

Title	Mixed-linker UiO-66: structure-property relationships revealed by a combination of high-resolution powder X-ray diffraction and density functional theory calculations
Authors	Taddei, Marco;Tiana, Davide;Casati, Nicola;van Bokhoven, Jeroen A.;Smit, Berend;Ranocchiari, Marco
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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

Marco Taddei,^a Davide Tiana,^b Nicola Casati,^c Jeroen A. van Bokhoven,^{a,d} Berend Smit,^{b,e} Marco Ranocchiari^{a*}

^a Laboratory for Catalysis and Sustainable Chemistry, Paul Scherrer Institute, 5232 Villigen-PSI, Switzerland

^b Laboratory of Molecular Simulation, EPFL, Rue de l'Industrie 17, 1951 Sion, Switzerland

^c Swiss Light Source, Paul Scherrer Institute, 5232 Villigen-PSI, Switzerland

^d Institute for Chemical and Bioengineering, ETH Zürich, Vladimir Prelog Weg 1, 8093 Zürich, Switzerland

^e Department of Chemical and Biomolecular Engineering, University of California, Berkeley, CA 94720, USA

ELECTRONIC SUPPLEMENTARY INFORMATION

Table S1. Amounts of BDC and ABDC used for the preparation of DS-MIXUiO-66-NH₂.

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

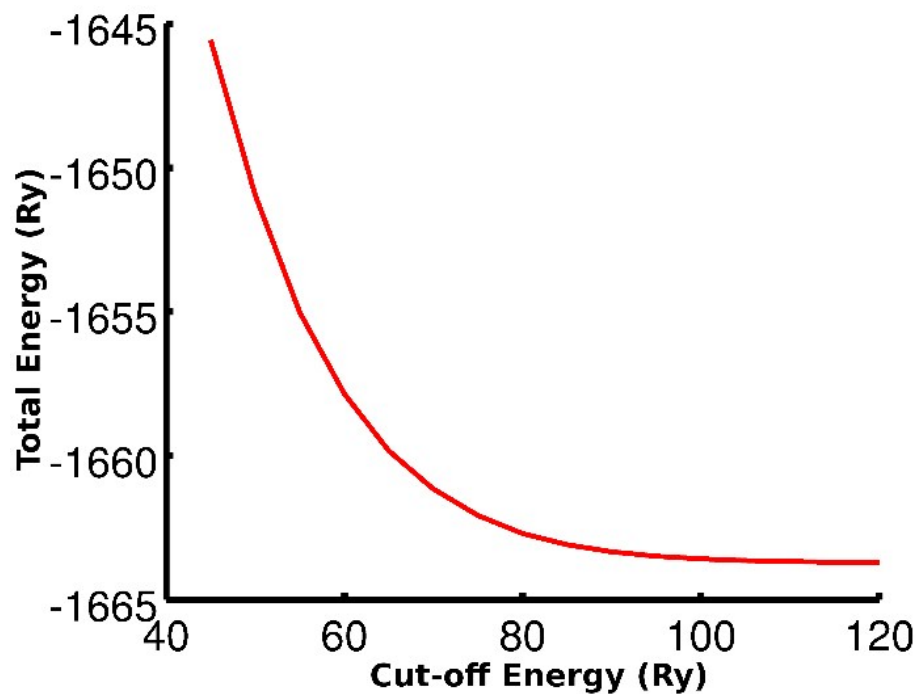


Figure S1. Energy cut-off convergence for the PBEsol norm-conserving pseudopotential.

Table S3. ABDC content of DS-MIXUiO-66-NH₂ from quantitative ¹H-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 ¹H-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-NH₂ after solvent evacuation.

Sample name	<i>a</i> (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)

