	-9.09691
Co-Cl-ZIF-7-8	2.120758 278	2.68	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	3.54	15	15	35.45	H2	2.76	2.01	-0.217	2.89	-10.5528
Co-Cl-ZIF-7-8	2.120758 278	2.89	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	3.54	15	15	35.45	O2	2.94	31.999	0.022	3.46	-13.5086
Co-Cl-ZIF-7-8	2.120758 278	2.94	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	3.54	15	15	35.45	CO2	3.24	44.01	0.225	3.3	-13.5686
Co-Cl-ZIF-7-8	2.120758 278	3.1	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	3.54	15	15	35.45	N2	3.13	28	0.037	3.64	-15.4949
Co-Cl-ZIF-7-8	2.120758 278	3.37	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	3.54	15	15	35.45	CH4	3.25	16.04	0.011	3.8	-19.7959
Co-Cl-ZIF-7-8	2.120758 278	3.38	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	3.54	15	15	35.45	ethylene	3.59	28.05	0.087	3.9	-20.2277
Co-Cl-ZIF-7-8	2.120758 278	3.42	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	3.54	15	15	35.45	ethane	3.72	30.07	0.099	4	-20.9208
Co-Cl-ZIF-7-8	2.120758 278	3.51	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	3.54	15	15	35.45	propylene	4.03	42.08	0.142	4.5	-22.5229

Co-Cl-ZIF-7-8	2.120758278	3.62	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	3.54	15	15	35.45	propane	4.16	44.1	0.152	4.3	-25.5686
tetr-ZIF8	3.81	3.84	0.325	0.7112	74	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-7.30103
tetr-ZIF8	3.81	3.83	0.325	0.7112	74	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-7.04576
tetr-ZIF8	3.81	3.85	0.325	0.7112	74	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	O2	2.94	31.999	0.022	3.46	-7.76955
tetr-ZIF8	3.81	3.81	0.325	0.7112	74	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-8.39794
tetr-ZIF8	3.81	3.86	0.325	0.7112	74	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-9
tetr-ZIF8	3.81	3.9	0.325	0.7112	74	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-8.88606
tetr-ZIF8	3.81	3.92	0.325	0.7112	74	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-8.62525
tetr-ZIF8	3.81	3.93	0.325	0.7112	74	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-8.64975
tetr-ZIF8	3.81	3.96	0.325	0.7112	74	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	propylene	4.03	42.08	0.142	4.5	-9.26122
tetr-ZIF8	3.81	3.99	0.325	0.7112	74	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	propane	4.16	44.1	0.152	4.3	-10.1707
tetr-ZIF8	3.81	3.99	0.325	0.7112	74	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	butane	4.52	58.12	0.2	4.5	-10.6655
tetr-ZIF8_Be	3.39	3.4	0.325	0.7112	41	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-7.30103
tetr-ZIF8_Be	3.39	3.41	0.325	0.7112	41	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-7.39794
tetr-ZIF8_Be	3.39	3.43	0.325	0.7112	41	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	O2	2.94	31.999	0.022	3.46	-8.19382
tetr-ZIF8_Be	3.39	3.39	0.325	0.7112	41	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-8.52288
tetr-ZIF8_Be	3.39	3.433	0.325	0.7112	41	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-8.92812
tetr-ZIF8_Be	3.39	3.503	0.325	0.7112	41	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-9.3279
tetr-ZIF8_Be	3.39	3.507	0.325	0.7112	41	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-10.567
tetr-ZIF8_Be	3.39	3.52	0.325	0.7112	41	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-11.0128
tetr-ZIF8_Be	3.39	3.56	0.325	0.7112	41	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	propylene	4.03	42.08	0.142	4.5	-12.2503
tetr-ZIF8_Be	3.39	3.6057	0.325	0.7112	41	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	propane	4.16	44.1	0.152	4.3	-14.2147
tetr-ZIF8_Be	3.39	3.602	0.325	0.7112	41	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	butane	4.52	58.12	0.2	4.5	-14.3279
tetr-ZIF8_Co	3.77	3.789	0.325	0.7112	72	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-7.33724
tetr-ZIF8_Co	3.77	3.8	0.325	0.7112	72	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-7.25964

tetr-ZIF8_Co	3.77	3.81	0.325	0.7112	72	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	O2	2.94	31.999	0.022	3.46	-7.82391
tetr-ZIF8_Co	3.77	3.77	0.325	0.7112	72	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-8.45593
tetr-ZIF8_Co	3.77	3.82	0.325	0.7112	72	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-8.95861
tetr-ZIF8_Co	3.77	3.86	0.325	0.7112	72	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-8.31876
tetr-ZIF8_Co	3.77	3.88	0.325	0.7112	72	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-8.77469
tetr-ZIF8_Co	3.77	3.88	0.325	0.7112	72	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-9.10902
tetr-ZIF8_Co	3.77	3.91	0.325	0.7112	72	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	propylene	4.03	42.08	0.142	4.5	-9.64589
tetr-ZIF8_Co	3.77	3.96	0.325	0.7112	72	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	propane	4.16	44.1	0.152	4.3	-10.5719
tetr-ZIF8_Co	3.77	3.96	0.325	0.7112	72	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	butane	4.52	58.12	0.2	4.5	-10.762
I-ZIF-7-8	2.09	2.38	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	He	2.66	4.002	-0.39	2.6	-8.1549
I-ZIF-7-8	2.09	2.63	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	H2	2.76	2.01	-0.217	2.89	-10.699
I-ZIF-7-8	2.09	2.83	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	O2	2.94	31.999	0.022	3.46	-13.0458
I-ZIF-7-8	2.09	2.86	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	CO2	3.24	44.01	0.225	3.3	-13.9136
I-ZIF-7-8	2.09	3.02	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	N2	3.13	28	0.037	3.64	-15.3757
I-ZIF-7-8	2.09	3.318	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	CH4	3.25	16.04	0.011	3.8	-18.5607
I-ZIF-7-8	2.09	3.35	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	ethylene	3.59	28.05	0.087	3.9	-19.7077
I-ZIF-7-8	2.09	3.39	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	ethane	3.72	30.07	0.099	4	-20.4989
I-ZIF-7-8	2.09	3.52	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	propylene	4.03	42.08	0.142	4.5	-22.4949
I-ZIF-7-8	2.09	3.62	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	propane	4.16	44.1	0.152	4.3	-26.6126
F-ZIF-7-8	2.175	2.57	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	He	2.66	4.002	-0.39	2.6	-10.1952
F-ZIF-7-8	2.175	2.84	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	H2	2.76	2.01	-0.217	2.89	-12.5186
F-ZIF-7-8	2.175	3.03	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	O2	2.94	31.999	0.022	3.46	-15.8539
F-ZIF-7-8	2.175	3.09	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	CO2	3.24	44.01	0.225	3.3	-15.2366
F-ZIF-7-8	2.175	3.2178	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	N2	3.13	28	0.037	3.64	-17.6576
F-ZIF-7-8	2.175	3.46	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	CH4	3.25	16.04	0.011	3.8	-24.6498
F-ZIF-7-8	2.175	3.46	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	ethylene	3.59	28.05	0.087	3.9	-23.6498
F-ZIF-7-8	2.175	3.48	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	ethane	3.72	30.07	0.099	4	-24.6882
F-ZIF-7-8	2.175	3.5	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	propylene	4.03	42.08	0.142	4.5	-27.1367
F-ZIF-7-8	2.175	3.65	0.25	0.0627	74	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	propane	4.16	44.1	0.152	4.3	-30.699

