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Mixed-Linker UiO-66: Structure-Properties Relations Revealed by a Combination of High-Resolution Powder X-Ray Diffraction and Density Functional Theory Calculations

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ELECTRONIC SUPPLEMENTARY INFORMATION

Table S1. Amounts of BDC and ABDC used for the preparation of DS-MIXUiO-66-NH_2.

Sample name	BDC (mg)	ABDC (mg)
UiO-66	237	0
DS_MIXUiO-66-NH_2_25	178	65
DS_MIXUiO-66-NH_2_50	119	130
DS_MIXUiO-66-NH_2_75	60	194
UiO-66-NH_2	0	259

Table S2. Amounts of BDC and BBDC used for the preparation of DS-MIXUiO-66-Br.

Sample name	BDC (mg)	BBDC (mg)
UiO-66	237	0
DS_MIXUiO-66-Br_25	178	88
DS_MIXUiO-66-Br_50	119	175
DS_MIXUiO-66-Br_75	60	263
UiO-66-Br	0	350

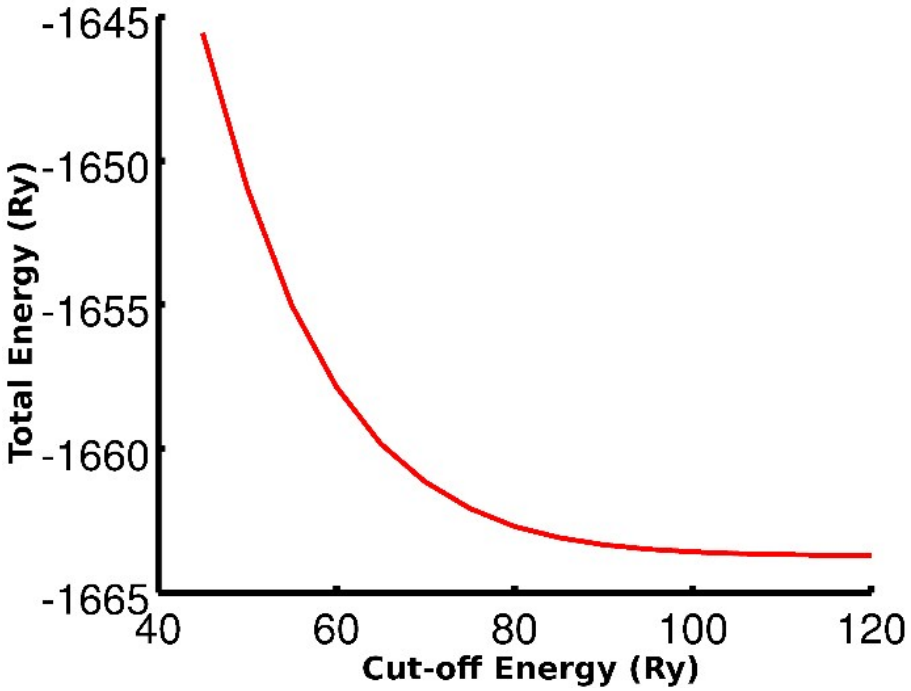


Figure S1. Energy cut-off convergence for the PBEsol norm-conserving pseudopotential.

Table S3. ABDC content of DS-MIXUiO-66-NH_2 from quantitative ^{1}H-NMR analysis.

Sample name	ABDC content (%)
DS_MIXUiO-66-NH_2_25	30
DS_MIXUiO-66-NH_2_50	53
DS_MIXUiO-66-NH_2_75	77

Table S4. BBDC content in DS-MIXUiO-66-Br from quantitative ^{1}H-NMR analysis.

Sample name	BBDC content (%)
DS_MIXUiO-66-Br_25	26
DS_MIXUiO-66-Br_50	51
DS_MIXUiO-66-Br_75	77

Table S5. Refined lattice parameters for DS-MIXUiO-66-NH_2 after solvent evacuation.

Sample name	***a*** **(Å)**
UiO-66	20.7520(4)
DS_MIXUiO-66-NH_2-25	20.766(2)
DS_MIXUiO-66-NH_2-50	20.784(3)
DS_MIXUiO-66-NH_2-75	20.783(2)
UiO-66-NH_2	20.798(2)

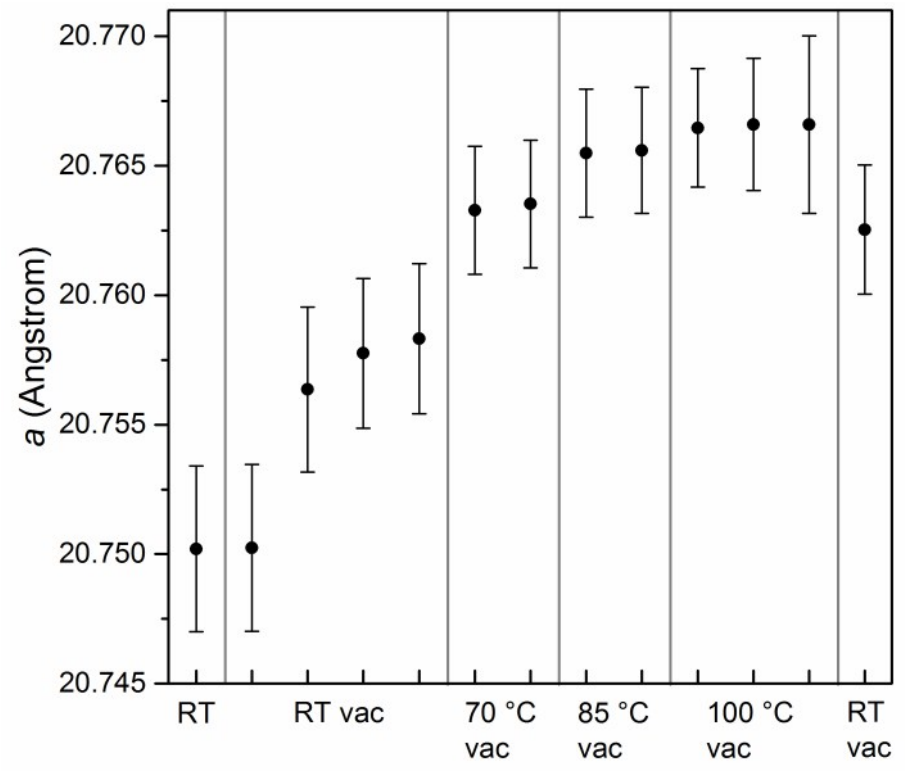


Figure S2. Refined lattice parameter for UiO-66 during in-situ solvent evacuation.

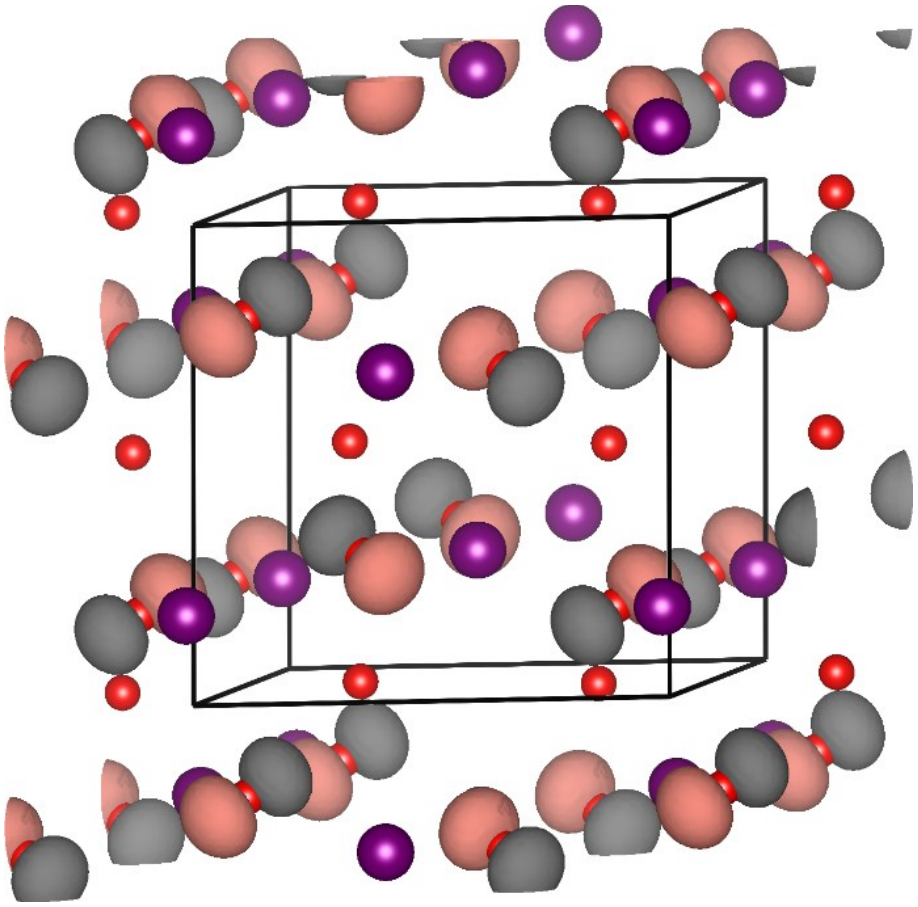


Figure S3. Highest Occupied Crystalline Orbital of ZrO_2. Adopted colour scheme: O red, Zr purple. Isovalue $5e^{-04}$.

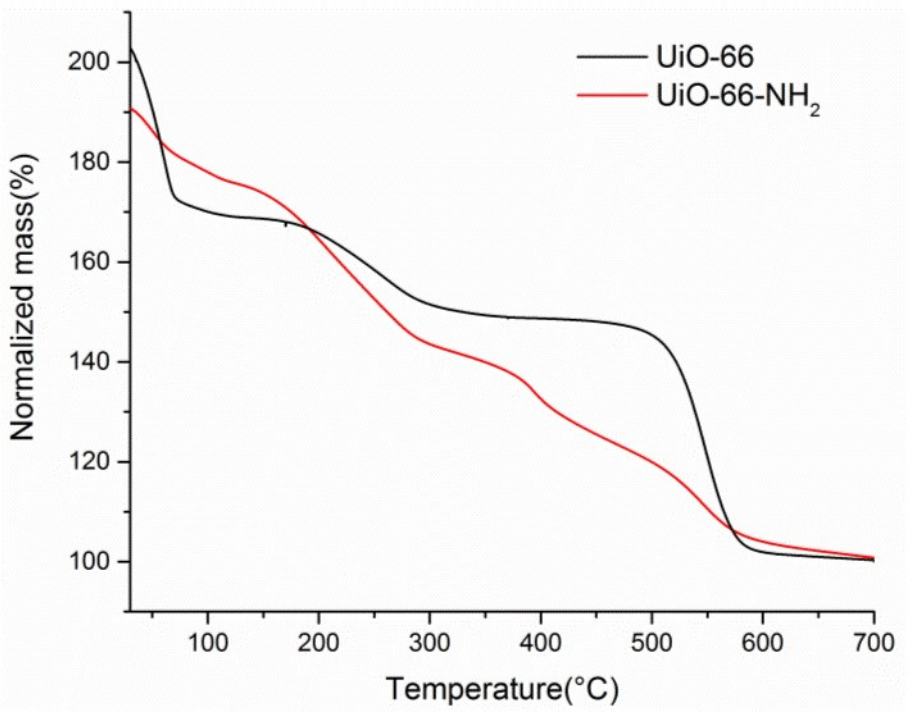


Figure S4. Thermogravimetric curves of UiO-66 (black) and UiO-66-NH_2 (red). Analysis was performed under a N_2 flow. The mass was normalized by taking the mass of ZrO_2 (123 g/mol) as a reference.