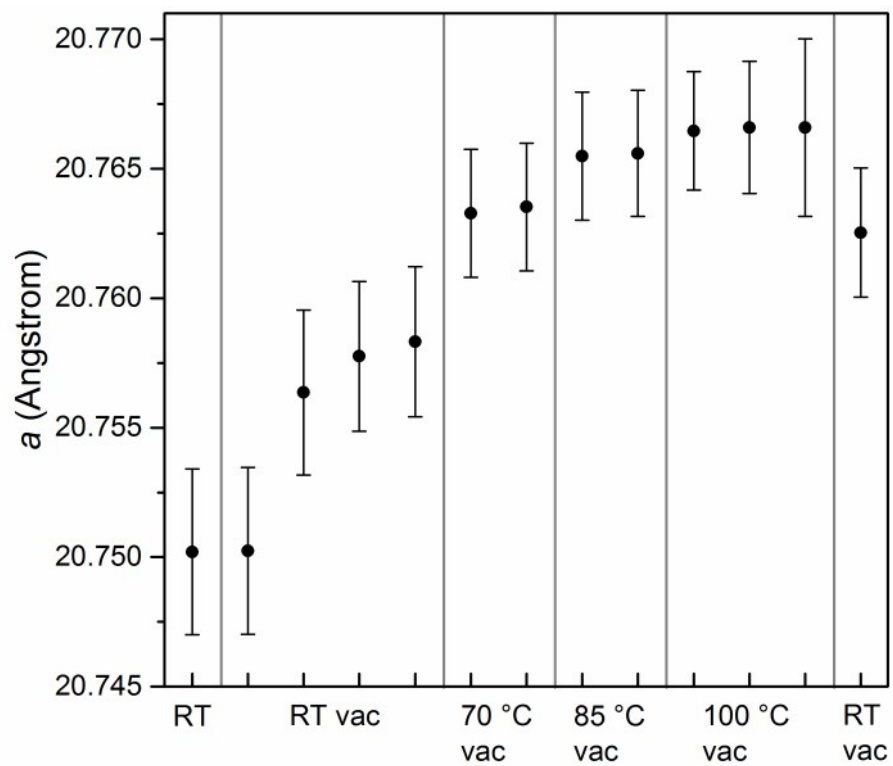


Figure S2. Refined lattice parameter for UiO-66 during in-situ solvent evacuation.

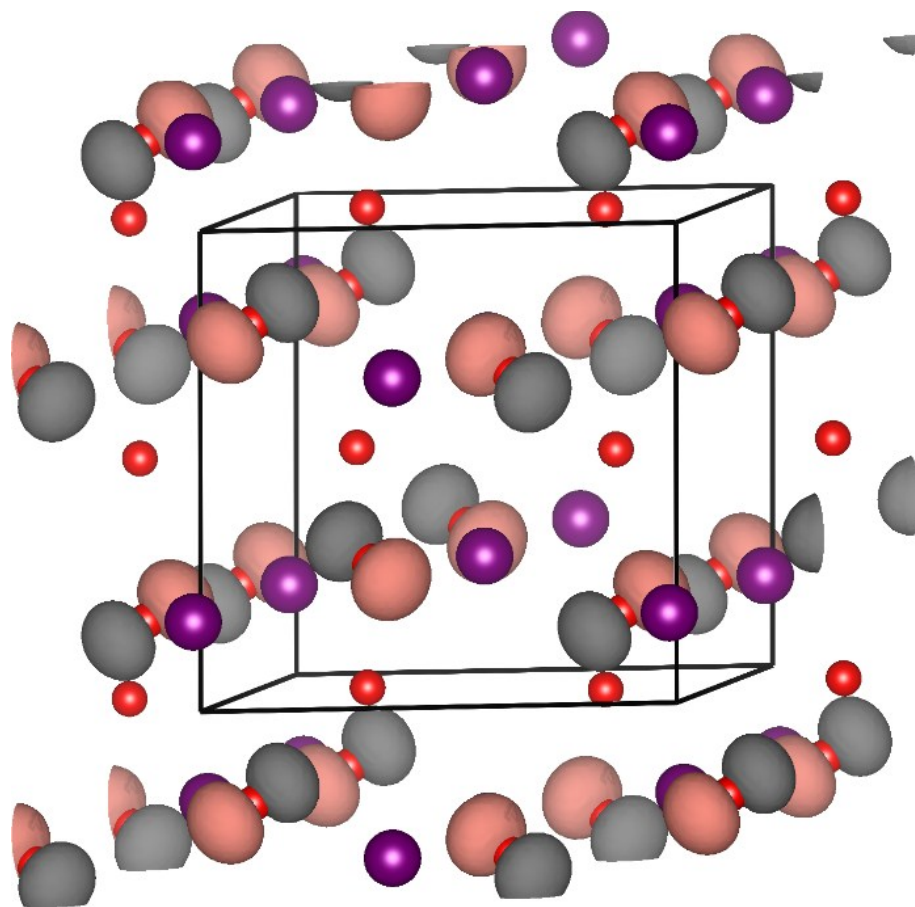


Figure S3. Highest Occupied Crystalline Orbital of ZrO_2 . Adopted colour scheme: O red, Zr purple. Isovalue 5e^{-04} .