Co-F-ZIF-7-8	2.185	2.55	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	He	2.66	4.002	-0.39	2.6	-9.55284
Co-F-ZIF-7-8	2.185	2.85	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	H2	2.76	2.01	-0.217	2.89	-11.8416
Co-F-ZIF-7-8	2.185	3.09	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	O2	2.94	31.999	0.022	3.46	-14.7773
Co-F-ZIF-7-8	2.185	3.14	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	CO2	3.24	44.01	0.225	3.3	-14.6162
Co-F-ZIF-7-8	2.185	3.31	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	N2	3.13	28	0.037	3.64	-17.2218
Co-F-ZIF-7-8	2.185	3.58	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	CH4	3.25	16.04	0.011	3.8	-21.3401
Co-F-ZIF-7-8	2.185	3.58	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	ethylene	3.59	28.05	0.087	3.9	-22.3325
Co-F-ZIF-7-8	2.185	3.6	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	ethane	3.72	30.07	0.099	4	-23.4202
Co-F-ZIF-7-8	2.185	3.66	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	propylene	4.03	42.08	0.142	4.5	-25.983
Co-F-ZIF-7-8	2.185	3.67	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	propane	4.16	44.1	0.152	4.3	-28.5031
Be-F-ZIF-7-8	2.048	2.4	0.25	0.0627	41	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	He	2.66	4.002	-0.39	2.6	-10.762
Be-F-ZIF-7-8	2.048	2.698	0.25	0.0627	41	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	H2	2.76	2.01	-0.217	2.89	-14.4089
Be-F-ZIF-7-8	2.048	2.914	0.25	0.0627	41	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	O2	2.94	31.999	0.022	3.46	-14.0044
Be-F-ZIF-7-8	2.048	2.924	0.25	0.0627	41	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	CO2	3.24	44.01	0.225	3.3	-19.3979
Be-F-ZIF-7-8	2.048	3.094	0.25	0.0627	41	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	N2	3.13	28	0.037	3.64	-23.7328
Be-F-ZIF-7-8	2.048	3.39	0.25	0.0627	41	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	CH4	3.25	16.04	0.011	3.8	-30.556
Be-F-ZIF-7-8	2.048	3.258	0.25	0.0627	41	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	ethylene	3.59	28.05	0.087	3.9	-34.279
Be-F-ZIF-7-8	2.048	3.271	0.25	0.0627	41	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	ethane	3.72	30.07	0.099	4	-35.7328
Be-F-ZIF-7-8	2.048	3.41	0.25	0.0627	41	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	propylene	4.03	42.08	0.142	4.5	-43.4685
Be-F-ZIF-7-8	2.048	3.48	0.25	0.0627	41	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	propane	4.16	44.1	0.152	4.3	-45.4559
Cu-ZIF-7-8	2.1214	2.47	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	He	2.66	4.002	-0.39	2.6	-9.5376

Cu-ZIF-7-8	2.1214	2.73	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	H2	2.76	2.01	-0.217	2.89	-11.4001
Cu-ZIF-7-8	2.1214	2.96	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	O2	2.94	31.999	0.022	3.46	-13.9508
Cu-ZIF-7-8	2.1214	2.99	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	CO2	3.24	44.01	0.225	3.3	-14.6576
Cu-ZIF-7-8	2.1214	3.148	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	N2	3.13	28	0.037	3.64	-16.4559
Cu-ZIF-7-8	2.1214	3.39	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	CH4	3.25	16.04	0.011	3.8	-20.3468
Cu-ZIF-7-8	2.1214	3.4	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	ethylene	3.59	28.05	0.087	3.9	-21.6676
Cu-ZIF-7-8	2.1214	3.38	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	ethane	3.72	30.07	0.099	4	-23.0386
Cu-ZIF-7-8	2.1214	3.49	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	propylene	4.03	42.08	0.142	4.5	-25.1079
Cu-ZIF-7-8	2.1214	3.53	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	propane	4.16	44.1	0.152	4.3	-26.8239
Cu-F-ZIF-7-8	2.1248	2.4	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	He	2.66	4.002	-0.39	2.6	-9.92082
Cu-F-ZIF-7-8	2.1248	2.7	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	H2	2.76	2.01	-0.217	2.89	-11.71
Cu-F-ZIF-7-8	2.1248	2.9	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	O2	2.94	31.999	0.022	3.46	-15.5258
Cu-F-ZIF-7-8	2.1248	2.96	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	CO2	3.24	44.01	0.225	3.3	-15.9586
Cu-F-ZIF-7-8	2.1248	3.09	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	N2	3.13	28	0.037	3.64	-17.757
Cu-F-ZIF-7-8	2.1248	3.277	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	CH4	3.25	16.04	0.011	3.8	-23.0555
Cu-F-ZIF-7-8	2.1248	3.28	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	ethylene	3.59	28.05	0.087	3.9	-24.2211
Cu-F-ZIF-7-8	2.1248	3.29	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	ethane	3.72	30.07	0.099	4	-24.8761
Cu-F-ZIF-7-8	2.1248	3.35	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	propylene	4.03	42.08	0.142	4.5	-27.5129
Cu-F-ZIF-7-8	2.1248	3.39	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	2.7	15	15	18.99	propane	4.16	44.1	0.152	4.3	-30.2472
Cu-Cl-ZIF-7-8	2.08	2.85	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	3.54	15	15	35.453	CO2	3.24	44.01	0.225	3.3	-14.9208
Cu-Cl-ZIF-7-8	2.08	3.24	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	3.54	15	15	35.453	CH4	3.25	16.04	0.011	3.8	-20.2757

Cd-I-ZIF-7-8	2.2	2.746	0.25	0.0627	92	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	H2	2.76	2.01	-0.217	2.89	-10
Cd-I-ZIF-7-8	2.2	2.98	0.25	0.0627	92	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	O2	2.94	31.999	0.022	3.46	-11.9066
Cd-I-ZIF-7-8	2.2	3.005	0.25	0.0627	92	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	CO2	3.24	44.01	0.225	3.3	-12.2628
Cd-I-ZIF-7-8	2.2	3.17	0.25	0.0627	92	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	N2	3.13	28	0.037	3.64	-13.6091
Cd-I-ZIF-7-8	2.2	3.44	0.25	0.0627	92	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	CH4	3.25	16.04	0.011	3.8	-16.1798
Cd-I-ZIF-7-8	2.2	3.48	0.25	0.0627	92	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	ethylene	3.59	28.05	0.087	3.9	-16.2366
Cd-I-ZIF-7-8	2.2	3.53	0.25	0.0627	92	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	ethane	3.72	30.07	0.099	4	-18
Cd-I-ZIF-7-8	2.2	3.65	0.25	0.0627	92	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	propylene	4.03	42.08	0.142	4.5	-18.5528
Co-I-ZIF-7-8	2.11	2.38	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	He	2.66	4.002	-0.39	2.6	-10.2255
Co-I-ZIF-7-8	2.11	2.61	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	H2	2.76	2.01	-0.217	2.89	-10.7696
Co-I-ZIF-7-8	2.11	2.85	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	O2	2.94	31.999	0.022	3.46	-13.2503
Co-I-ZIF-7-8	2.11	2.87	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	CO2	3.24	44.01	0.225	3.3	-13.699
Co-I-ZIF-7-8	2.11	3.03	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	N2	3.13	28	0.037	3.64	-14.7747
Co-I-ZIF-7-8	2.11	3.327	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	CH4	3.25	16.04	0.011	3.8	-18.7352
Co-I-ZIF-7-8	2.11	3.36	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	ethylene	3.59	28.05	0.087	3.9	-19.1308
Co-I-ZIF-7-8	2.11	3.4	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	ethane	3.72	30.07	0.099	4	-20.0862
Co-I-ZIF-7-8	2.11	3.53	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	propylene	4.03	42.08	0.142	4.5	-22.9586
Co-I-ZIF-7-8	2.11	3.61	0.25	0.0627	72	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	propane	4.16	44.1	0.152	4.3	-25.7696
NH2-tetrz	3.36	3.37981	0.325	0.7112	74	3.66	3.66	3.66	83	83	83	3.927	3.927	3.927	16	16	16	He	2.66	4.002	-0.39	2.6	-7.39794
NH2-tetrz	3.36	3.39125	0.325	0.7112	74	3.66	3.66	3.66	83	83	83	3.927	3.927	3.927	16	16	16	H2	2.76	2.01	-0.217	2.89	-7.39794
NH2-tetrz	3.36	3.38	0.325	0.7112	74	3.66	3.66	3.66	83	83	83	3.927	3.927	3.927	16	16	16	CO2	3.24	44.01	0.225	3.3	-8.69897
NH2-tetrz	3.36	3.43	0.325	0.7112	74	3.66	3.66	3.66	83	83	83	3.927	3.927	3.927	16	16	16	N2	3.13	28	0.037	3.64	-8.55284
NH2-tetrz	3.36	3.51	0.325	0.7112	74	3.66	3.66	3.66	83	83	83	3.927	3.927	3.927	16	16	16	CH4	3.25	16.04	0.011	3.8	-9.39794