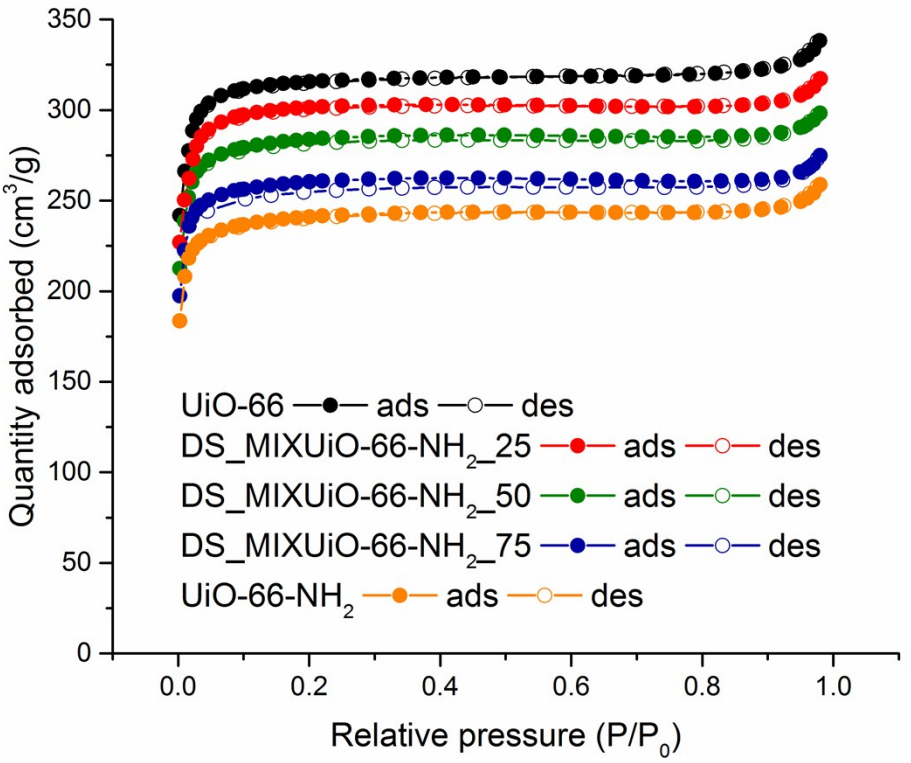


Figure S5. Nitrogen sorption isotherms of DS_MIXUiO-66-NH_2 samples obtained from reaction mixtures containing 0% (black), 25% (red), 50% (green), 75% (blue) and 100% (orange) ABDC.

Table S6. BET value and micropore volume measured for the samples of Figure S5.

Sample name	**BET value (m^2/g)**	**Micropore volume (cm^3/g)**
UiO-66	1288	0.46
DS_MIXUiO-66-NH_2_25	1227	0.43
DS_MIXUiO-66-NH_2_50	1161	0.40
DS_MIXUiO-66-NH_2_75	1065	0.37
UiO-66-NH_2	978	0.34

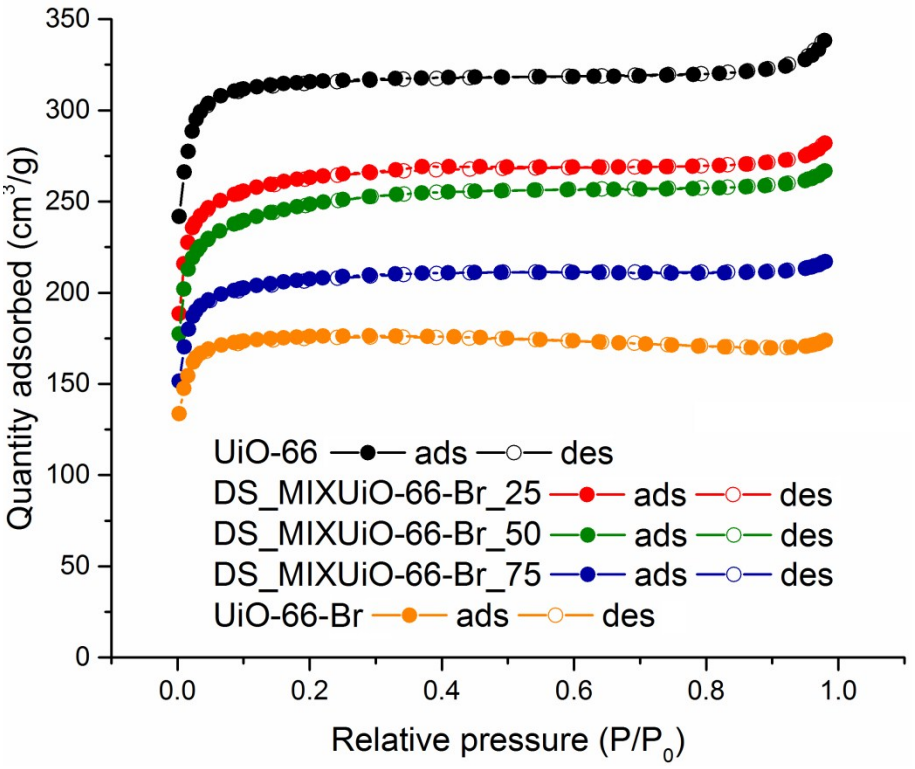


Figure S6. Nitrogen sorption isotherms of DS_MIXUiO-66-Br samples obtained from reaction mixtures containing 0% (black), 25% (red), 50% (green), 75% (blue) and 100% (orange) BBDC.

Table S7. BET value and micropore volume measured for the samples of Figure S6.

Sample name	BET value (m^2/g)	Micropore volume (cm^3/g)
UiO-66	1288	0.46
DS_MIXUiO-66-Br_25	1045	0.34
DS_MIXUiO-66-Br_50	971	0.31
DS_MIXUiO-66-Br_75	833	0.28
UiO-66-Br	718	0.25

Table S8. ABDC content of PSE_MIXUiO-66 from quantitative ^{1}H-NMR analysis.

Sample name	ABDC content (%)
PSE_MIXUiO-66-NH_2_A(42%)	42
PSE_MIXUiO-66-NH_2_A(66%)	66
PSE_MIXUiO-66-NH_2_A(86%)	86
PSE_MIXUiO-66-NH_2_B(65%)	65
PSE_MIXUiO-66-NH_2_B(57%)	57
PSE_MIXUiO-66-NH_2_B(47%)	47

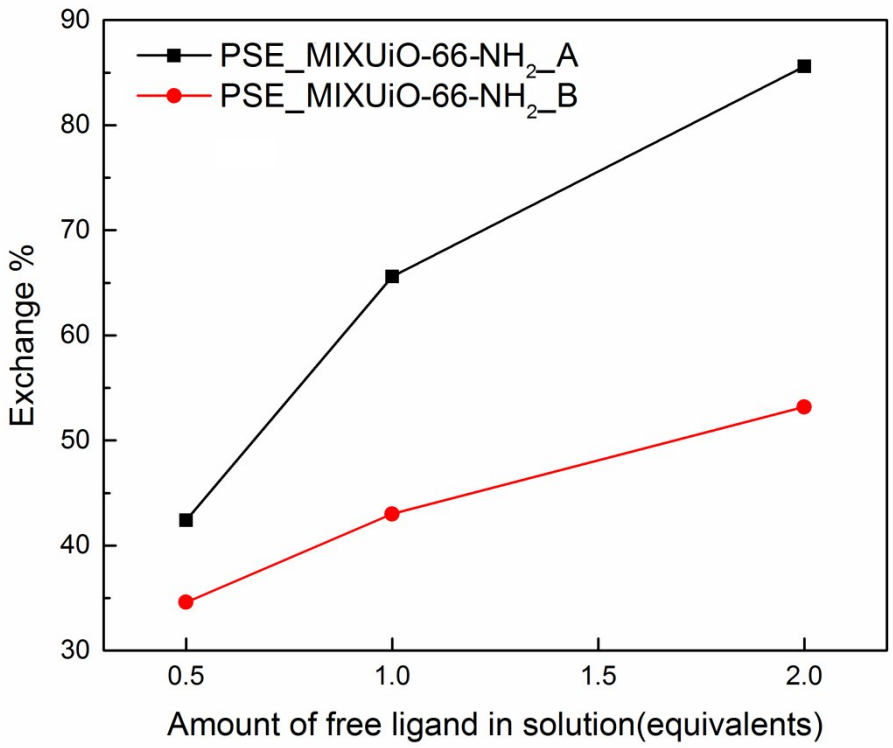


Figure S7. Degree of ligand exchange for PSE of ABDC into UiO-66 (black) and of BDC into UiO-66-NH_2 (red).

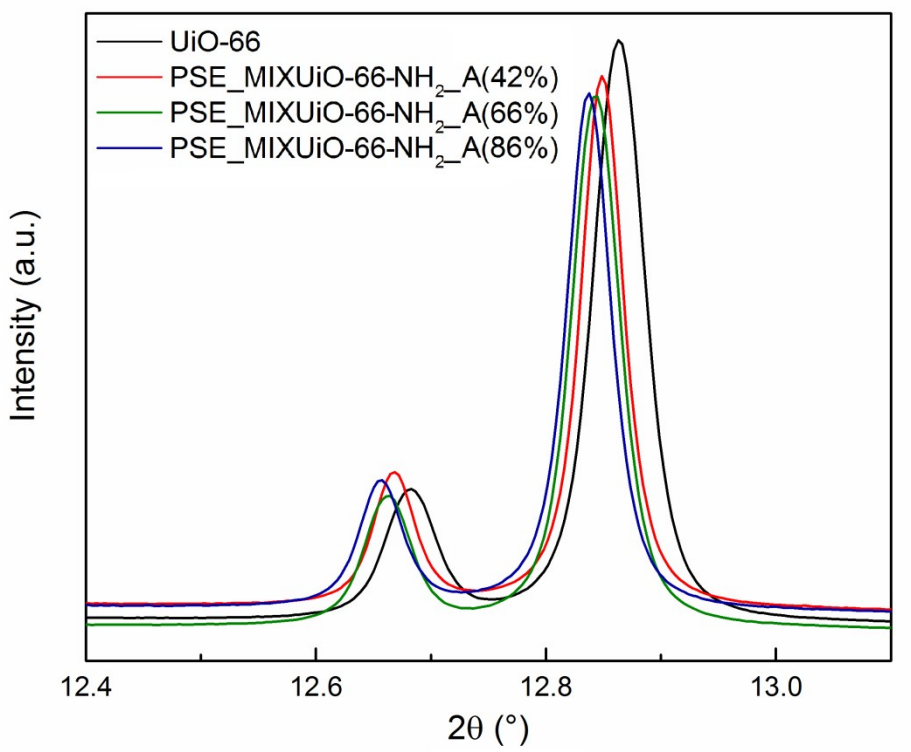


Figure S8. (531) and (006) reflections in the HR-PXRD patterns of UiO-66 (black), UiO-66 exchanged with 0.5 equivalents of ABDC (red), UiO-66 exchanged with 1.0 equivalents of ABDC (green) and UiO-66 exchanged with 2.0 equivalents of ABDC (blue). Intensities were scaled to allow easier visualization of the peak shift.