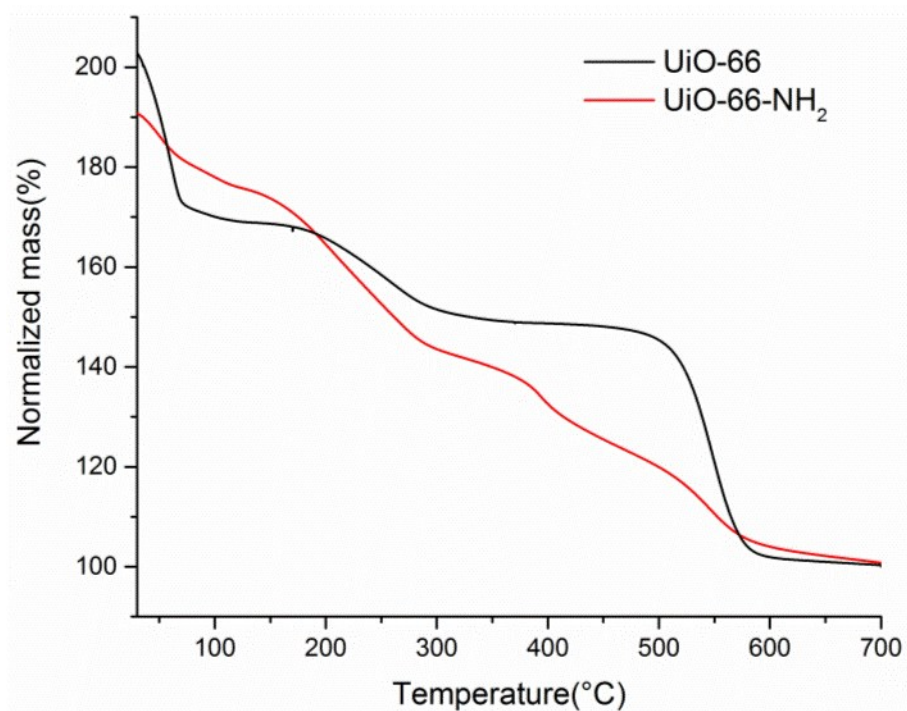


Figure S4. Thermogravimetric curves of UiO-66 (black) and UiO-66-NH₂ (red). Analysis was performed under a N₂ flow. The mass was normalized by taking the mass of ZrO₂ (123 g/mol) as a reference.

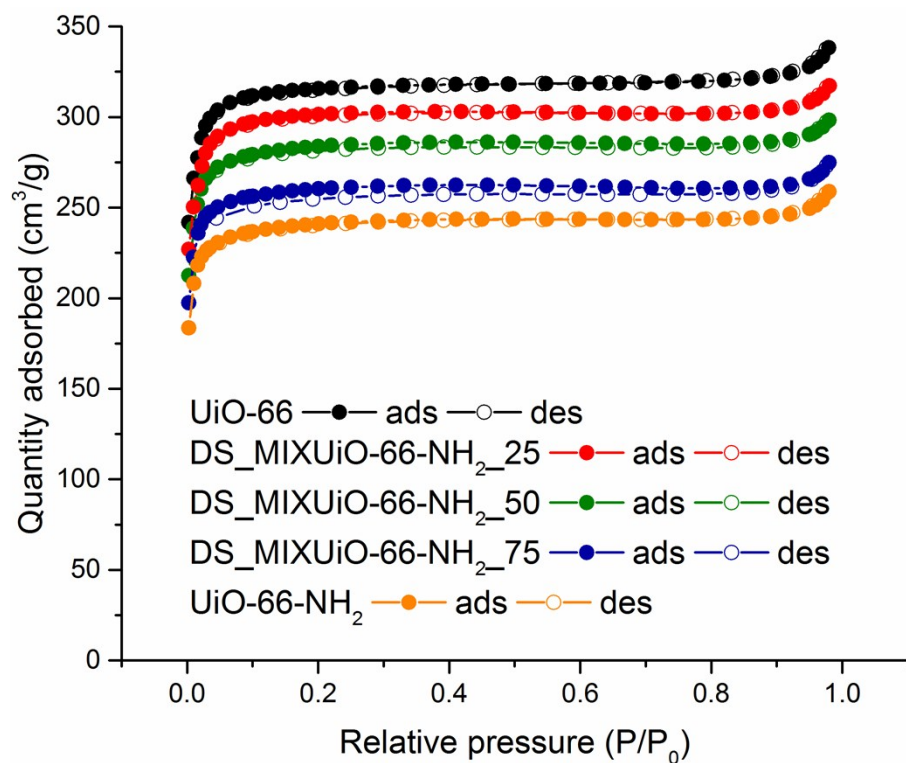


Figure S5. Nitrogen sorption isotherms of DS_MIXUiO-66-NH₂ samples obtained from reaction mixtures containing 0% (black), 25% (red), 50% (green), 75% (blue) and 100% (orange) ABDC.