NH2-tetrz	3.36	3.52	0.325	0.7112	74	3.66	3.66	3.66	83	83	83	3.927	3.927	3.927	16	16	16	ethylene	3.59	28.05	0.087	3.9	-10.3979
NH2-tetrz	3.36	3.53	0.325	0.7112	74	3.66	3.66	3.66	83	83	83	3.927	3.927	3.927	16	16	16	ethane	3.72	30.07	0.099	4	-10.4921
NH2-tetrz	3.36	3.57	0.325	0.7112	74	3.66	3.66	3.66	83	83	83	3.927	3.927	3.927	16	16	16	propylene	4.03	42.08	0.142	4.5	-11.0825
NH2-tetrz	3.36	3.63	0.325	0.7112	74	3.66	3.66	3.66	83	83	83	3.927	3.927	3.927	16	16	16	propane	4.16	44.1	0.152	4.3	-12.71
NH2-tetrz	3.36	3.63	0.325	0.7112	74	3.66	3.66	3.66	83	83	83	3.927	3.927	3.927	16	16	16	butane	4.52	58.12	0.2	4.5	-12.7696
NH2_tetr z_Be	3.022	3.035	0.325	0.7112	41	3.66	3.66	3.66	83	83	83	3.927	3.927	3.927	16	16	16	He	2.66	4.002	-0.39	2.6	-7.63827
NH2_tetr z_Be	3.022	3.053	0.325	0.7112	41	3.66	3.66	3.66	83	83	83	3.927	3.927	3.927	16	16	16	H2	2.76	2.01	-0.217	2.89	-7.85387
NH2_tetr z_Be	3.022	3.075	0.325	0.7112	41	3.66	3.66	3.66	83	83	83	3.927	3.927	3.927	16	16	16	O2	2.94	31.999	0.022	3.46	-9.1549
NH2_tetr z_Be	3.022	3.044	0.325	0.7112	41	3.66	3.66	3.66	83	83	83	3.927	3.927	3.927	16	16	16	CO2	3.24	44.01	0.225	3.3	-10
NH2_tetr z_Be	3.022	3.096	0.325	0.7112	41	3.66	3.66	3.66	83	83	83	3.927	3.927	3.927	16	16	16	N2	3.13	28	0.037	3.64	-9.79588
NH2_tetr z_Be	3.022	3.1968	0.325	0.7112	41	3.66	3.66	3.66	83	83	83	3.927	3.927	3.927	16	16	16	CH4	3.25	16.04	0.011	3.8	-12.5935
NH2_tetr z_Be	3.022	3.2	0.325	0.7112	41	3.66	3.66	3.66	83	83	83	3.927	3.927	3.927	16	16	16	ethylene	3.59	28.05	0.087	3.9	-13.5719
NH2_tetr z_Be	3.022	3.21	0.325	0.7112	41	3.66	3.66	3.66	83	83	83	3.927	3.927	3.927	16	16	16	ethane	3.72	30.07	0.099	4	-13.9031
NH2_tetr z_Be	3.022	3.26	0.325	0.7112	41	3.66	3.66	3.66	83	83	83	3.927	3.927	3.927	16	16	16	propylene	4.03	42.08	0.142	4.5	-15.9547
NH2_tetr z_Be	3.022	3.31	0.325	0.7112	41	3.66	3.66	3.66	83	83	83	3.927	3.927	3.927	16	16	16	propane	4.16	44.1	0.152	4.3	-18.4089
NH2_tetr z_Be	3.022	3.31	0.325	0.7112	41	3.66	3.66	3.66	83	83	83	3.927	3.927	3.927	16	16	16	butane	4.52	58.12	0.2	4.5	-18.8539
NH2- tetrz_Co	3.57	3.57913	0.325	0.7112	72	3.66	3.66	3.66	83	83	83	3.927	3.927	3.927	16	16	16	He	2.66	4.002	-0.39	2.6	-7.39794
NH2- tetrz_Co	3.57	3.58743	0.325	0.7112	72	3.66	3.66	3.66	83	83	83	3.927	3.927	3.927	16	16	16	H2	2.76	2.01	-0.217	2.89	-7.39794
NH2- tetrz_Co	3.57	3.60014	0.325	0.7112	72	3.66	3.66	3.66	83	83	83	3.927	3.927	3.927	16	16	16	O2	2.94	31.999	0.022	3.46	-8.04576
NH2- tetrz_Co	3.57	3.57372	0.325	0.7112	72	3.66	3.66	3.66	83	83	83	3.927	3.927	3.927	16	16	16	CO2	3.24	44.01	0.225	3.3	-8.04576
NH2- tetrz_Co	3.57	3.61001	0.325	0.7112	72	3.66	3.66	3.66	83	83	83	3.927	3.927	3.927	16	16	16	N2	3.13	28	0.037	3.64	-10
NH2- tetrz_Co	3.57	3.64852	0.325	0.7112	72	3.66	3.66	3.66	83	83	83	3.927	3.927	3.927	16	16	16	CH4	3.25	16.04	0.011	3.8	-8.69897
NH2- tetrz_Co	3.57	3.65904	0.325	0.7112	72	3.66	3.66	3.66	83	83	83	3.927	3.927	3.927	16	16	16	ethylene	3.59	28.05	0.087	3.9	-9.09691