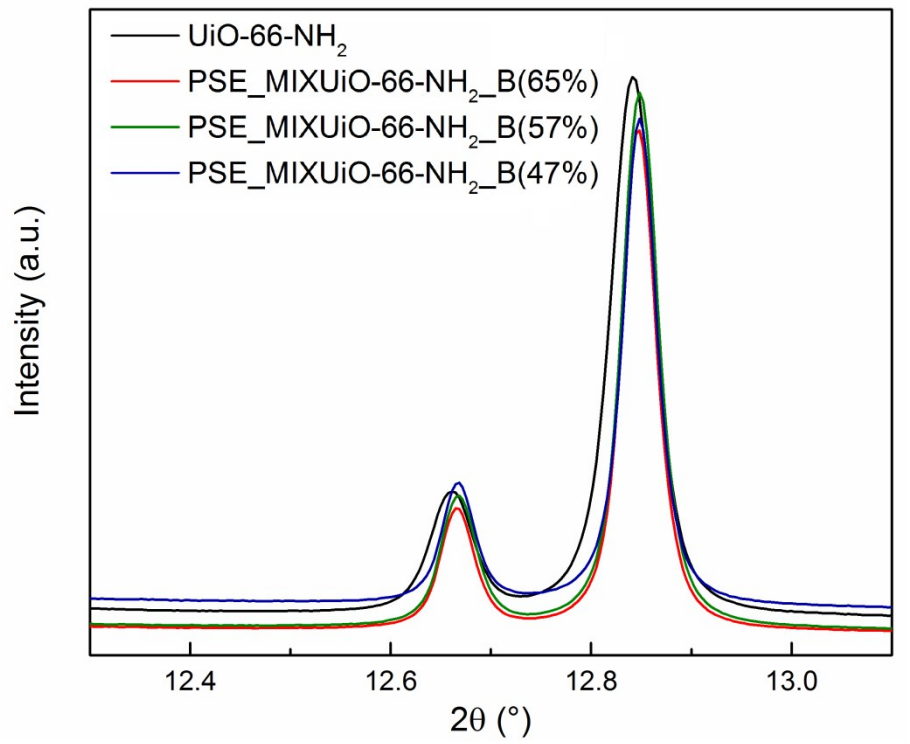


Figure S9 (531) and (006) reflections in the HR-PXRD patterns of UiO-66-NH_2 (black), UiO-66-NH_2 exchanged with 0.5 equivalents of BDC (red), UiO-66-NH_2 exchanged with 1.0 equivalents of BDC (green) and UiO-66-NH_2 exchanged with 2.0 equivalents of BDC (blue). Intensities were scaled to allow easier visualization of the peak shift.

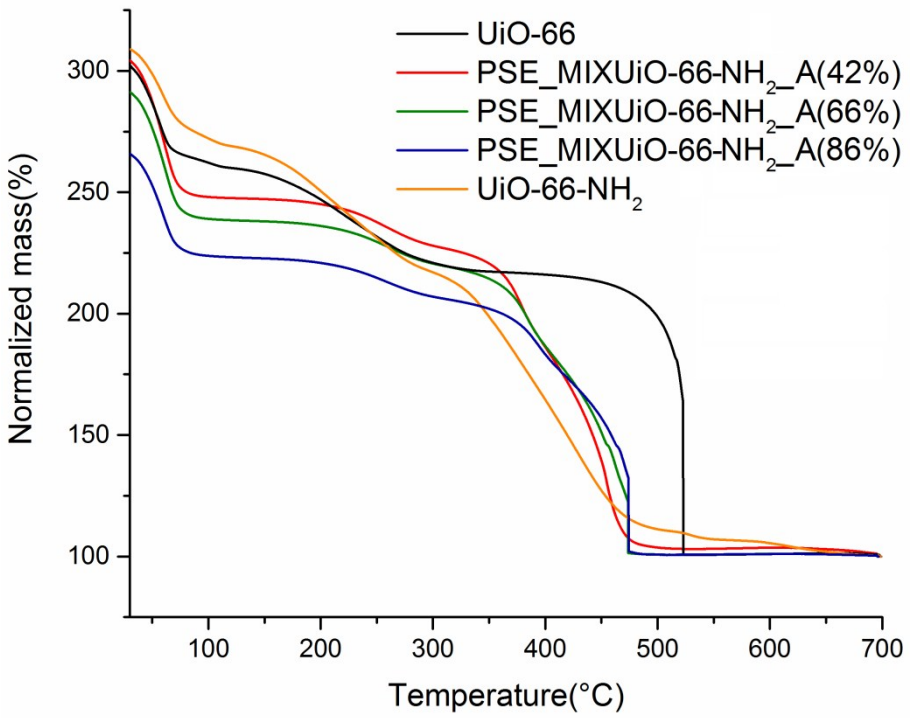


Figure S10. Thermogravimetric curves of UiO-66 (black), UiO-66 exchanged with 0.5 equivalents of ABDC (red), UiO-66 exchanged with 1.0 equivalents of ABDC (green), UiO-66 exchanged with 2.0 equivalents of ABDC (blue) and UiO-66-NH_2 (orange). The analysis was performed under a 80/20 N_2:O_2 flow. The mass was normalized by taking the mass of ZrO_2 (123 g/mol) as a reference.

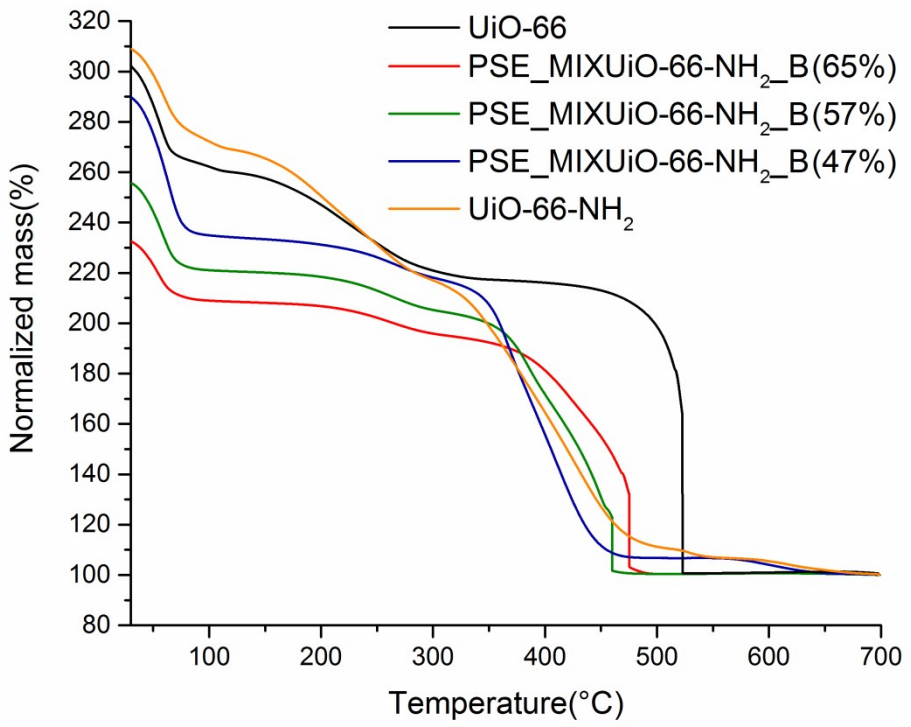


Figure S11. Thermogravimetric curves of UiO-66 (black), UiO-66-NH_2 exchanged with 0.5 equivalents of BDC (red), UiO-66-NH_2 exchanged with 1.0 equivalents of BDC (green), UiO-66-NH_2 exchanged with 2.0 equivalents of BDC (blue) and UiO-66-NH_2 (orange). The analysis was performed under a 80/20 N_2:O_2 flow. The mass was normalized by taking the mass of ZrO_2 (123 g/mol) as a reference.

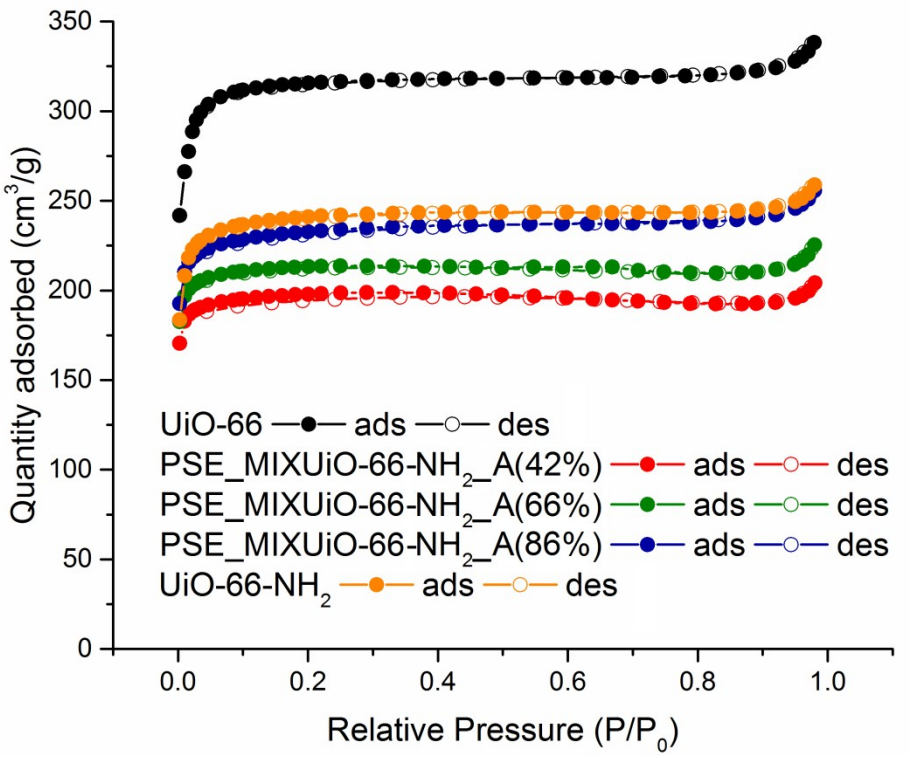


Figure S12. Nitrogen sorption isotherms of UiO-66 (black), UiO-66 exchanged with 0.5 equivalents of ABDC (red), UiO-66 exchanged with 1.0 equivalents of ABDC (green), UiO-66 exchanged with 2.0 equivalents of ABDC (blue) and UiO-66-NH_2 (orange).