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

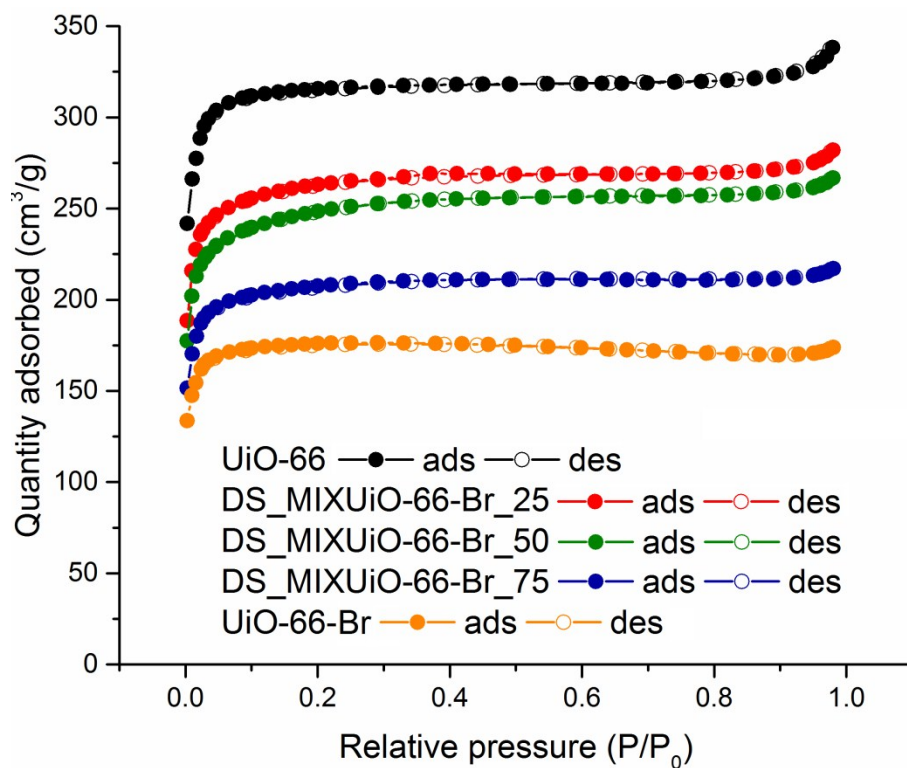


Figure S6. Nitrogen sorption isotherms of DS_MIXUiO-66-Br samples obtained from reaction mixtures containing 0% (black), 25% (red), 50% (green), 75% (blue) and 100% (orange) BBDC.

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 ^1H -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

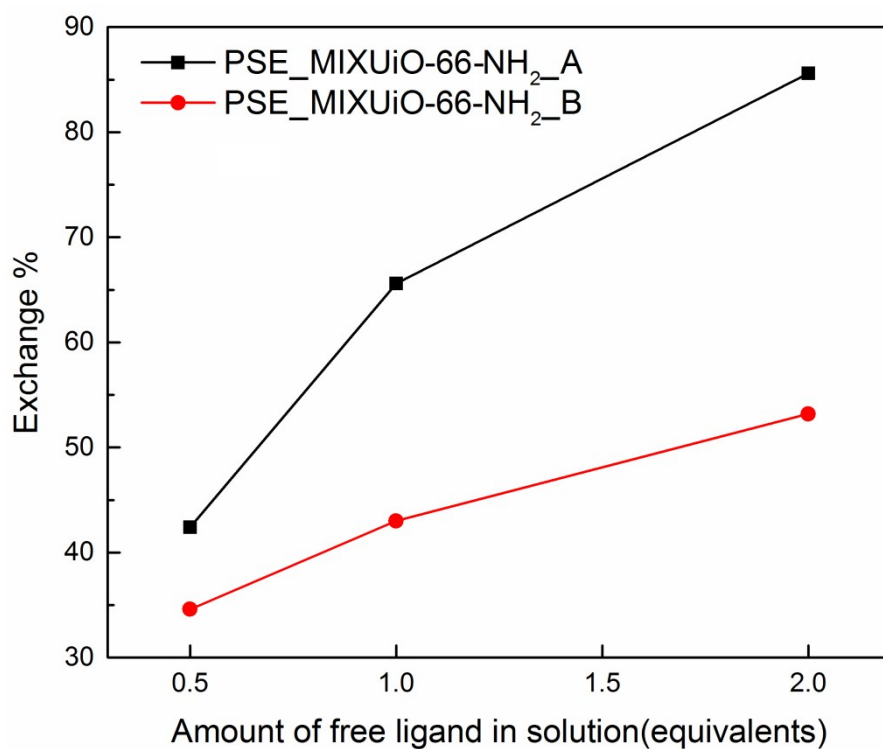


Figure S7. Degree of ligand exchange for PSE of ABDC into UiO-66 (black) and of BDC into UiO-66-NH₂ (red).