NH2-tetrz_Co	3.57	3.66677	0.325	0.7112	72	3.66	3.66	3.66	83	83	83	3.927	3.927	3.927	16	16	16	ethane	3.72	30.07	0.099	4	-9.30103
NH2-tetrz_Co	3.57	3.69374	0.325	0.7112	72	3.66	3.66	3.66	83	83	83	3.927	3.927	3.927	16	16	16	propylene	4.03	42.08	0.142	4.5	-9.85387
NH2-tetrz_Co	3.57	3.73719	0.325	0.7112	72	3.66	3.66	3.66	83	83	83	3.927	3.927	3.927	16	16	16	propane	4.16	44.1	0.152	4.3	-10.8239
dClm_Zn	2.99	3.01	0.34	1.2552	74	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-7.31876
dClm_Zn	2.99	3.02	0.34	1.2552	74	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-7.72125
dClm_Zn	2.99	3.05	0.34	1.2552	74	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	O2	2.94	31.999	0.022	3.46	-9.36653
dClm_Zn	2.99	3.02	0.34	1.2552	74	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-8.74473
dClm_Zn	2.99	3.07	0.34	1.2552	74	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-9.95861
dClm_Zn	2.99	3.17	0.34	1.2552	74	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-12.0088
dClm_Zn	2.99	3.17	0.34	1.2552	74	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-12.699
dClm_Zn	2.99	3.19	0.34	1.2552	74	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-13.1487
dClm_Zn	2.99	3.24	0.34	1.2552	74	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	propylene	4.03	42.08	0.142	4.5	-15.1871
dClm_Zn	2.99	3.3	0.34	1.2552	74	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	propane	4.16	44.1	0.152	4.3	-19.0969
dClm_Co	2.94	2.95	0.34	1.2552	72	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-7.49485
dClm_Co	2.94	2.96	0.34	1.2552	72	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-7.82391
dClm_Co	2.94	2.98	0.34	1.2552	72	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	O2	2.94	31.999	0.022	3.46	-9.4318
dClm_Co	2.94	2.96	0.34	1.2552	72	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-8.83863
dClm_Co	2.94	3.01	0.34	1.2552	72	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-10.301
dClm_Co	2.94	3.11	0.34	1.2552	72	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-12.699
dClm_Co	2.94	3.11	0.34	1.2552	72	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-13
dClm_Co	2.94	3.13	0.34	1.2552	72	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-13.9208
dClm_Co	2.94	3.18	0.34	1.2552	72	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	propylene	4.03	42.08	0.142	4.5	-15.699
dClm_Co	2.94	3.23	0.34	1.2552	72	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	propane	4.16	44.1	0.152	4.3	-20.585
dClm_Be	2.79278	2.8	0.34	1.2552	41	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-7.52288
dClm_Be	2.79278	2.82	0.34	1.2552	41	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-8.04576
dClm_Be	2.79278	2.84	0.34	1.2552	41	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	O2	2.94	31.999	0.022	3.46	-9.85387
dClm_Be	2.79278	2.82	0.34	1.2552	41	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-9.30103
dClm_Be	2.79278	2.87	0.34	1.2552	41	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-10.9208
dClm_Be	2.79278	2.98	0.34	1.2552	41	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-16.2218
dClm_Be	2.79278	2.98	0.34	1.2552	41	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-16.6576
dClm_Be	2.79278	2.99	0.34	1.2552	41	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-17.5686
dClm_Be	2.79278	3.05	0.34	1.2552	41	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	propylene	4.03	42.08	0.142	4.5	-20.7399
dClm_Cd	3.12	3.13	0.34	1.2552	92	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-7.34199

dClm_Cd	3.12	3.144	0.34	1.2552	92	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-7.65758
dClm_Cd	3.12	3.17	0.34	1.2552	92	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	O2	2.94	31.999	0.022	3.46	-9.02228
dClm_Cd	3.12	3.14	0.34	1.2552	92	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-8.69897
dClm_Cd	3.12	3.2	0.34	1.2552	92	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-9.55284
dClm_Cd	3.12	3.29	0.34	1.2552	92	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-10.3979
dClm_Cd	3.12	3.29	0.34	1.2552	92	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-12.5622
dClm_Cd	3.12	3.3	0.34	1.2552	92	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-13.1238
dClm_Cd	3.12	3.36	0.34	1.2552	92	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	propylene	4.03	42.08	0.142	4.5	-14.8069
dClm_Cd	3.12	3.42	0.34	1.2552	92	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	propane	4.16	44.1	0.152	4.3	-15.9208
dClm_Mg	3.02	3.03261	0.34	1.2552	71	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-7.52288
dClm_Mg	3.02	3.04558	0.34	1.2552	71	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-7.69897
dClm_Mg	3.02	3.06858	0.34	1.2552	71	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	O2	2.94	31.999	0.022	3.46	-8.34679
dClm_Mg	3.02	3.0425	0.34	1.2552	71	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-8.69897
dClm_Mg	3.02	3.09184	0.34	1.2552	71	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-10.0088
dClm_Mg	3.02	3.18925	0.34	1.2552	71	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-11.3979
dClm_Mg	3.02	3.19323	0.34	1.2552	71	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-13.5686
dClm_Mg	3.02	3.209	0.34	1.2552	71	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-14.1469
dClm_Mg	3.02	3.26248	0.34	1.2552	71	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	propylene	4.03	42.08	0.142	4.5	-16.0362
dClm_Mg	3.02	3.32219	0.34	1.2552	71	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	propane	4.16	44.1	0.152	4.3	-18.1549
Be-I-ZIF-7-8	1.96	2.51	0.25	0.0627	41	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	H2	2.76	2.01	-0.217	2.89	-12.301
Be-I-ZIF-7-8	1.96	2.72	0.25	0.0627	41	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	O2	2.94	31.999	0.022	3.46	-16.1549
Be-I-ZIF-7-8	1.96	2.74	0.25	0.0627	41	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	CO2	3.24	44.01	0.225	3.3	-16.4191
Be-I-ZIF-7-8	1.96	2.9	0.25	0.0627	41	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	N2	3.13	28	0.037	3.64	-19.3439
Be-I-ZIF-7-8	1.96	3.22	0.25	0.0627	41	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	CH4	3.25	16.04	0.011	3.8	-24.7122
Be-I-ZIF-7-8	1.96	3.246	0.25	0.0627	41	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	ethylene	3.59	28.05	0.087	3.9	-25.7144
Be-I-ZIF-7-8	1.96	3.3	0.25	0.0627	41	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	ethane	3.72	30.07	0.099	4	-27.1062
Be-I-ZIF-7-8	1.96	3.42	0.25	0.0627	41	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	propylene	4.03	42.08	0.142	4.5	-30.6383
Be-I-ZIF-7-8	1.96	3.497	0.25	0.0627	41	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	propane	4.16	44.1	0.152	4.3	-35.3251
CHO_Zn	3.81	3.80095	0.25	0.0627	71	4.438	4.438	4.438	81	81	81	4.093	4.093	4.093	31	31	31	He	2.66	4.002	-0.39	2.6	-7.22185