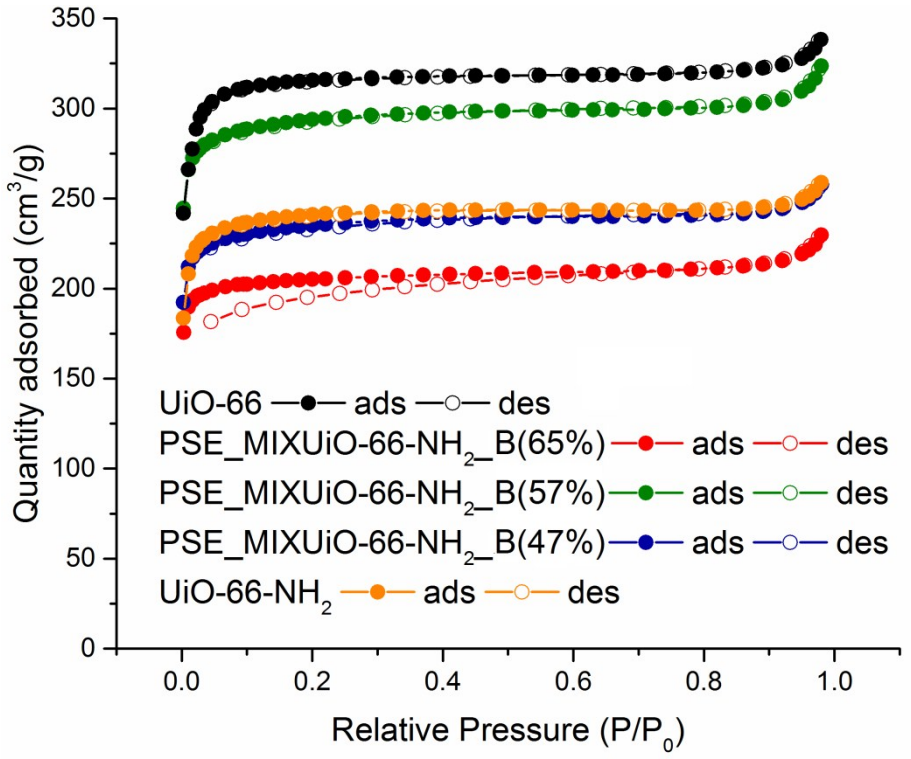


Figure S13. Nitrogen sorption isotherms of UiO-66 (black), UiO-66-NH_2 exchanged with 0.5 equivalents of BDC (red), UiO-66-NH_2 exchanged with 1.0 equivalents of BDC (green), UiO-66-NH_2 exchanged with 2.0 equivalents of BDC (blue) and UiO-66-NH_2 (orange).

Table S9. BET value and micropore volume measured for the samples of Figures S12 and S13.

Sample name	BET value (m^2/g)	Micropore volume (cm^3/g)
PSE_MIXUiO-66-NH_2_A(42%)	807	0.28
PSE_MIXUiO-66-NH_2_A(66%)	870	0.31
PSE_MIXUiO-66-NH_2_A(86%)	941	0.32
PSE_MIXUiO-66-NH_2_B(65%)	837	0.29
PSE_MIXUiO-66-NH_2_B(57%)	1188	0.41
PSE_MIXUiO-66-NH_2_B(47%)	948	0.32

Norm-conserving PBEsol Optimized geometries:

UiO-66

```
CELL_PARAMETERS (angstrom)
  14.854685481   0.075930553   0.076439828
   7.427387162  12.877607134   0.076445316
   7.427398865   4.317891784  12.150814330

ATOMIC_POSITIONS (angstrom)
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H       18.227930606   8.165666391   1.958980085
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H       16.961154663   3.783181720   5.029823451
H       16.753188010  11.211264243  10.559451944
H       12.748154914   3.750802166   4.998020545
H       12.959361028  11.183723712  10.530139279
H       16.958781065   5.966622744   1.944796273
H       16.750585655  13.640863937   7.133755254
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H       22.281648247  12.952666814   3.605148424
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C       17.503657550  10.978059484  11.319360762
C       11.990410216   3.115466013   5.463947779
C       12.206897772  10.948600051  11.287579815
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O	11.418635015	5.031388659	11.260522447
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O        7.432083095  11.082184126   0.708541746
O        7.433519191   4.321141563  10.245259141
O        1.569272574   0.911305509   0.647770504
Zr       9.246024234  11.839454853   1.563522197
Zr      20.465462938   5.432292506  10.740937614
Zr       9.247580973   5.375861289  10.681179399
Zr      20.463952833  11.896561043   1.622289710
Zr      14.855210595   2.170687820   1.563052794
Zr      14.855736922  15.101959879  10.741363668
```