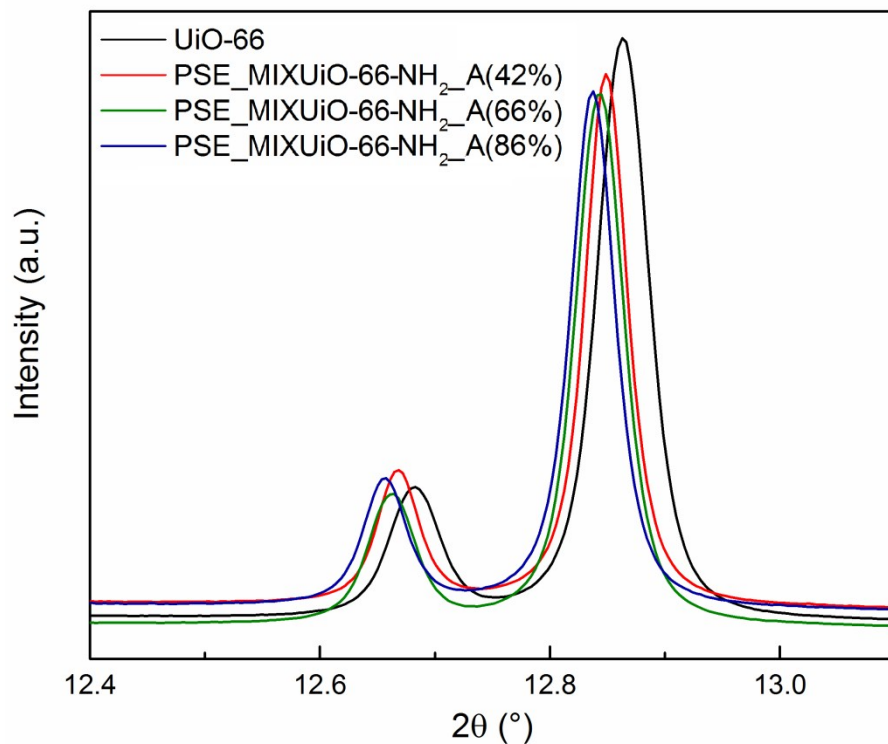


Figure S8. (531) and (006) reflections in the HR-PXRD patterns of UiO-66 (black), UiO-66 exchanged with 0.5 equivalents of ABDC (red), UiO-66 exchanged with 1.0 equivalents of ABDC (green) and UiO-66 exchanged with 2.0 equivalents of ABDC (blue). Intensities were scaled to allow easier visualization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

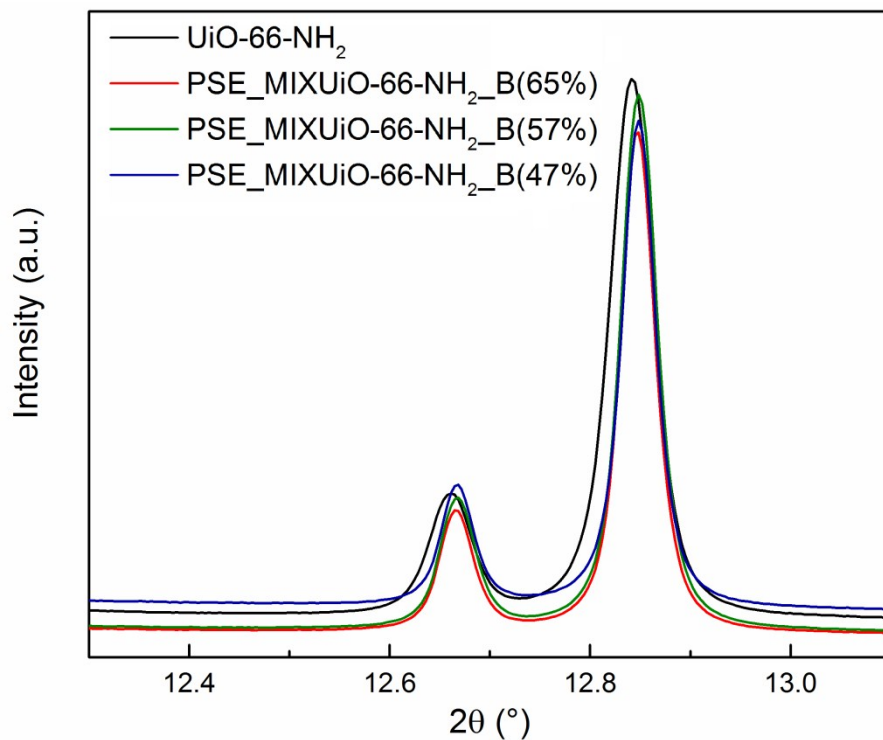


Figure S9 (531) and (006) reflections in the HR-PXRD patterns of UiO-66-NH₂ (black), UiO-66-NH₂ exchanged with 0.5 equivalents of BDC (red), UiO-66-NH₂ exchanged with 1.0 equivalents of BDC (green) and UiO-66-NH₂ exchanged with 2.0 equivalents of BDC (blue). Intensities were scaled to allow easier visualization of the peak shift.