CHO_Zn	3.81	3.80505	0.25	0.0627	71	4.438	4.438	4.438	81	81	81	4.093	4.093	4.093	31	31	31	H2	2.76	2.01	-0.217	2.89	-7.39794
CHO_Zn	3.81	3.83978	0.25	0.0627	71	4.438	4.438	4.438	81	81	81	4.093	4.093	4.093	31	31	31	O2	2.94	31.999	0.022	3.46	-8
CHO_Zn	3.81	3.87196	0.25	0.0627	71	4.438	4.438	4.438	81	81	81	4.093	4.093	4.093	31	31	31	CO2	3.24	44.01	0.225	3.3	-8.72125
CHO_Zn	3.81	3.88193	0.25	0.0627	71	4.438	4.438	4.438	81	81	81	4.093	4.093	4.093	31	31	31	N2	3.13	28	0.037	3.64	-8.35655
CHO_Zn	3.81	3.88193	0.25	0.0627	71	4.438	4.438	4.438	81	81	81	4.093	4.093	4.093	31	31	31	CH4	3.25	16.04	0.011	3.8	-8.22915
CHO_Zn	3.81	3.90142	0.25	0.0627	71	4.438	4.438	4.438	81	81	81	4.093	4.093	4.093	31	31	31	ethylene	3.59	28.05	0.087	3.9	-9
CHO_Zn	3.81	3.91	0.25	0.0627	71	4.438	4.438	4.438	81	81	81	4.093	4.093	4.093	31	31	31	ethane	3.72	30.07	0.099	4	-9.48413
CHO_Zn	3.81	3.95	0.25	0.0627	71	4.438	4.438	4.438	81	81	81	4.093	4.093	4.093	31	31	31	propylene	4.03	42.08	0.142	4.5	-10.1549
CHO_Zn	3.81	4.008	0.25	0.0627	71	4.438	4.438	4.438	81	81	81	4.093	4.093	4.093	31	31	31	propane	4.16	44.1	0.152	4.3	-11.2848
tetr-ZIF8_Cu	3.6	3.61166	0.325	0.7112	71	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-7.30103
tetr-ZIF8_Cu	3.6	3.62196	0.325	0.7112	71	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-7.30103
tetr-ZIF8_Cu	3.6	3.63791	0.325	0.7112	71	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	O2	2.94	31.999	0.022	3.46	-8
tetr-ZIF8_Cu	3.6	3.59472	0.325	0.7112	71	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-8.60206
tetr-ZIF8_Cu	3.6	3.65091	0.325	0.7112	71	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-8.74473
tetr-ZIF8_Cu	3.6	3.7	0.325	0.7112	71	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-8.52288
tetr-ZIF8_Cu	3.6	3.718	0.325	0.7112	71	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-9.57025
tetr-ZIF8_Cu	3.6	3.72	0.325	0.7112	71	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-9.7986
tetr-ZIF8_Cu	3.6	3.76	0.325	0.7112	71	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	propylene	4.03	42.08	0.142	4.5	-10.8729
tetr-ZIF8_Cu	3.6	3.81	0.325	0.7112	71	3.66	3.66	3.66	83	83	83	3.78	3.78	3.78	15	15	15	propane	4.16	44.1	0.152	4.3	-12.1713
dClm_Cu	2.98	2.99566	0.34	1.2552	71	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-7.4437
dClm_Cu	2.98	3.00789	0.34	1.2552	71	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-7.58503
dClm_Cu	2.98	3.03031	0.34	1.2552	71	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	O2	2.94	31.999	0.022	3.46	-9.20761
dClm_Cu	2.98	3.00852	0.34	1.2552	71	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-8.69897
dClm_Cu	2.98	3.05694	0.34	1.2552	71	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-10
dClm_Cu	2.98	3.15134	0.34	1.2552	71	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-13.0809
dClm_Cu	2.98	3.15391	0.34	1.2552	71	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-13.4112
dClm_Cu	2.98	3.17166	0.34	1.2552	71	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-14.1688
dClm_Cu	2.98	3.22101	0.34	1.2552	71	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	propylene	4.03	42.08	0.142	4.5	-15.699

dClm_Cu	2.98	3.27701	0.34	1.2552	71	5.7	5.7	5.7	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	propane	4.16	44.1	0.152	4.3	-19.5229
dFm_Zn	3.32	3.41	0.285	0.255	74	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-7.36653
dFm_Zn	3.32	3.43	0.285	0.255	74	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-7.74473
dFm_Zn	3.32	3.47	0.285	0.255	74	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	O2	2.94	31.999	0.022	3.46	-8.56703
dFm_Zn	3.32	3.4	0.285	0.255	74	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-8.85387
dFm_Zn	3.32	3.5	0.285	0.255	74	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-8.88606
dFm_Zn	3.32	3.63	0.285	0.255	74	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-10.2218
dFm_Zn	3.32	3.64	0.285	0.255	74	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-10.699
dFm_Zn	3.32	3.65	0.285	0.255	74	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-11
dFm_Zn	3.32	3.8	0.285	0.255	74	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	propane	4.16	44.1	0.152	4.3	-14.1549
dBrm_Zn	3.437	3.44314	0.4	1.8731	74	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-7.48545
dBrm_Zn	3.437	3.45257	0.4	1.8731	74	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-7.60206
dBrm_Zn	3.437	3.47006	0.4	1.8731	74	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	O2	2.94	31.999	0.022	3.46	-9.39794
dBrm_Zn	3.437	3.45387	0.4	1.8731	74	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-9.284
dBrm_Zn	3.437	3.48695	0.4	1.8731	74	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-10.2366
dBrm_Zn	3.437	3.5512	0.4	1.8731	74	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-11.1549
dBrm_Zn	3.437	3.56103	0.4	1.8731	74	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-14.1215
dBrm_Zn	3.437	3.57348	0.4	1.8731	74	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-14.5346
dBrm_Zn	3.437	3.61546	0.4	1.8731	74	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	propylene	4.03	42.08	0.142	4.5	-15.8327
dBrm_Zn	3.437	3.66077	0.4	1.8731	74	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	propane	4.16	44.1	0.152	4.3	-18.7375
dIm_Zn	2.9	2.91908	0.367	2.4267	74	6.41	6.41	6.41	317.8	317.8	317.8	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-7.4318
dIm_Zn	2.9	2.92823	0.367	2.4267	74	6.41	6.41	6.41	317.8	317.8	317.8	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-7.63827
dIm_Zn	2.9	2.94368	0.367	2.4267	74	6.41	6.41	6.41	317.8	317.8	317.8	3.78	3.78	3.78	15	15	15	O2	2.94	31.999	0.022	3.46	-9
dIm_Zn	2.9	2.92	0.367	2.4267	74	6.41	6.41	6.41	317.8	317.8	317.8	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-9.16749
dIm_Zn	2.9	2.9654	0.367	2.4267	74	6.41	6.41	6.41	317.8	317.8	317.8	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-9.72125
dIm_Zn	2.9	3.03585	0.367	2.4267	74	6.41	6.41	6.41	317.8	317.8	317.8	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-12.4949
dIm_Zn	2.9	3.04297	0.367	2.4267	74	6.41	6.41	6.41	317.8	317.8	317.8	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-12.7122
dIm_Zn	2.9	3.05554	0.367	2.4267	74	6.41	6.41	6.41	317.8	317.8	317.8	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-13.1778
dIm_Zn	2.9	3.10287	0.367	2.4267	74	6.41	6.41	6.41	317.8	317.8	317.8	3.78	3.78	3.78	15	15	15	propylene	4.03	42.08	0.142	4.5	-13.3279
dIm_Zn	2.9	3.15286	0.367	2.4267	74	6.41	6.41	6.41	317.8	317.8	317.8	3.78	3.78	3.78	15	15	15	propane	4.16	44.1	0.152	4.3	-15.4437
Cu-Br-zif-7-8	2.12	2.38	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	He	2.66	4.002	-0.39	2.6	-8.92082
Cu-Br-zif-7-8	2.12	2.6	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	H2	2.76	2.01	-0.217	2.89	-10.3979
Cu-Br-zif-7-8	2.12	2.8	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	O2	2.94	31.999	0.022	3.46	-12.7447