MIXUiO-66-NH_2-17

```
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   7.396385583  12.861123005   0.055481900
   7.399429961   4.288623028  12.158372308

ATOMIC_POSITIONS (angstrom)
H        9.611851875   9.179076630   4.917922179
H       16.161324449   5.645243559  10.449801200
H       13.609677483  11.699172780   1.814838724
H       20.166553294   7.648618339   6.973820919
H       11.513841709   4.408022996   6.976269993
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H        9.612064934   7.699008140   6.982301315
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H       22.295214407  12.878223049   3.483426368
H       26.904066922  15.506000057  11.014249792
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C	14.188615934	12.248316731	1.067862545
C	21.094932507	8.003456568	6.518930941
C	11.331615687	3.442266800	6.498083831
C	18.449291245	7.322576601	1.081212436
C	11.539905536	9.667360348	11.187724997
C	18.195968717	13.801813788	5.408709445
C	12.010394482	6.076892673	1.063899394
C	12.269815599	14.120519397	6.466278253
C	17.749120179	3.075713908	5.428306380
C	17.527278643	10.898822158	11.219426985
C	12.019843777	3.047909510	5.361664654
C	12.240598223	10.863397302	11.202324048
C	17.748889655	6.126216599	1.067331707
C	17.507582310	14.196668363	6.544798585
C	8.684230189	8.011441149	6.496158906
C	15.574999125	12.251265876	1.073873209
C	14.196429020	5.101598716	11.197720197
C	21.094848664	8.811638167	5.392655674
C	11.322699230	7.280098280	1.074054307
C	18.472516229	3.417363887	6.553226196
C	11.517533359	13.785649265	5.325780863
C	18.214696395	9.695583908	11.209088231
C	4.620911356	0.045866503	-0.018086322
C	7.466443980	6.788272580	8.292000129
C	7.465559480	10.124540458	3.632640710
C	10.355102955	0.054029156	0.002624960
C	2.379199024	3.880556378	-0.040657216
C	12.544492185	1.345576480	3.621884528
C	9.696849482	2.974938474	8.318333310
C	5.270735100	8.831122111	0.010531748
C	2.369903274	1.340066533	3.589807630
C	9.696740503	8.858978167	0.035086296
C	12.548566141	3.890188321	0.004403297
C	5.270337440	2.930834493	8.274350996
C	7.466632583	9.205749919	4.798505768
C	8.870970005	0.096179861	0.028496208
C	6.104710111	0.091154801	0.017620377
C	7.466969044	7.593868441	7.045269821
C	10.387923393	2.579497948	7.066364107
C	4.563936453	7.525653639	0.031923443
C	3.165867634	5.138896760	0.004370942
C	11.760874370	1.793292552	4.799726037
C	11.763753648	5.149043855	0.045933829
C	4.598339334	2.510640914	7.037829573
C	3.157782356	1.782987596	4.768585597
C	10.391630402	7.548304912	0.065095612
O	8.608894896	10.498477295	3.202616598
O	18.325257888	4.975652826	11.210162010
O	11.448006947	12.216604948	0.949270244
O	21.167055942	6.530088374	8.832872604
O	10.008558010	4.113173294	8.805820717
O	19.799801000	9.711370573	0.985922992
O	10.046319164	7.364375825	11.162442496

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O       19.685945837  13.035352532   3.236236829
O       13.427971093   3.745961074   0.919339199
O       13.518627160  14.971076760   8.850486519
O       16.329163661   2.193621488   3.208808597
O       16.272814432  13.326726962  11.233057662
O       13.418824479   2.162047827   3.176392635
O       13.509087843  13.298948107  11.221708970
O       16.335393340   3.777341788   0.925586501
O       16.270894749  14.989542906   8.863522799
O        8.608824215   6.500270595   8.784975600
O       18.319016464  12.229748625   0.974266453
O       11.452448211   4.967877390  11.187577913
O       21.167433244  10.523795162   3.246906368
O       10.003349100   9.694219954   0.950642068
O       19.796731391   4.112003949   8.833409152
O       10.031207565  13.034798882   3.193373216
O       19.692289096   7.373035322  11.205907576
O       16.902577334  15.953019916  11.315234939
O       22.298102184   6.630588867  11.294928123
O       22.291861949  12.874193980   2.512287839
O       27.686728912  15.969832479  11.353851368
O       13.353554139   0.890237527   0.589696117
O        7.470948964  11.024194552   0.616740392
O        7.476684397   4.247181224  10.163288310
O        1.618937956   0.872578553   0.553354882
Zr       9.278969393  11.790389284   1.463709513
Zr      20.490480460   5.322921997  10.627941196
Zr       9.283791614   5.306177842  10.594919265
Zr      20.487224000  11.812391767   1.505586546
Zr      14.892179853   2.103751363   1.449920397
Zr      14.883710272  15.020613528  10.662268423
N       13.214326593  13.251062989   6.917847823
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H       13.313631055  12.346660119   6.473113324
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CELL_PARAMETERS (angstrom)
  14.847819153   0.020266931   0.064001383
   7.375444361  12.849661791   0.041107261
   7.395686568   4.261340009  12.151343399

ATOMIC_POSITIONS (angstrom)
H        9.590565790   9.169057225   4.906422547
H       16.160746093   5.641964520  10.473352966
H       13.584421610  11.653282286   1.781415417
H       20.158922084   7.602729463   6.976839394
H       11.495402232   4.384635299   6.967358621
H       18.246491036   8.055080341   1.829976161
H       11.736741173   8.845020403  10.443266887
H       18.004046139  12.799178928   4.900272577
H       16.923286008   3.636580499   5.040449223
H       16.875277319  11.071113883  10.334260625
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H	12.777210861	3.663325483	4.895980789
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H	16.986372861	5.849529714	1.821903401
H	16.721604014	13.520860234	6.971007265
H	9.600162642	7.694683650	6.976135613
H	16.125204733	11.662509839	1.801307539
H	13.621702669	5.632957239	10.454421911
H	20.149862840	9.075535453	4.908308825
H	11.305842194	8.030311904	1.870773623
H	18.234410998	4.283958854	7.109762720
H	11.764491436	12.861449668	4.725127172
H	18.196117298	8.909406727	10.421746063
H	22.287132194	12.822615586	3.468394459
H	26.872862221	15.454768714	10.993384296
H	17.660215936	15.437711864	10.956027937
H	22.295873940	7.493802832	10.983083174
C	8.665172081	8.805517569	5.360413087
C	15.581107110	5.086721778	11.215190391
C	14.165256246	12.214797924	1.045161704
C	21.085335825	7.958884412	6.519047319
C	11.318992500	3.419720549	6.485507127
C	18.438520723	7.283318580	1.080326067
C	11.548890281	9.614506435	11.196334237
C	18.173814778	13.768071076	5.376534736
C	11.937327707	6.071591103	1.168919462
C	12.315892186	14.142282536	6.393051837
C	17.722499947	3.010018317	5.440758032
C	17.561620807	10.842392261	11.151647611
C	12.018003967	3.025826737	5.355715287
C	12.237558457	10.817216610	11.201698160
C	17.750640893	6.080336894	1.075569375
C	17.474912470	14.161900166	6.506464555
C	8.670615281	8.001528000	6.489785435
C	15.551446631	12.219422796	1.055954284
C	14.194437259	5.082089890	11.204917181
C	21.080284960	8.763010587	5.389255519
C	11.202253911	7.268130163	1.092203482
C	18.440880263	3.358099674	6.566290006
C	11.565143457	13.798396185	5.254545082
C	18.282470532	9.667044150	11.205063258
C	4.620290864	0.027507877	-0.027628893
C	7.460092548	6.771536028	8.287589662
C	7.442316670	10.095085932	3.613966218
C	10.355268397	0.045383423	0.012364125
C	2.393142881	3.856071514	-0.027318331
C	12.561741114	1.318934201	3.625606137
C	9.676781530	2.949071208	8.294805140
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C	5.264096990	2.925313782	8.262998379
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C	8.870959037	0.090527165	0.037530270

C	6.103914845	0.081280924	0.016801129
C	7.456056652	7.579847789	7.041747433
C	10.371941295	2.555531461	7.045145597
C	4.548333783	7.512843669	0.027572254
C	3.176234944	5.114780487	0.017446395
C	11.765571504	1.770788050	4.792390263
C	11.781287847	5.134252590	0.104803045
C	4.607741942	2.510469580	7.016731368
C	3.177456014	1.769928126	4.747651397
C	10.349889804	7.518651016	0.030918140
O	8.585954016	10.462132271	3.177569308
O	18.322329156	4.942867372	11.215091336
O	11.426050140	12.180403897	0.920584553
O	21.165094429	6.485858369	8.832751479
O	9.992412149	4.085583787	8.784697695
O	19.760240939	9.681071408	0.969739488
O	10.056709697	7.314306137	11.167644847
O	19.681520672	12.997729235	3.225301676
O	13.452630518	3.707852795	0.953283202
O	13.490437263	14.951506910	8.821118808
O	16.340886350	2.138348132	3.205532253
O	16.228310724	13.269988810	11.173588115
O	13.446903236	2.129424112	3.188928255
O	13.464247385	13.272101355	11.194773251
O	16.352762064	3.725269550	0.941505727
O	16.225929313	14.954428102	8.821061084
O	8.603555095	6.480211801	8.776654271
O	18.296978921	12.203587505	0.966000289
O	11.449091122	4.920721950	11.169768210
O	21.147068873	10.468160541	3.231239352
O	9.955024540	9.667990337	0.899314500
O	19.781843578	4.071626567	8.835592125
O	10.022608908	12.996366847	3.170719123
O	19.719088332	7.346513360	11.224717954
O	16.870516335	15.902823437	11.277164650
O	22.306313998	6.573894485	11.294250070
O	22.281226304	12.814509853	2.497392374
O	27.657158201	15.915442672	11.333651084
O	13.354240506	0.860885818	0.597611642
O	7.441295366	11.005172030	0.593570315
O	7.463095030	4.225322010	10.158528983
O	1.630981614	0.850880566	0.546017413
Zr	9.257966696	11.754405914	1.437393029
Zr	20.484821260	5.286492835	10.630603982
Zr	9.279702901	5.270231433	10.579109094
Zr	20.465793694	11.768832799	1.492347669
Zr	14.910694486	2.048902449	1.449338422
Zr	14.847006036	14.983218555	10.631220253
N	13.313381033	13.313722518	6.805485293
H	13.784376176	13.546876110	7.680277747
H	13.460678607	12.433156407	6.326460429
N	12.753505010	5.861240178	2.236660000
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H	12.847712771	6.580896544	2.943448117

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CELL_PARAMETERS (angstrom)
  14.857108219   0.030978794   0.057712681
   7.389288387  12.859784544   0.025852961
   7.398242696   4.256819436  12.132307717

ATOMIC_POSITIONS (angstrom)
H        9.645767208   9.173716497   4.837516388
H       16.209583794   5.623839715  10.381134058
H       13.647326436  11.656360435   1.700149408
H       20.220390937   7.591865212   6.873027024
H       11.557106780   4.376442756   6.874581341
H       18.290481647   8.134289250   1.612246596
H       11.790987117   8.716775652  10.454856914
H       18.046707778  12.795483489   4.812745624
H       16.966547601   3.629361871   4.967459030
H       16.968521588  11.077120826  10.199877213
H       12.830490050   3.635098867   4.804125754
N       13.309447117  10.842816026  10.134260477
H       16.981329631   5.965460139   1.713469331
H       16.767969630  13.539695687   6.878745835
H        9.650307490   7.713974121   6.917042025
H       16.187882377  11.659198892   1.711956317
H       13.668809920   5.619882756  10.369316388
H       20.216707619   9.048396153   4.793400351
H       11.320522481   8.011786779   1.801563807
H       18.301068149   4.287677424   7.019912347
H       11.845166597  12.878904815   4.605291821
H       18.265417282   8.902638376  10.311096290
H       22.343251410  12.814774263   3.377481949
H       26.950097083  15.444671371  10.875905326
H       17.725025492  15.445498012  10.850574233
H       22.343954789   7.493442595  10.907819471
C        8.719689856   8.804255032   5.285306249
C       15.629782421   5.070854927  11.124636208
C       14.227079144  12.216810461   0.962112766
C       21.147654725   7.953554213   6.421774094
C       11.373633521   3.410207621   6.397581430
C       18.483061316   7.313873801   0.916367470
C       11.603106405   9.527694525  11.165279956
C       18.223741600  13.765260508   5.284723872
C       11.954868478   6.052473046   1.103982157
C       12.405461107  14.162260120   6.267475306
C       17.778117772   3.011116964   5.355626535
C       17.628821222  10.837571608  11.035453027
C       12.068087856   3.005556109   5.269279839
C       12.347775862  10.717040009  11.095401960
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C	18.509154843	3.365711482	6.470658373
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C	18.338512706	9.656250717	11.099664350
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C	7.499828549	10.074839079	3.521733386