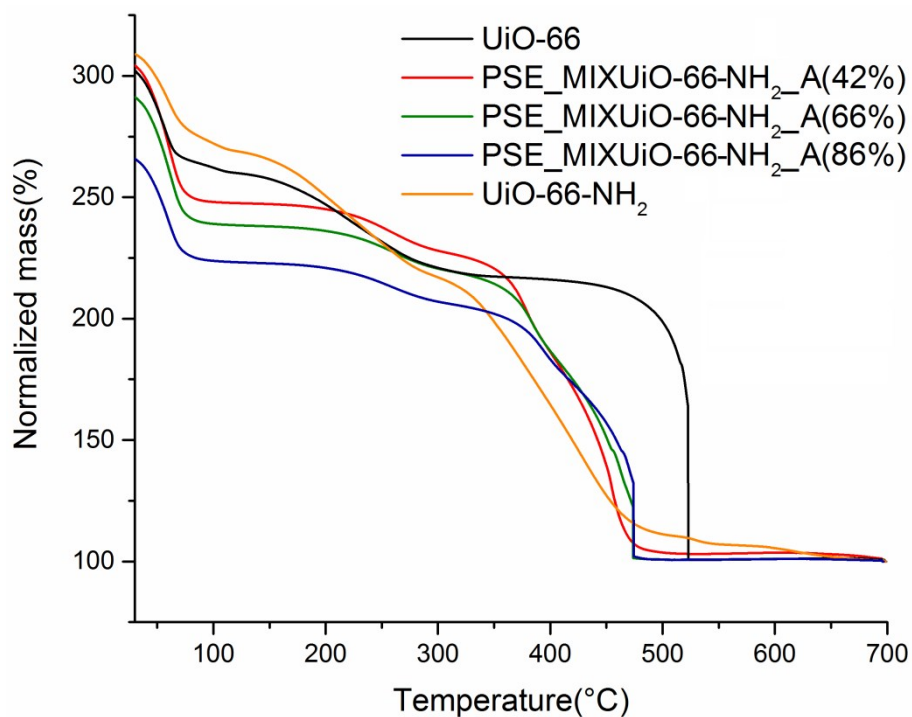


Figure S10. Thermogravimetric curves of UiO-66 (black), UiO-66 exchanged with 0.5 equivalents of ABDC (red), UiO-66 exchanged with 1.0 equivalents of ABDC (green), UiO-66 exchanged with 2.0 equivalents of ABDC (blue) and UiO-66-NH₂ (orange). The analysis was performed under a 80/20 N₂:O₂ flow. The mass was normalized by taking the mass of ZrO₂ (123 g/mol) as a reference.

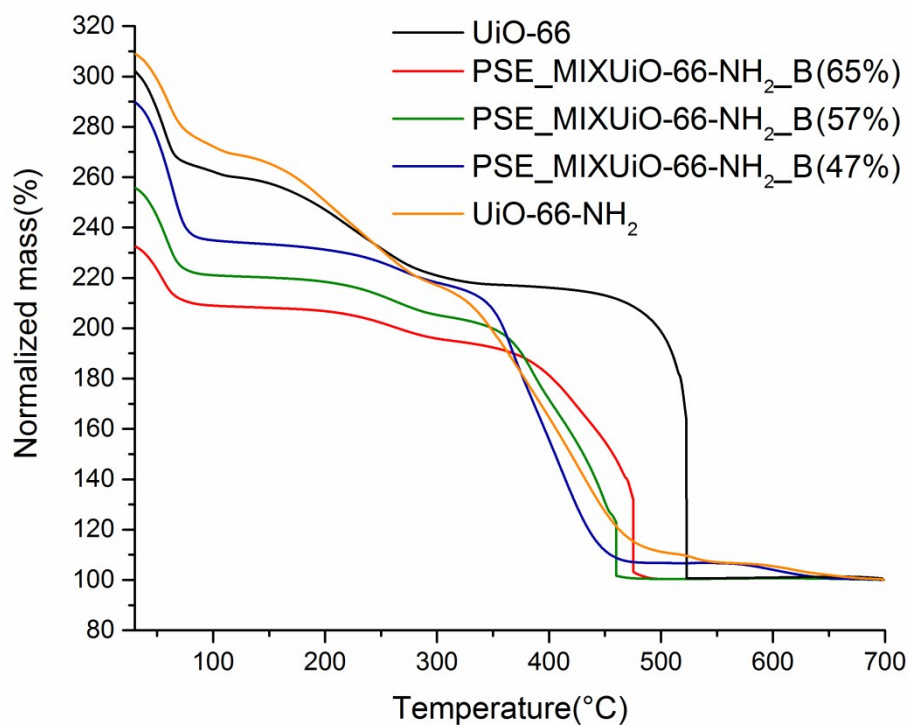


Figure S11. Thermogravimetric curves of UiO-66 (black), UiO-66-NH₂ exchanged with 0.5 equivalents of BDC (red), UiO-66-NH₂ exchanged with 1.0 equivalents of BDC (green), UiO-66-NH₂ exchanged with 2.0 equivalents of BDC (blue) and UiO-66-NH₂ (orange). The analysis was performed under a 80/20 N₂:O₂ flow. The mass was normalized by taking the mass of ZrO₂ (123 g/mol) as a reference.