Cu-Br-zif-7-8	2.12	2.85	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	CO2	3.24	44.01	0.225	3.3	-13.6778
Cu-Br-zif-7-8	2.12	2.99	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	N2	3.13	28	0.037	3.64	-14.4318
Cu-Br-zif-7-8	2.12	3.29	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	CH4	3.25	16.04	0.011	3.8	-17.8601
Cu-Br-zif-7-8	2.12	3.32	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	ethylene	3.59	28.05	0.087	3.9	-19.2262
Cu-Br-zif-7-8	2.12	3.35	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	ethane	3.72	30.07	0.099	4	-20.2218
Cu-Br-zif-7-8	2.12	3.48	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	propylene	4.03	42.08	0.142	4.5	-22.9355
Cu-Br-zif-7-8	2.12	3.57	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	propane	4.16	44.1	0.152	4.3	-25.1391
Cu-I-zif-7-8	2.1227	2.344	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	127	He	2.66	4.002	-0.39	2.6	-9
Cu-I-zif-7-8	2.1227	2.58	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	127	H2	2.76	2.01	-0.217	2.89	-10.7447
Cu-I-zif-7-8	2.1227	2.8	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	127	O2	2.94	31.999	0.022	3.46	-13.4559
Cu-I-zif-7-8	2.1227	2.82	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	127	CO2	3.24	44.01	0.225	3.3	-13.6345
Cu-I-zif-7-8	2.1227	2.97	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	127	N2	3.13	28	0.037	3.64	-15.3615
Cu-I-zif-7-8	2.1227	3.25	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	127	CH4	3.25	16.04	0.011	3.8	-18.8268
Cu-I-zif-7-8	2.1227	3.29	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	127	ethylene	3.59	28.05	0.087	3.9	-20.0625
Cu-I-zif-7-8	2.1227	3.33	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	127	ethane	3.72	30.07	0.099	4	-20.6234
Cu-I-zif-7-8	2.1227	3.46	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	127	propylene	4.03	42.08	0.142	4.5	-22.618
Cu-I-zif-7-8	2.1227	3.55	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	127	propane	4.16	44.1	0.152	4.3	-26.2549
Mg-zif-7-8	2.4328	2.75	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	He	2.66	4.002	-0.39	2.6	-8.30103
Mg-zif-7-8	2.4328	2.99	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	H2	2.76	2.01	-0.217	2.89	-9
Mg-zif-7-8	2.4328	3.21	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	O2	2.94	31.999	0.022	3.46	-11.7645
Mg-zif-7-8	2.4328	3.23	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	CO2	3.24	44.01	0.225	3.3	-11.5229

Mg-zif-7-8	2.4328	3.39	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	N2	3.13	28	0.037	3.64	-13.0701
Mg-zif-7-8	2.4328	3.62	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	CH4	3.25	16.04	0.011	3.8	-14.8447
Mg-zif-7-8	2.4328	3.65	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	ethylene	3.59	28.05	0.087	3.9	-16.0555
Mg-zif-7-8	2.4328	3.7	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	ethane	3.72	30.07	0.099	4	-16.6271
Mg-zif-7-8	2.4328	3.7	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	propylene	4.03	42.08	0.142	4.5	-18.7122
Mg-zif-7-8	2.4328	3.7	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	propane	4.16	44.1	0.152	4.3	-19.3161
Mg-Br-zif-7-8	2.35	2.59	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	He	2.66	4.002	-0.39	2.6	-8.52288
Mg-Br-zif-7-8	2.35	2.8	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	H2	2.76	2.01	-0.217	2.89	-9.1549
Mg-Br-zif-7-8	2.35	3	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	O2	2.94	31.999	0.022	3.46	-10.7696
Mg-Br-zif-7-8	2.35	3	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	CO2	3.24	44.01	0.225	3.3	-11.0809
Mg-Br-zif-7-8	2.35	3.17	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	N2	3.13	28	0.037	3.64	-12.2328
Mg-Br-zif-7-8	2.35	3.42	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	CH4	3.25	16.04	0.011	3.8	-13.4498
Mg-Br-zif-7-8	2.35	3.45	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	ethylene	3.59	28.05	0.087	3.9	-14.2958
Mg-Br-zif-7-8	2.35	3.49	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	ethane	3.72	30.07	0.099	4	-14.8601
Mg-Br-zif-7-8	2.35	3.5	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	propylene	4.03	42.08	0.142	4.5	-15.8041
Mg-Br-zif-7-8	2.35	3.55	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	propane	4.16	44.1	0.152	4.3	-16.6126
Mg-I-zif-7-8	2.3	2.56	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	He	2.66	4.002	-0.39	2.6	-8.34679
Mg-I-zif-7-8	2.3	2.78	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	H2	2.76	2.01	-0.217	2.89	-9.16749
Mg-I-zif-7-8	2.3	3	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	CO2	3.24	44.01	0.225	3.3	-11.0835
Mg-I-zif-7-8	2.3	3.16	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	N2	3.13	28	0.037	3.64	-12.7167
Mg-I-zif-7-8	2.3	3.42	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	CH4	3.25	16.04	0.011	3.8	-14.1068

Mg-I-zif-7-8	2.3	3.46	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	ethylene	3.59	28.05	0.087	3.9	-14.6234
Mg-I-zif-7-8	2.3	3.5	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	ethane	3.72	30.07	0.099	4	-15.2518
Mg-I-zif-7-8	2.3	3.53	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	propylene	4.03	42.08	0.142	4.5	-16.7959
Mg-I-zif-7-8	2.3	3.67	0.25	0.0627	71	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	propane	4.16	44.1	0.152	4.3	-16.9586
Mn-zif-7-8	2.456	2.78	0.25	0.0627	80	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	He	2.66	4.002	-0.39	2.6	-8.22185
Mn-zif-7-8	2.456	3.29	0.25	0.0627	80	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	CO2	3.24	44.01	0.225	3.3	-11.699
Mn-zif-7-8	2.456	3.65	0.25	0.0627	80	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	CH4	3.25	16.04	0.011	3.8	-13.7905
Mn-zif-7-8	2.456	3.73	0.25	0.0627	80	4.438	4.438	5.996	81	81	117	3.78	3.78	2.278	15	15	1	propane	4.16	44.1	0.152	4.3	-17.6459
Mn-Br-zif-7-8	2.463	2.68	0.25	0.0627	80	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	He	2.66	4.002	-0.39	2.6	-8.09691
Mn-Br-zif-7-8	2.463	2.82	0.25	0.0627	80	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	H2	2.76	2.01	-0.217	2.89	-8.69897
Mn-Br-zif-7-8	2.463	3.06	0.25	0.0627	80	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	O2	2.94	31.999	0.022	3.46	-10.7696
Mn-Br-zif-7-8	2.463	3.09	0.25	0.0627	80	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	CO2	3.24	44.01	0.225	3.3	-10.699
Mn-Br-zif-7-8	2.463	3.45	0.25	0.0627	80	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	CH4	3.25	16.04	0.011	3.8	-12.3439
Mn-Br-zif-7-8	2.463	3.57	0.25	0.0627	80	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	propylene	4.03	42.08	0.142	4.5	-14.3116
Mn-Br-zif-7-8	2.463	3.71	0.25	0.0627	80	4.438	4.438	5.996	81	81	117	3.78	3.78	3.85	15	15	79.9	propane	4.16	44.1	0.152	4.3	-15.3872
Mn-I-zif-7-8	2.387	2.63	0.25	0.0627	80	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	He	2.66	4.002	-0.39	2.6	-8.30103
Mn-I-zif-7-8	2.387	2.82	0.25	0.0627	80	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	H2	2.76	2.01	-0.217	2.89	-9.88606
Mn-I-zif-7-8	2.387	3.03	0.25	0.0627	80	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	O2	2.94	31.999	0.022	3.46	-10.7235
Mn-I-zif-7-8	2.387	3.07	0.25	0.0627	80	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	CO2	3.24	44.01	0.225	3.3	-11.063
Mn-I-zif-7-8	2.387	3.42	0.25	0.0627	80	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	CH4	3.25	16.04	0.011	3.8	-13.1945
Mn-I-zif-7-8	2.387	3.55	0.25	0.0627	80	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	propylene	4.03	42.08	0.142	4.5	-15.1349