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C	19.986569543	8.131836409	12.105981590
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C	16.316722583	4.333992631	12.095743871
C	13.548440736	4.331622861	12.083812292
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C	10.421790574	2.554551795	6.961050307
C	4.628392842	7.490029206	-0.106268536
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C	11.806851999	1.748911358	4.712741019
C	11.811815198	5.119504959	0.034842578
C	4.679040782	2.514141124	6.913319768
C	3.225302717	1.762857332	4.665768330
C	17.797772713	11.770478485	12.072706131
O	8.643323364	10.446337263	3.088378066
O	18.371008180	4.924387150	11.117015187
O	11.485354322	12.183361385	0.840014612
O	21.221342412	6.494639966	8.748213996
O	10.040912664	4.091133349	8.698933241
O	19.825356191	9.673345938	0.836934108
O	10.082293296	7.297489926	11.124285679
O	19.735260231	12.979896164	3.131517022
O	13.476375742	3.690063617	0.892095003
O	13.564875865	14.954113766	8.709380819
O	16.371387742	2.123407878	3.144175404
O	16.299010638	13.269365339	11.048036202
O	13.486129130	2.102329677	3.113764644
O	13.565174717	13.261151293	11.079833988
O	16.376845867	3.736829214	0.899991381
O	16.297105864	14.965062468	8.722569813
O	8.650278468	6.492395220	8.710514590
O	18.359450907	12.192556202	0.866555469
O	11.497136355	4.917989484	11.091368815
O	21.213432366	10.452175802	3.128448997
O	10.013837445	9.666327907	0.801129664
O	19.854017441	4.076515608	8.733686897
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O       27.729537267  15.914869444  11.214532818
O       13.401704825   0.841805404   0.522971613
O        7.503258217  10.996326117   0.506454549
O        7.511295604   4.223747253  10.070311295
O        1.666831186   0.838279998   0.487614801
Zr       9.314914109  11.750239473   1.355453341
Zr      20.535113467   5.281546932  10.539480937
Zr       9.324591341   5.268083143  10.503317162
Zr      20.527121381  11.753484035   1.393441656
Zr      14.948958796   2.038083473   1.383357687
Zr      14.917481903  14.995919228  10.524480112
N       13.426323422  13.347326157   6.658590742
H       13.844056709  13.551991566   7.567935990
H       13.491325113  12.422999900   6.246736429
N       12.747362652   5.829786497   2.187810557
H       13.345460974   5.002773047   2.163402379
H       12.882229830   6.573067425   2.863407957
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H       13.629289232  10.001763128   9.665908972
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CELL_PARAMETERS (angstrom)
  14.881046027   0.037715652   0.044796762
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   7.401606028   4.255059977  12.114423387

ATOMIC_POSITIONS (angstrom)
H        9.646088162   9.198343127   4.821727522
N       16.190559824   5.947292386  10.134663228
H       13.734805890  11.593140393   1.680015031
H       20.264386569   7.574285891   6.843431469
H       11.568621242   4.371575653   6.880519429
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MIXUiO-66-NH_2-83

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UiO-66-NH_2

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O        8.694289694   6.510303971   8.752140368
O       18.324239778  12.195975442   0.773819530
O       11.459185520   4.877075013  11.132478905
O       21.139617234  10.399197629   3.076321859
O        9.964741591   9.635155447   0.807086123
O       19.854595152   4.088729461   8.693359337
O       10.019144790  12.959477360   3.104339990
O       19.762602007   7.330131592  11.096156649
O       16.898255033  15.871839291  11.191713964
O       22.348247111   6.552281075  11.214920637
O       22.279730125  12.768101209   2.383923339
O       27.698442996  15.894780179  11.156980789
O       13.389117034   0.837403968   0.487681533
O        7.462771058  10.999037643   0.478880565
O        7.514047849   4.217074999  10.060701326
O        1.656128860   0.832452433   0.519383408
Zr       9.271291457  11.723093972   1.361641929
Zr      20.549470813   5.274123487  10.504599408
Zr       9.312144161   5.246652324  10.548382779
Zr      20.475105210  11.734578351   1.341841825
Zr      14.926889025   2.019663916   1.380298489
Zr      14.888726915  14.972725070  10.500481472
N       13.397156860  13.347111087   6.647056654
H       13.950717274  13.637111792   7.453106165
H       13.673287817  12.575090305   6.051966678
N       12.749780600   5.827942733   2.165221785
H       13.380707795   5.026119630   2.102331045
H       12.963567164   6.616784155   2.765568155
H       14.094361900  11.553783333  10.449749286
H       13.963303771   9.828257552  10.124323352
H       15.569536673   6.192116066   9.303580426
H       17.152014732   5.800972157   9.997083956
H       11.998708462   5.374734315   6.083747636
H       11.029807428   5.066000932   7.509301306
H       10.748865116   8.519003530   6.709764022
H       10.008281211   7.443239081   7.879144133
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MIXUiO-66-Br-17

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CELL_PARAMETERS (angstrom)
  14.845583769   0.038072374   0.070580895
   7.389678592  12.855551993   0.056057464
   7.404968607   4.280244852  12.166969742
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ATOMIC_POSITIONS (angstrom)
H        9.602960555   9.183968755   4.926539889
H       16.164429096   5.640321272  10.458511297
H       13.599183766  11.716736317   1.828721781
H       20.159091225   7.648045295   6.994727969
H       11.531997057   4.405871280   6.992248501
H       18.262641906   8.074003514   1.867792070
H       11.698839281   8.910262064  10.427930403
H       17.990972428  12.845005218   4.926001428
H       12.753633021   5.828736061   1.827173882
H       17.010726972   3.707906626   5.036784426
H       16.784477150  11.125847769  10.467077916
H       12.790750644   3.681843963   4.908761494
H       12.974338142  11.105812186  10.452457043
H       16.981637320   5.881173278   1.838670005
H       16.723305129  13.573997540   7.002319596
H        9.604701638   7.703463938   6.987816701
H       16.136603530  11.712384179   1.834618229
H       13.625781288   5.647816521  10.454559074
H       20.157544138   9.128920833   4.932876154
H       11.493166461   8.033782516   1.841742037
H       18.341337067   4.315802156   7.106656938
H       11.699280024  12.813356266   4.798622569
H       18.044926748   8.920635451  10.452702800
H       22.275646974  12.861631754   3.491749613
H       26.899842358  15.479096730  11.045189653
H       17.693252597  15.483718841  11.000067242
H       22.297966805   7.530971369  10.985229195
C        8.674700080   8.824104881   5.377664744
C       15.585696889   5.102186349  11.213635754
C       14.177178931  12.260631532   1.077216263
C       21.087629918   8.000570741   6.538336754
C       11.342262514   3.444120188   6.508805390
C       18.441449398   7.311635364   1.105133684
C       11.525737308   9.668567431  11.195750583
C       18.177215747  13.809188927   5.405770730
C       12.006985960   6.071129650   1.066791099
C       12.259616287  14.103031972   6.440922263
C       17.773969846   3.042572517   5.447708256
C       17.524792684  10.879622826  11.232410328
C       12.029476116   3.048899344   5.371900904
C       12.223924056  10.865977894  11.210412704
C       17.742260138   6.114797910   1.089238474
C       17.488267731  14.205024532   6.541812162
C        8.675691305   8.015266532   6.503657277
C       15.563678989  12.257697731   1.080198489
C       14.199103709   5.106366595  11.211512252
C       21.086579617   8.809582881   5.412199912
C       11.319125387   7.274574821   1.074851411
C       18.502017524   3.373133494   6.577185644
C       11.530789541  13.763884066   5.308797871
C       18.212678731   9.676177000  11.224526245
C        4.616539515   0.056308536  -0.015795531
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C	7.460299493	6.785056311	8.297460720
C	7.456041172	10.126613929	3.637579977
C	10.351435823	0.046513355	-0.002997888
C	2.370713489	3.882432282	-0.036694638
C	12.546524185	1.346581872	3.630247936
C	9.702953555	2.979878468	8.325617088
C	5.256148551	8.832431058	0.022341874
C	2.372418491	1.340874399	3.579616579
C	9.690683272	8.849931705	0.036146382
C	12.542719453	3.881435341	0.011510186
C	5.296496406	2.909368214	8.297496151
C	7.457143623	9.210585109	4.806493971
C	8.867654716	0.099839859	0.029196682
C	6.100528961	0.106750632	0.024098531
C	7.459132710	7.596368015	7.053613022
C	10.389885715	2.586721146	7.070622143
C	4.548031153	7.528343029	0.041379265
C	3.154777709	5.141364893	0.010318015
C	11.760776328	1.798134429	4.804752067
C	11.757936202	5.140461821	0.051673491
C	4.626458440	2.469097424	7.041251972
C	3.168636836	1.775195859	4.758558021
C	10.386039332	7.539662029	0.067161642
O	8.599626643	10.496860567	3.204036595
O	18.326998088	4.943370027	11.200756633
O	11.436852923	12.216006422	0.948312109
O	21.161843102	6.510194449	8.844453630
O	10.013477165	4.120286155	8.812141761
O	19.781856048	9.706949223	1.004784336
O	10.042802051	7.358990226	11.174125187
O	19.679764436	13.032073517	3.242603851
O	13.423216597	3.738504866	0.925727045
O	13.515486179	14.954373887	8.873444774
O	16.335539546	2.192374441	3.219740494
O	16.271387707	13.307691701	11.243866038
O	13.427733168	2.159122957	3.188751730
O	13.504356091	13.288116435	11.247494818
O	16.328869505	3.767995933	0.939955329
O	16.276684829	14.986876452	8.874400857
O	8.602011647	6.498394673	8.791706773
O	18.309448024	12.224196203	0.973754292
O	11.453093956	4.968765884	11.198110282
O	21.159229436	10.519269869	3.261056738
O	9.996759824	9.687545665	0.950258696
O	19.801917037	4.090296286	8.828053589
O	10.027418720	13.031408865	3.187656687
O	19.691992295	7.353369899	11.223303583
O	16.898569836	15.939678360	11.321962460
O	22.298066091	6.615399225	11.309219915
O	22.286074161	12.863672995	2.520743628
O	27.686383960	15.947326788	11.369294701
O	13.345965584	0.886963998	0.596712059
O	7.459525921	11.021386511	0.613671596
O	7.477562087	4.234923650	10.172627288

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O        1.612917121   0.872480693   0.552507838
Zr       9.268240718  11.781100019   1.458366796
Zr      20.494728273   5.304668584  10.643166888
Zr       9.283093344   5.300127402  10.601232136
Zr      20.478170323  11.802450542   1.513803165
Zr      14.887066320   2.096615054   1.455179082
Zr      14.883450439  14.995376816  10.666252949
Br      13.536859263  12.791523960   6.966994051
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CELL_PARAMETERS (angstrom)
  14.853213453   0.008720107   0.083402168
   7.368134377  12.851338251   0.049866652
   7.410885207   4.257203373  12.162490936

ATOMIC_POSITIONS (angstrom)
H        9.584152101   9.167457657   4.909375680
H       16.172551266   5.629611034  10.475485454
H       13.571764634  11.666057583   1.794190561
H       20.154014594   7.604107451   7.003675561
H       11.510115163   4.386266463   6.960524332
H       18.227291087   8.045001310   1.848344140
H       11.739177712   8.859177918  10.438253728
H       17.986278802  12.790252244   4.934246142
H       16.957642569   3.621528874   5.078087656
H       16.899327804  11.048250913  10.377310034
H       12.773203774   3.652126567   4.881823124
H       12.995206549  11.066657419  10.456708808
H       16.965046717   5.841139643   1.824527155
H       16.707639320  13.533442249   7.000081510
H        9.592398427   7.696001783   6.974527386
H       16.107437571  11.668390404   1.812615869
H       13.634803813   5.628308699  10.457585063
H       20.145438734   9.075525006   4.936186084
H       11.310129219   8.036131914   1.897399149
H       18.286227324   4.246865427   7.145682433
H       11.761012752  12.845564094   4.731680620
H       18.226980122   8.890287476  10.485322991
H       22.267377896  12.810199243   3.490770143
H       26.878347052  15.435513786  11.042545297
H       17.667196617  15.450018857  10.966173462
H       22.322977142   7.480118183  11.003324706
C        8.656452141   8.809181287   5.362761713