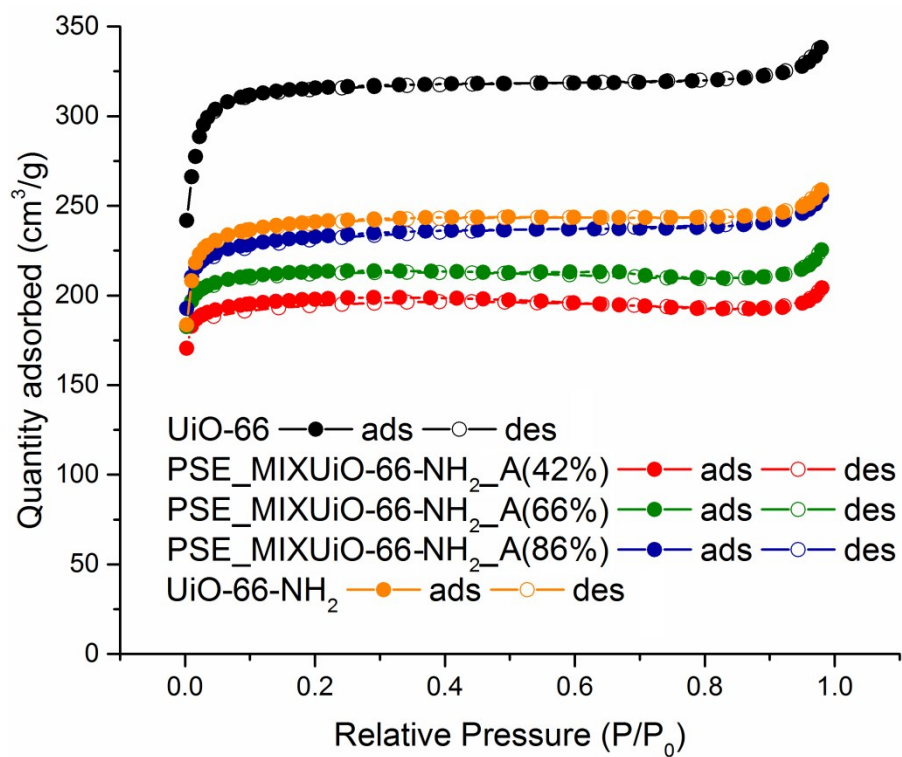


Figure S12. Nitrogen sorption isotherms of UiO-66 (black), UiO-66 exchanged with 0.5 equivalents of ABDC (red), UiO-66 exchanged with 1.0 equivalents of ABDC (green), UiO-66 exchanged with 2.0 equivalents of ABDC (blue) and UiO-66-NH₂ (orange).

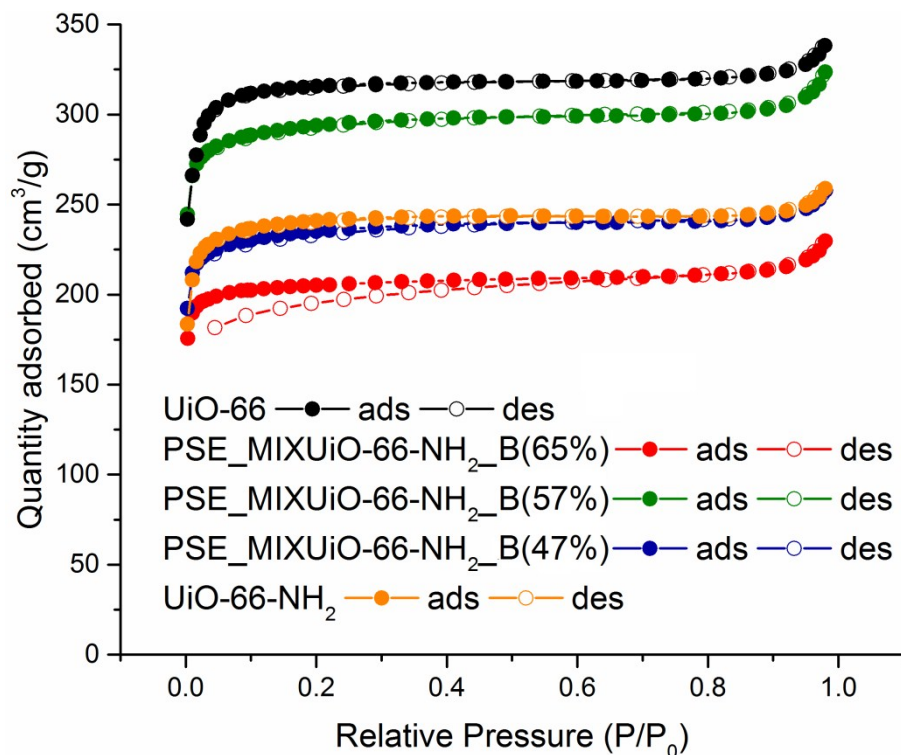


Figure S13. Nitrogen sorption isotherms of UiO-66 (black), UiO-66-NH₂ exchanged with 0.5 equivalents of BDC (red), UiO-66-NH₂ exchanged with 1.0 equivalents of BDC (green), UiO-66-NH₂ exchanged with 2.0 equivalents of BDC (blue) and UiO-66-NH₂ (orange).