Mn-I-zif-7-8	2.387	3.71	0.25	0.0627	80	4.438	4.438	5.996	81	81	117	3.78	3.78	4.25	15	15	126.9	propane	4.16	44.1	0.152	4.3	-16.3665
dBrm_Be	3.306	3.3128	0.4	1.8731	41	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-8.39794
dBrm_Be	3.306	3.32389	0.4	1.8731	41	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-8.89279
dBrm_Be	3.306	3.34171	0.4	1.8731	41	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	O2	2.94	31.999	0.022	3.46	-9.91721
dBrm_Be	3.306	3.32989	0.4	1.8731	41	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-9.25181
dBrm_Be	3.306	3.36195	0.4	1.8731	41	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-11
dBrm_Be	3.306	3.4312	0.4	1.8731	41	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-14.301
dBrm_Be	3.306	3.43959	0.4	1.8731	41	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-15.5834
dBrm_Be	3.306	3.45211	0.4	1.8731	41	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-16.3507
dBrm_Be	3.306	3.49206	0.4	1.8731	41	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	propylene	4.03	42.08	0.142	4.5	-17.9547
dBrm_Be	3.306	3.53933	0.4	1.8731	41	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	propane	4.16	44.1	0.152	4.3	-21.585
dBrm_Co	3.43279	3.43901	0.4	1.8731	72	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-7.35655
dBrm_Co	3.43279	3.44721	0.4	1.8731	72	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-7.61979
dBrm_Co	3.43279	3.46611	0.4	1.8731	72	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	O2	2.94	31.999	0.022	3.46	-9.41908
dBrm_Co	3.43279	3.45088	0.4	1.8731	72	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-9.33724
dBrm_Co	3.43279	3.48407	0.4	1.8731	72	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-10.2596
dBrm_Co	3.43279	3.54652	0.4	1.8731	72	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-12.6459
dBrm_Co	3.43279	3.5548	0.4	1.8731	72	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-14.0301
dBrm_Co	3.43279	3.56758	0.4	1.8731	72	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-14.9101
dBrm_Co	3.43279	3.6072	0.4	1.8731	72	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	propylene	4.03	42.08	0.142	4.5	-16.1385
dBrm_Co	3.43279	3.65414	0.4	1.8731	72	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	propane	4.16	44.1	0.152	4.3	-19.0177
dBrm_Cu	3.41563	3.42413	0.4	1.8731	71	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-7.45593
dBrm_Cu	3.41563	3.43113	0.4	1.8731	71	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-7.67778
dBrm_Cu	3.41563	3.44917	0.4	1.8731	71	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	O2	2.94	31.999	0.022	3.46	-9.55284
dBrm_Cu	3.41563	3.43516	0.4	1.8731	71	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-9.26761
dBrm_Cu	3.41563	3.46657	0.4	1.8731	71	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-10.2518
dBrm_Cu	3.41563	3.53182	0.4	1.8731	71	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-12.8861
dBrm_Cu	3.41563	3.53904	0.4	1.8731	71	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-14.2218
dBrm_Cu	3.41563	3.55074	0.4	1.8731	71	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-14.7959
dBrm_Cu	3.41563	3.59301	0.4	1.8731	71	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	propylene	4.03	42.08	0.142	4.5	-16.6162
dBrm_Cu	3.41563	3.63806	0.4	1.8731	71	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	propane	4.16	44.1	0.152	4.3	-19.3979
dBrm_Cd	3.54973	3.55667	0.4	1.8731	92	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-7.37161
dBrm_Cd	3.54973	3.56555	0.4	1.8731	92	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-7.55284
dBrm_Cd	3.54973	3.5851	0.4	1.8731	92	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	O2	2.94	31.999	0.022	3.46	-9.1549

dBrm_Cd	3.54973	3.56476	0.4	1.8731	92	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-9.22185
dBrm_Cd	3.54973	3.59846	0.4	1.8731	92	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-9.82391
dBrm_Cd	3.54973	3.6618	0.4	1.8731	92	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-11.8539
dBrm_Cd	3.54973	3.67105	0.4	1.8731	92	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-12.8928
dBrm_Cd	3.54973	3.68336	0.4	1.8731	92	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-13.6635
dBrm_Cd	3.54973	3.72367	0.4	1.8731	92	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	propylene	4.03	42.08	0.142	4.5	-14.7375
dBrm_Cd	3.54973	3.7709	0.4	1.8731	92	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	propane	4.16	44.1	0.152	4.3	-17.284
dBrm_Mg	3.47101	3.47776	0.4	1.8731	71	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-7.34679
dBrm_Mg	3.47101	3.48758	0.4	1.8731	71	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-7.65758
dBrm_Mg	3.47101	3.50635	0.4	1.8731	71	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	O2	2.94	31.999	0.022	3.46	-9.34679
dBrm_Mg	3.47101	3.48973	0.4	1.8731	71	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-9.284
dBrm_Mg	3.47101	3.52549	0.4	1.8731	71	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-10.0809
dBrm_Mg	3.47101	3.58425	0.4	1.8731	71	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-12.4815
dBrm_Mg	3.47101	3.59323	0.4	1.8731	71	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-13.6696
dBrm_Mg	3.47101	3.60784	0.4	1.8731	71	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-14.4949
dBrm_Mg	3.47101	3.64561	0.4	1.8731	71	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	propylene	4.03	42.08	0.142	4.5	-15.5058
dBrm_Mg	3.47101	3.69382	0.4	1.8731	71	6.01	6.01	6.01	223.8	223.8	223.8	3.78	3.78	3.78	15	15	15	propane	4.16	44.1	0.152	4.3	-18.7447
dFm_Co	3.349	3.3722	0.285	0.255	72	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-7.63827
dFm_Co	3.349	3.39904	0.285	0.255	72	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-7.56864
dFm_Co	3.349	3.43517	0.285	0.255	72	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	O2	2.94	31.999	0.022	3.46	-8.67778
dFm_Co	3.349	3.36292	0.285	0.255	72	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-8.69897
dFm_Co	3.349	3.46386	0.285	0.255	72	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-9.14267
dFm_Co	3.349	3.59899	0.285	0.255	72	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-11.0783
dFm_Co	3.349	3.60335	0.285	0.255	72	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-11.7447
dFm_Co	3.349	3.621	0.285	0.255	72	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-11.9208
dFm_Co	3.349	3.69801	0.285	0.255	72	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	propylene	4.03	42.08	0.142	4.5	-13.2403
dFm_Co	3.349	3.77328	0.285	0.255	72	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	propane	4.16	44.1	0.152	4.3	-15.0711
dFm_Cd	3.72625	3.76542	0.285	0.255	92	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-7.24413
dFm_Cd	3.72625	3.77416	0.285	0.255	92	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-7.3279
dFm_Cd	3.72625	3.79589	0.285	0.255	92	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	O2	2.94	31.999	0.022	3.46	-8.10791
dFm_Cd	3.72625	3.73385	0.285	0.255	92	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-8.31876
dFm_Cd	3.72625	3.84349	0.285	0.255	92	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-8.284
dFm_Cd	3.72625	3.93404	0.285	0.255	92	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-8.69897
dFm_Cd	3.72625	3.93446	0.285	0.255	92	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-9.30103
dFm_Cd	3.72625	3.96042	0.285	0.255	92	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-9.52288