C       15.592377556   5.078640399  11.220168275
C       14.150892882  12.223587994   1.053731434
C       21.081400960   7.957084538   6.545204059
C       11.330730457   3.416869110   6.488884100
C       18.423851947   7.276139692   1.096800729
C       11.550464353   9.623640858  11.196317201
C       18.165217828  13.759979091   5.405449558
C       11.927940651   6.094351389   1.174281263
C       12.287820911  14.128017026   6.390947194
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C	17.752027393	2.981313232	5.469365758
C	17.586057696	10.833459057	11.199660475
C	12.023248914	3.014867545	5.357671705
C	12.237121242	10.827493140	11.207146440
C	17.736307371	6.072786369	1.085233771
C	17.470807395	14.163079728	6.535129712
C	8.661333723	8.004758489	6.492346842
C	15.537606083	12.224506634	1.063765110
C	14.205539815	5.078192201	11.210380899
C	21.076423807	8.761086517	5.415206427
C	11.206022049	7.278937985	1.117525887
C	18.478736835	3.321393678	6.596748763
C	11.560342214	13.779365582	5.260917374
C	18.310624152	9.656247074	11.260746228
C	4.613471791	0.035176307	-0.030299320
C	7.452239185	6.775811036	8.292563931
C	7.432351375	10.102095613	3.617137544
C	10.351280871	0.040573708	0.009423516
C	2.385044428	3.860803612	-0.040822401
C	12.558925814	1.297899485	3.640090897
C	9.693471729	2.955627807	8.306468126
C	5.221480701	8.833080678	0.001111684
C	2.381631340	1.318868658	3.572624988
C	9.642477557	8.831843449	-0.004765467
C	12.574524319	3.870243814	0.065541975
C	5.291117383	2.912479438	8.286079474
C	7.437238401	9.191410145	4.791426913
C	8.866519862	0.088247030	0.033684729
C	6.097902706	0.086593510	0.014104140
C	7.446919392	7.585844038	7.047163857
C	10.384889572	2.556981704	7.057355251
C	4.531304530	7.520841246	0.028288358
C	3.163112018	5.122270190	0.005455058
C	11.765949444	1.755091112	4.806019197
C	11.795462720	5.137300781	0.149373303
C	4.633310962	2.475536389	7.022675538
C	3.179713736	1.763254854	4.745153795
C	10.346160978	7.523858277	0.049674188
O	8.575858788	10.471954600	3.181147937
O	18.335284698	4.932413746	11.220600716
O	11.410910477	12.187927576	0.925401908
O	21.161449139	6.481248035	8.861291685
O	10.005419747	4.096126718	8.792369694
O	19.738974377	9.682631145	0.986793295
O	10.055064632	7.321028649	11.156650053
O	19.666443906	12.979185430	3.245595944
O	13.470871665	3.699076249	0.950124162
O	13.478770396	14.945205909	8.859093540
O	16.346814870	2.137853359	3.231233007
O	16.239745183	13.257800795	11.190520547
O	13.448934671	2.102907368	3.205767752
O	13.477582828	13.269014298	11.224163881
O	16.361930251	3.709048910	0.956383026
O	16.240309432	14.962240812	8.847208869

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O        8.594065713   6.478631002   8.779064072
O       18.286653818  12.203260269   0.971793647
O       11.456398636   4.926479423  11.180406407
O       21.142951719  10.461781835   3.251317883
O        9.943680043   9.669465143   0.909171256
O       19.803801444   4.062011361   8.833905843
O       10.014667195  13.005787750   3.173096062
O       19.709229801   7.341680011  11.258713663
O       16.872921201  15.902393754  11.294023441
O       22.316645448   6.561774250  11.319107889
O       22.275289884  12.809778257   2.519719829
O       27.665243918  15.904796552  11.364563002
O       13.353825084   0.858094163   0.611414474
O        7.429210177  11.010489337   0.592865515
O        7.469267525   4.219408231  10.164435146
O        1.619380791   0.857392670   0.541759482
Zr       9.242841262  11.762320886   1.439043251
Zr      20.500950435   5.272294810  10.656906915
Zr       9.284715328   5.271073258  10.584167633
Zr      20.457317827  11.763915649   1.511543349
Zr      14.909270465   2.049479606   1.471230151
Zr      14.852154119  14.973672649  10.640570732
Br      13.625715330  12.861622608   6.873719851
Br      13.049175603   5.941746594   2.705967309
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CELL_PARAMETERS (angstrom)
  14.867763726   0.032013919   0.068507823
   7.395456625  12.869884263   0.029148523
   7.412598112   4.258519965  12.141647683

ATOMIC_POSITIONS (angstrom)
H        9.636296950   9.167349840   4.833279923
H       16.207703718   5.576920018  10.344007811
H       13.638492979  11.691782022   1.711712829
H       20.211547829   7.658433496   6.918120965
H       11.469448630   4.430994938   6.790574144
H       18.211357361   8.200931237   1.490935903
H       11.948566140   8.633191544  10.599812632
H       18.136984641  12.745028430   4.917592577
H       16.955247052   3.611278121   5.021638135
H       16.894320451  11.039278345  10.332792294
H       12.720172632   3.682905661   4.710922749
H       16.863366656   6.055996138   1.572293224
H       16.873427031  13.501065323   6.988064605
H        9.636519815   7.711788537   6.907700798
H       16.172506589  11.684659439   1.720091514
H       13.673260847   5.584024475  10.334601790
H       20.211211055   9.113240062   4.839978707
H       11.473107725   8.105555062   1.754570190
H       18.302800275   4.253546449   7.071436503
H       11.883743833  12.912721059   4.574894137
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H	18.203641212	8.868759442	10.442522309
H	22.327981482	12.822254552	3.387951593
H	26.967215379	15.453283870	10.894012924
H	17.731959086	15.474166857	10.858123578
H	22.350859509	7.496884160	10.916081630
C	8.706266771	8.816250516	5.287438942
C	15.629930924	5.037113688	11.098569880
C	14.215621363	12.234795351	0.958953658
C	21.140932501	8.004453307	6.458781385
C	11.325514294	3.437814719	6.357348698
C	18.455482833	7.346040229	0.855377648
C	11.697738795	9.472797972	11.251062341
C	18.279988254	13.738251431	5.350892066
C	12.040667859	6.137717978	1.060611410
C	12.406357105	14.193769381	6.235862948
C	17.778216131	2.993294566	5.389069630
C	17.619247092	10.840266495	11.125501490
C	12.011292765	3.028082293	5.224840786
C	12.436558570	10.647398298	11.214751239
C	17.718551285	6.175721492	0.902014229
C	17.593591116	14.148848348	6.482153193
C	8.706254334	8.019842087	6.423280493
C	15.602864803	12.229692675	0.962935566
C	14.242635275	5.042061747	11.094289812
C	21.140836562	8.799826630	5.322300395
C	11.329919156	7.328587261	1.000925220
C	18.516364840	3.342962117	6.505328039
C	11.663049785	13.832604454	5.120570325
C	18.330982381	9.655738215	11.190233609
C	12.059415188	4.289900960	12.042664738
C	7.489982063	6.799911757	8.226810327
C	7.487638545	10.098179493	3.527863464
C	17.802669745	4.272067033	12.058246095
C	9.809335647	8.109314122	12.074080175
C	12.587477972	1.279734331	3.554009520
C	9.741524012	2.962306917	8.220751550
C	12.739382685	13.063565632	12.024968673
C	2.403435397	1.308275314	3.506501239
C	17.138020162	13.117999961	12.049813270
C	20.018637946	8.131342619	12.138307481
C	5.346775951	2.927911003	8.181356197
C	7.489126248	9.197747816	4.710603148
C	16.316999714	4.316859106	12.083044708
C	13.545696323	4.327398232	12.075274757
C	7.489872836	7.608408102	6.979586646
C	10.432737574	2.555930684	6.974932556
C	4.670615602	7.469077327	-0.096356798
C	3.198969903	5.099303901	-0.026219064
C	11.799445223	1.739234500	4.721731207
C	11.851865459	5.153811222	0.070243459
C	4.693108570	2.500189829	6.913815893
C	3.215351690	1.767077949	4.661809711
C	17.840868849	11.810791840	12.104871364
O	8.630303472	10.467939507	3.090823639

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O       18.375156817   4.915938194  11.112975759
O       11.470569335  12.210362947   0.840796394
O       21.213484151   6.528324589   8.779385534
O       10.039601551   4.109059102   8.699983274
O       19.842719621   9.658319418   0.866617070
O       10.075317579   7.309461207  11.115142277
O       19.725148919  12.979963729   3.136547162
O       13.491349303   3.690780973   0.889688864
O       13.556491085  14.974467354   8.733312778
O       16.372408373   2.141949149   3.156657411
O       16.327150068  13.289172453  11.082162559
O       13.474496720   2.088728917   3.121135951
O       13.559103495  13.286567847  11.079786937
O       16.376417652   3.743259374   0.903949939
O       16.324166297  14.982103220   8.745915603
O        8.632231303   6.503247120   8.715590229
O       18.354569245  12.188862750   0.854059118
O       11.490033404   4.929482642  11.094414359
O       21.212338524  10.474109360   3.140837840
O       10.023840853   9.694442979   0.826629917
O       19.868339437   4.096973337   8.722143726
O       10.064308311  13.011684983   3.091132253
O       19.733952666   7.343348073  11.172790568
O       16.938956869  15.927210758  11.188145828
O       22.351267170   6.578906748  11.233109065
O       22.336399530  12.824389267   2.416834635
O       27.745701280  15.926780142  11.230093413
O       13.390737162   0.849586700   0.530839675
O        7.493079631  11.011656212   0.497926175
O        7.503153693   4.221842963  10.073635403
O        1.643093976   0.850097338   0.483250367
Zr       9.300449001  11.771770246   1.354930932
Zr      20.542397070   5.286100900  10.557596837
Zr       9.314767875   5.271674593  10.504408968
Zr      20.526979311  11.767238408   1.398672361
Zr      14.937251513   2.049425379   1.398838620
Zr      14.927021513  14.993714193  10.521087263
Br      13.809981270  12.983833160   6.661515711
Br      13.229337626   6.020521595   2.545887198
Br      13.891143860  10.620668959   9.990483372
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CELL_PARAMETERS (angstrom)
  14.906005865   0.043917377   0.049099964
   7.424808817  12.868218027   0.014297675
   7.419266341   4.257015782  12.113386568

ATOMIC_POSITIONS (angstrom)
H        9.636088856   9.186563501   4.805121338
Br      16.272253858   6.069870736   9.531104260
H       13.774323079  11.709199529   1.730831254
H       20.280710036   7.628779871   6.886571330
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H	11.341727715	4.473928201	6.680408514
H	18.447243872	8.107325738	1.638435180
H	11.720116729	8.767378201	10.328483483
H	18.404187111	12.642995043	5.053373080
H	16.708748164	3.364534306	5.278334982
H	16.649392061	10.867307853	10.555056875
H	12.584931036	3.734576488	4.593997279
Br	13.495016152	10.841863468	9.542845512
H	17.128966845	5.945379883	1.755269771
H	17.171692113	13.382021980	7.149412493
H	9.666272910	7.730857950	6.879577097
H	16.299795926	11.788142485	1.622136643
H	13.591436965	5.535812911	10.297675291
H	20.250142268	9.084644993	4.809301324
H	11.730918532	8.247305178	1.528629892
H	18.086110528	4.038875891	7.294194024
H	12.153358672	13.185690337	4.299527697
H	18.001954951	8.725971642	10.635689057
H	22.369798777	12.827428973	3.360586257
H	27.035745522	15.480918288	10.809297162
H	17.760429195	15.450227660	10.844422433
H	22.414619164	7.507214607	10.874926546
C	8.713315477	8.821807355	5.263239899
C	15.582089837	5.061092957	10.993692973
C	14.297283015	12.257536295	0.943291527
C	21.202746489	7.988493025	6.422791656
C	11.276738115	3.449867967	6.303965161
C	18.597508464	7.304284991	0.912489263
C	11.565422859	9.553166795	11.070573521
C	18.466271021	13.667674489	5.428636564
C	12.223434964	6.234257483	0.915421837
C	12.591960099	14.391765271	6.040771223
C	17.651728641	2.869197408	5.522792980
C	17.495992019	10.745828343	11.236591931
C	11.955811345	3.045911116	5.164691969
C	12.282232605	10.740543214	11.005720308
C	17.878331622	6.124163934	0.980098077
C	17.791362569	14.071277978	6.569681084
C	8.729945053	8.025206696	6.398410961
C	15.680112994	12.300763804	0.881753098
C	14.194527189	5.021824889	11.049158508
C	21.186302947	8.784230264	5.287171192
C	11.487014087	7.409049491	0.872942160
C	18.409567860	3.240631206	6.619663729
C	11.823454271	13.994149126	4.955642587
C	18.235120407	9.576197266	11.283632929
C	12.061613023	4.264276534	12.054677525
C	7.530123756	6.794421192	8.206925311
C	7.476434137	10.089262305	3.511305661
C	17.841468414	4.320506976	11.975460444
C	9.831956528	8.097672062	12.061129164
C	12.607734569	1.278419429	3.541355263
C	9.782698083	2.939879907	8.231595508
C	12.726074202	13.078929328	11.962782687

C	2.372504855	1.294675772	3.533744862
C	17.140547699	13.099507525	12.032781010
C	20.081938791	8.151965228	12.086378286
C	5.378317072	2.951144139	8.143929600
C	7.488645222	9.187111744	4.691775954
C	16.350210801	4.383378350	11.960968209
C	13.550841784	4.313256874	12.062571703
C	7.520898381	7.598272535	6.958205784
C	10.489911404	2.524826922	6.997766171
C	12.055530878	11.750173554	11.961679006
C	10.620293174	9.357313444	12.075357681
C	11.839467454	1.721043225	4.728934365
C	19.324201461	9.429459437	12.160442641
C	4.710274187	2.546076262	6.877568455
C	3.190088503	1.767038138	4.677119511
C	17.850788950	11.796663226	12.086858423
O	8.619030454	10.465123898	3.079384273
O	18.449445629	4.955429013	11.055517973
O	11.507923220	12.185184546	0.871693830
O	21.292567050	6.543376260	8.744045146
O	10.069854026	4.093503594	8.701025339
O	19.860074718	9.685970769	0.815606656
O	10.094927825	7.293677442	11.103933066
O	19.767535608	12.981021052	3.100358962
O	13.525012168	3.697391038	0.886209666
O	13.604797646	14.977584350	8.674400673
O	16.362548697	2.129103886	3.178594473
O	16.322453427	13.264661126	11.070712447
O	13.482918726	2.094934025	3.101805175
O	13.573766389	13.294890862	11.042112876
O	16.444612949	3.738398982	0.912318475
O	16.388812369	14.961313199	8.737955338
O	8.671309370	6.493233916	8.695626847
O	18.384892468	12.229031612	0.798140197
O	11.488652971	4.903124415	11.110148214
O	21.238919763	10.472214107	3.102100829
O	10.027423859	9.684963937	0.829052683
O	19.942811177	4.127617821	8.675459181
O	10.077603004	13.003610558	3.094647683
O	19.814601434	7.375515749	11.108144218
O	16.970169885	15.911228979	11.169855318
O	22.414094764	6.591811909	11.199268461
O	22.378211117	12.828338129	2.389436094
O	27.812950425	15.946157162	11.159514994
O	13.427649803	0.864416715	0.512486831
O	7.501503470	11.014530476	0.489482736
O	7.521734978	4.216690823	10.051137596
O	1.639493268	0.842890899	0.503846694
Zr	9.310307692	11.762010235	1.358512652
Zr	20.607952234	5.309397728	10.509518967
Zr	9.328980592	5.260723478	10.496060269
Zr	20.567742122	11.781517277	1.357777941
Zr	14.970099708	2.059295173	1.393679608
Zr	14.955582737	14.987102055	10.485086011

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Br      14.269508238  13.517955383   6.211398574
Br      13.646135033   6.254792893   2.183064034
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CELL_PARAMETERS (angstrom)
  14.894221987   0.036856591   0.035628200
   7.412770231  12.864371196   0.030416006
   7.400320523   4.274913639  12.134252087

ATOMIC_POSITIONS (angstrom)
H        9.613705400   9.004130800   4.701622762
Br      16.237981077   5.873609096   9.402325894
H       13.759681161  11.815288032   1.811755268
H       20.236281144   7.812447273   6.996125550
Br      12.040730684   5.191477871   6.910505192
H       18.320760640   8.189261817   1.514678022
H       11.860513244   8.681134596  10.534480947
H       18.042030056  12.809380456   4.915766278
H       16.841449760   3.519951463   5.115666582
H       16.842043658  11.019133874  10.350464845
H       12.869069782   3.605122648   4.699110854
Br      13.748141907  10.687457885   9.829840165
H       16.978884007   6.044065501   1.637342361
H       16.862948251  13.675799679   6.986365372
H        9.629179909   7.560027584   6.783456182
H       16.285711705  11.862894070   1.676033039
H       13.559377275   5.430271596  10.232551902
H       20.220315851   9.245884208   4.903376074
H       11.454368533   8.085357116   1.764358656
H       18.217898871   4.182948532   7.136006843
H       11.947376881  12.971386174   4.512866271
H       18.160287418   8.855720884  10.455262054
H       22.340300368  12.804329668   3.356462388
H       27.007292330  15.481252363  10.819894060
H       17.744850534  15.492397391  10.873384201
H       22.366217642   7.531321591  10.896756324
C        8.687796035   8.722372672   5.209305759
C       15.552674691   4.985018705  10.941693702
C       14.280913076  12.306948334   0.986550503
C       21.160327869   8.091329622   6.483329580
C       11.477435137   3.462026769   6.347812994
C       18.530293144   7.344769428   0.853535201
C       11.644878985   9.509981143  11.211603789
C       18.265394995  13.791992359   5.338517067
C       12.019841892   6.116743389   1.074302994
C       12.457891066  14.240492976   6.187448626
C       17.713151918   2.942450483   5.432955190
C       17.576983319  10.828328532  11.136479869
C       12.119682173   2.995731408   5.208985557
C       12.379023428  10.686593006  11.148999095
C       17.796694809   6.173546059   0.923589786
C       17.625921470  14.264252013   6.470509607
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C	8.697175344	7.935875623	6.351892527
C	15.663280185	12.332721120	0.910003543
C	14.165387460	4.964971280	11.013268281
C	21.151428862	8.874524964	5.339344066
C	11.309871616	7.307763723	1.011551756
C	18.470147550	3.306458745	6.532493841
C	11.694611803	13.862074304	5.091800942
C	18.293833509	9.646395011	11.198812749
C	12.037257791	4.300074253	12.084590404
C	7.492462857	6.825989874	8.232782051
C	7.466372772	10.078739102	3.511295761
C	17.811987034	4.304740635	11.960765843
C	9.802748024	8.130756732	12.104363416
C	12.581384238	1.260065258	3.517661068
C	9.787069154	3.029801422	8.232076188
C	12.731752128	13.087010342	11.987761628
C	2.356672912	1.289012424	3.541198994
C	17.125052718	13.121974359	12.040616798
C	20.020297905	8.148144229	12.120724704
C	5.366920405	2.951811667	8.156195446
C	7.469378276	9.182001671	4.695050239
C	16.322230069	4.365779643	11.946301707
C	13.526083709	4.331453265	12.077798407
C	7.486421967	7.616809557	6.976500163
C	10.513648552	2.659508992	6.987749549
C	12.070664410	11.753466161	12.014166937
C	10.605961430	9.379564563	12.131114425
C	11.818185709	1.733080417	4.700917133
C	19.239239459	9.411585903	12.212421953
C	4.688155788	2.513877525	6.905884732
C	3.171120995	1.752123211	4.691926377
C	17.809760756	11.806246379	12.106955627
O	8.611938372	10.443889978	3.077143802
O	18.419285870	4.944091923	11.043758962
O	11.491067373	12.196085313	0.895695309
O	21.240410135	6.567912901	8.754873612
O	10.059484648	4.161162150	8.746313046
O	19.863573293	9.674959588	0.797275055
O	10.064180126	7.332554627	11.142440051
O	19.716380381	12.961751726	3.099019424
O	13.511732378	3.696938365	0.876368997
O	13.604883975	14.994587123	8.699299976
O	16.344019490	2.123473139	3.166348779
O	16.332313571	13.303836910	11.058640940
O	13.468557999	2.064742400	3.082587567
O	13.567155532	13.305712352	11.056091241
O	16.413803697	3.745840514	0.912492312
O	16.378101531	15.030180271	8.720164324
O	8.631302879	6.533154483	8.728233843
O	18.363936900	12.194226908	0.780716886
O	11.463992789	4.953490307	11.151411161
O	21.220109396	10.464326392	3.088080632
O	10.019610315	9.681737728	0.826056043
O	19.922391556	4.126390980	8.662247770

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O       10.042698660  12.992195735   3.118630185
O       19.756154629   7.370448346  11.142704553
O       16.949028530  15.944648012  11.197643218
O       22.370325182   6.612576266  11.211321273
O       22.348840598  12.811574689   2.385343057
O       27.784575170  15.950602629  11.164717014
O       13.407333687   0.858687456   0.494373857
O        7.496382530  11.012520640   0.485703544
O        7.507736909   4.249645174  10.072223041
O        1.635683137   0.849852188   0.510838870
Zr       9.298174869  11.758115556   1.367702428
Zr      20.572947927   5.319309098  10.509171776
Zr       9.306302639   5.306647482  10.528297372
Zr      20.547997012  11.767780402   1.344681900
Zr      14.950997987   2.052876936   1.379820597
Zr      14.947696018  15.013241523  10.499694127
Br      13.955635051  13.116884186   6.521330699
Br      13.184649260   5.991769932   2.576508728
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UiO-66-Br

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CELL_PARAMETERS (angstrom)
  14.885548478   0.018777779   0.054924702
   7.392927760  12.856029457   0.019449021
   7.406518823   4.246783953  12.148621544

ATOMIC_POSITIONS (angstrom)
H        9.505502402   9.154524103   4.741764776
H        6.374157645  -1.114425382   1.781935851
H        5.373097620   7.524992524   6.943600307
Br      11.693021271   5.304726501   6.688269758
H        3.978025583   7.827260798   1.834349373
H        3.713897890   4.828833022  -2.116541982
H       10.874240754  -0.204233871   5.077308447
H        1.888004607   3.385511582   5.196086552
H        9.421567664   6.692324671  -1.747816397
H       12.622862629   3.685571690   4.541051637
Br       5.163778718   7.131296231  -3.053612639
H        2.692804317   5.650838333   1.978101001
H        9.701628600   0.647292892   7.158275673
H        9.661724933   7.717424058   6.818377159
H        8.898192340  -1.044555548   1.635526019
H        6.153779534   1.220183853  -1.818465963
Br       4.417403227   8.995408212   4.703840462
H       11.480742464   8.080675810   1.757505554
H        3.280331558   4.052882187   7.200273424
H        4.640057255   0.181382737   4.405226334
H       10.758977631   4.544688658  -1.646367690
H        0.031174469  -0.101397514   3.306261487
H       -2.691893334  -1.678421760  -1.388418472
H        2.946237418  -1.673953369  -1.261415779
H        0.109885405   3.204456965  -1.264359334
C        8.610745314   8.778865223   5.244404622
C        8.153538902   0.762472957  -1.136751335
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C	6.887528763	-0.589671512	0.972255189
C	6.276708772	7.887349300	6.449463751
C	11.338286409	3.483324449	6.268699166
C	3.899149119	7.151543054	0.977175694
C	3.780074255	5.495755866	-1.254369357
C	10.985012605	0.827201793	5.422164580
C	12.056924788	6.114946111	1.069420096
C	5.126053919	1.420898492	6.109286684
C	2.798045348	2.845004784	5.468200595
C	10.167026417	6.515380320	-0.968404962
C	11.978866923	3.024347318	5.126299327
C	4.458339644	6.702863931	-1.339719255
C	3.201332731	5.958841936	1.061062526
C	10.348178934	1.292731238	6.558233702
C	8.698717928	7.998706387	6.384341735
C	8.269027453	-0.551408448	0.890256220
C	6.766981094	0.729027054	-1.059930267
C	6.196653846	8.664310001	5.301872741
C	11.329315846	7.296220600	1.013306109
C	3.564661133	3.212422677	6.560633181
C	4.352152854	1.033863869	5.024162228
C	10.898886596	5.341718179	-0.910756030
C	4.649051780	0.003226074	-0.011129770
C	7.549300504	6.780679748	8.257330474
C	7.406829852	10.046865589	3.504489403
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C	9.815394223	2.974725124	8.270650951
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C	2.366019738	1.269526017	3.570246497
C	9.702776321	8.811158507	-0.066045041
C	12.651670707	3.861193275	-0.003714511
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C	7.370556471	9.141036516	4.687943263
C	8.930775744	0.110612676	-0.159982993
C	6.137026418	0.050781881	-0.016671348
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C	3.155526913	5.130170084	-0.062216782
C	11.812098219	1.703094056	4.715593298
C	11.866170082	5.123407709	0.086514294
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C	3.189396525	1.736001671	4.713861169
C	10.404010206	7.502333063	-0.007447201
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O	1.575959683	3.673950627	0.907592082
O	4.076577143	0.652244447	-0.947877065
O	2.632181251	0.104229417	3.122645044
O	2.151137994	-1.222326980	-0.934357263
O	0.110966488	2.286728302	-0.946919684
O	0.046074417	-0.099157162	2.335185560
O	-1.907454717	-1.224981305	-1.038435137

O	-1.466103284	0.825309014	0.462813715
O	0.088607452	-1.852587583	0.468070354
O	0.135989860	-0.040281677	-2.057461476
O	1.650245142	0.824136266	0.532082168
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Zr	1.933351472	1.006837012	-1.583398537
Zr	-1.758780639	-1.128387024	1.274626134
Zr	0.080704231	2.008178563	1.359483205
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Br	6.717825248	0.407305998	6.349878406
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O	13.539860709	3.681334435	0.889532796
O	5.072406261	4.066748500	8.641115693
O	6.225549948	2.100282801	8.680934333
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C	12.579314201	1.239088203	3.533294169
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