dFm_Cd	3.72625	4.01873	0.285	0.255	92	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	propylene	4.03	42.08	0.142	4.5	-10
dFm_Cd	3.72625	4.09548	0.285	0.255	92	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	propane	4.16	44.1	0.152	4.3	-11.0969
dFm_Mg	3.39995	3.43393	0.285	0.255	71	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-7.73755
dFm_Mg	3.39995	3.45148	0.285	0.255	71	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-7.69897
dFm_Mg	3.39995	3.48902	0.285	0.255	71	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	O2	2.94	31.999	0.022	3.46	-8.52288
dFm_Mg	3.39995	3.41894	0.285	0.255	71	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-8.56864
dFm_Mg	3.39995	3.5227	0.285	0.255	71	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-8.85387
dFm_Mg	3.39995	3.66	0.285	0.255	71	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-10.2676
dFm_Mg	3.39995	3.66157	0.285	0.255	71	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-11.3298
dFm_Mg	3.39995	3.68128	0.285	0.255	71	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-11.752
dFm_Mg	3.39995	3.7511	0.285	0.255	71	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	propylene	4.03	42.08	0.142	4.5	-12.1605
dFm_Mg	3.39995	3.83066	0.285	0.255	71	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	propane	4.16	44.1	0.152	4.3	-14.4089
dFm_Be	3.023	3.05112	0.285	0.255	41	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-7.60206
dFm_Be	3.023	3.07777	0.285	0.255	41	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-7.92082
dFm_Be	3.023	3.11179	0.285	0.255	41	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	O2	2.94	31.999	0.022	3.46	-9.45593
dFm_Be	3.023	3.06132	0.285	0.255	41	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-9.63827
dFm_Be	3.023	3.16096	0.285	0.255	41	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-10.2366
dFm_Be	3.023	3.32957	0.285	0.255	41	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-14
dFm_Be	3.023	3.32484	0.285	0.255	41	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-14.7447
dFm_Be	3.023	3.3459	0.285	0.255	41	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-15.4547
dFm_Be	3.023	3.4257	0.285	0.255	41	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	propylene	4.03	42.08	0.142	4.5	-17.9788
dFm_Be	3.023	3.5069	0.285	0.255	41	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	propane	4.16	44.1	0.152	4.3	-21.7799
dFm_Cu	3.37185	3.39685	0.285	0.255	71	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-7.45593
dFm_Cu	3.37185	3.41459	0.285	0.255	71	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-7.56864
dFm_Cu	3.37185	3.44863	0.285	0.255	71	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	O2	2.94	31.999	0.022	3.46	-8.79048
dFm_Cu	3.37185	3.37579	0.285	0.255	71	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-8.5376
dFm_Cu	3.37185	3.474	0.285	0.255	71	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-8.81531
dFm_Cu	3.37185	3.60307	0.285	0.255	71	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-10.5686
dFm_Cu	3.37185	3.60961	0.285	0.255	71	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-11.2534
dFm_Cu	3.37185	3.62236	0.285	0.255	71	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-11.6383
dFm_Cu	3.37185	3.69051	0.285	0.255	71	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	propylene	4.03	42.08	0.142	4.5	-13.2034
dFm_Cu	3.37185	3.78	0.285	0.255	71	4.86	4.86	4.86	101.98	101.98	101.98	3.78	3.78	3.78	15	15	15	propane	4.16	44.1	0.152	4.3	-15.2351
dIm_Be	2.75316	2.76198	0.34	1.2552	41	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-7.50864
dIm_Be	2.75316	2.77747	0.34	1.2552	41	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-7.76955
dIm_Be	2.75316	2.79688	0.34	1.2552	41	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	O2	2.94	31.999	0.022	3.46	-9.49485

dIm_Be	2.75316	2.77121	0.34	1.2552	41	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-9.11919
dIm_Be	2.75316	2.81784	0.34	1.2552	41	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-10.1024
dIm_Be	2.75316	2.90166	0.34	1.2552	41	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-13.301
dIm_Be	2.75316	2.90884	0.34	1.2552	41	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-14.2218
dIm_Be	2.75316	2.91996	0.34	1.2552	41	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-14.4685
dIm_Be	2.75316	2.96338	0.34	1.2552	41	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	propylene	4.03	42.08	0.142	4.5	-16
dIm_Be	2.75316	3.01459	0.34	1.2552	41	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	propane	4.16	44.1	0.152	4.3	-17.7212
dIm_Co	2.91071	2.92661	0.34	1.2552	72	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-7.23657
dIm_Co	2.91071	2.942	0.34	1.2552	72	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-7.69897
dIm_Co	2.91071	2.94424	0.34	1.2552	72	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	O2	2.94	31.999	0.022	3.46	-9.18842
dIm_Co	2.91071	2.92065	0.34	1.2552	72	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-8.94692
dIm_Co	2.91071	2.96588	0.34	1.2552	72	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-9.55284
dIm_Co	2.91071	3.0371	0.34	1.2552	72	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-12.6021
dIm_Co	2.91071	3.04392	0.34	1.2552	72	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-12.8239
dIm_Co	2.91071	3.05574	0.34	1.2552	72	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-13.2366
dIm_Co	2.91071	3.09884	0.34	1.2552	72	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	propylene	4.03	42.08	0.142	4.5	-13.9208
dIm_Co	2.91071	3.14551	0.34	1.2552	72	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	propane	4.16	44.1	0.152	4.3	-16.0969
dIm_Cu	2.89378	2.90368	0.34	1.2552	71	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-7.50864
dIm_Cu	2.89378	2.91359	0.34	1.2552	71	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-7.52288
dIm_Cu	2.89378	2.93049	0.34	1.2552	71	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	O2	2.94	31.999	0.022	3.46	-9.11351
dIm_Cu	2.89378	2.90805	0.34	1.2552	71	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-8.88606
dIm_Cu	2.89378	2.95139	0.34	1.2552	71	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-9.58503
dIm_Cu	2.89378	3.01634	0.34	1.2552	71	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-11.5229
dIm_Cu	2.89378	3.02567	0.34	1.2552	71	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-12.9393
dIm_Cu	2.89378	3.03895	0.34	1.2552	71	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-13.3468
dIm_Cu	2.89378	3.07926	0.34	1.2552	71	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	propylene	4.03	42.08	0.142	4.5	-14.3809
dIm_Cu	2.89378	3.12849	0.34	1.2552	71	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	propane	4.16	44.1	0.152	4.3	-16.2366
dIm_Cd	2.99	3.00007	0.34	1.2552	92	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-7.38722
dIm_Cd	2.99	3.00819	0.34	1.2552	92	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-7.67778
dIm_Cd	2.99	3.02663	0.34	1.2552	92	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	O2	2.94	31.999	0.022	3.46	-8.93554
dIm_Cd	2.99	2.99964	0.34	1.2552	92	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-9
dIm_Cd	2.99	3.04975	0.34	1.2552	92	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-9.39794
dIm_Cd	2.99	3.10757	0.34	1.2552	92	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-10.9208
dIm_Cd	2.99	3.11696	0.34	1.2552	92	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-12.1739
dIm_Cd	2.99	3.12911	0.34	1.2552	92	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-12.5229

dIm_Cd	2.99	3.16762	0.34	1.2552	92	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	propylene	4.03	42.08	0.142	4.5	-13.9508
dIm_Mg	2.95	2.95572	0.34	1.2552	71	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	He	2.66	4.002	-0.39	2.6	-7.46852
dIm_Mg	2.95	2.96666	0.34	1.2552	71	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	H2	2.76	2.01	-0.217	2.89	-7.45593
dIm_Mg	2.95	2.98282	0.34	1.2552	71	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	O2	2.94	31.999	0.022	3.46	-9.18046
dIm_Mg	2.95	2.95545	0.34	1.2552	71	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	CO2	3.24	44.01	0.225	3.3	-9.09691
dIm_Mg	2.95	3.0024	0.34	1.2552	71	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	N2	3.13	28	0.037	3.64	-9.63827
dIm_Mg	2.95	3.06987	0.34	1.2552	71	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	CH4	3.25	16.04	0.011	3.8	-11.5229
dIm_Mg	2.95	3.07875	0.34	1.2552	71	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	ethylene	3.59	28.05	0.087	3.9	-12.6576
dIm_Mg	2.95	3.08837	0.34	1.2552	71	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	ethane	3.72	30.07	0.099	4	-13.0506
dIm_Mg	2.95	3.12791	0.34	1.2552	71	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	propylene	4.03	42.08	0.142	4.5	-13.8539
dIm_Mg	2.95	3.1705	0.34	1.2552	71	6.41	6.41	6.41	134.906	134.906	134.906	3.78	3.78	3.78	15	15	15	propane	4.16	44.1	0.152	4.3	-17.3979