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)

H	9.573794500	9.224242713	4.999353760
H	16.126305311	5.725177628	10.530629252
H	13.581332306	11.788042455	1.944524515
H	20.135533152	7.804525235	7.132322743
H	11.472323993	4.479948357	7.073004793
H	18.227930606	8.165666391	1.958980085
H	11.690251172	8.984648294	10.516214815
H	18.026273425	12.911673006	5.058608751
H	12.745655245	5.937941424	1.914150466
H	12.956786609	13.609355568	7.103690438
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
H	9.573941866	7.753890501	7.073614603
H	16.120878372	11.802037417	1.958643293
H	13.586758107	5.711148977	10.516784835
H	20.135339614	9.274816868	5.057932750
H	11.470123083	8.137111553	1.914246963
H	18.228506320	4.520348983	7.101687897
H	11.689404050	12.872333371	5.031786057
H	18.028682825	9.011995833	10.559333491
H	22.281648247	12.952666814	3.605148424
H	26.890317363	15.632981455	11.137712585
H	17.682697088	15.582632971	11.085469328
H	22.283666652	7.650573556	11.085007708
C	8.646223600	8.880674000	5.464710225
C	15.549014486	5.187851509	11.287757652
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C	21.063202458	8.140886688	6.661860567
C	11.295380729	3.512948085	6.594683851
C	18.409908650	7.400323787	1.199644747
C	11.513380825	9.747214033	11.279522914
C	18.197099443	13.882345466	5.531744190
C	11.989081039	6.167594089	1.159232305
C	12.205161254	14.247886920	6.631753797
C	17.717460171	3.147437425	5.498056658
C	17.503657550	10.978059484	11.319360762
C	11.990410216	3.115466013	5.463947779
C	12.206897772	10.948600051	11.287579815
C	17.716311468	6.198977980	1.191520179
C	17.502083699	14.279830661	6.662644249

C	8.646534277	8.079425920	6.595122490
C	15.545632426	12.339318780	1.199885960
C	14.162151661	5.179987097	11.279713301
C	21.062887949	8.942159548	5.531288987
C	11.293903556	7.366248794	1.159250256
C	18.410597101	3.550582020	6.630561224
C	11.512056685	13.844759763	5.499241412
C	18.198881070	9.779266169	11.319356265
C	4.558988204	0.086414487	0.067020311
C	7.428658221	6.875924237	8.399171813
C	7.426680753	10.183576568	3.731544582
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C	2.334945398	3.920824010	0.066928220
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C	9.648083321	3.051514724	8.399737207
C	5.208900381	8.890052236	0.104585374
C	2.334735626	1.356761497	3.685223650
C	9.646971900	8.917436088	0.124325305
C	12.516957213	3.967367723	0.124414686
C	5.208720791	3.028507358	8.371664947
C	7.427041775	9.279067765	4.905912139
C	8.810349185	0.161092434	0.128056049
C	6.042930959	0.144693397	0.111515773
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C	4.505349939	7.580609859	0.127865481
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O	8.570862891	10.547208696	3.295665669
O	18.293942214	5.078675790	11.306406378
O	11.416419730	12.268487006	1.051205235
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O	13.471766605	13.389353514	11.305904253
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O	18.291891411	12.316588624	1.097313514
O	11.418635015	5.031388659	11.260522447
O	21.137800830	10.610483388	3.360731680
O	9.959887711	9.753831968	1.037635689
O	19.751023355	4.244637044	8.933388098

O	10.024811386	13.065131839	3.317810890
O	19.683268856	7.477634548	11.320892081
O	16.885662345	16.035523504	11.406198129
O	22.281520911	6.733890195	11.405853327
O	22.279902269	12.952080484	2.633931324
O	27.680723395	16.092610949	11.465096230
O	13.299933471	0.968349224	0.707848119
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-NH₂-17

CELL_PARAMETERS (angstrom)

14.844632673	0.046401639	0.061439222
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
H	18.266636582	8.088535317	1.839143867
H	11.718157039	8.903388614	10.426737448
H	18.020365437	12.832519149	4.935231897
H	12.755610552	5.831548718	1.824955847
H	16.986442352	3.730320775	5.002566708
H	16.788020305	11.147314173	10.453777059
H	12.775523250	3.684641449	4.894421543
H	13.002133879	11.094475855	10.453020913
H	16.984935647	5.895976291	1.814498210
H	16.757144100	13.556302385	7.015137597
H	9.612064934	7.699008140	6.982301315
H	16.150339090	11.705742239	1.826336375
H	13.621428216	5.640616722	10.440396677
H	20.166567707	9.129409783	4.910943448
H	11.495035834	8.036832948	1.843757016
H	18.306913406	4.366854090	7.068917671
H	11.679048218	12.828013018	4.821252991
H	18.048175415	8.941976710	10.435047166
H	22.295214407	12.878223049	3.483426368
H	26.904066922	15.506000057	11.014249792
H	17.696997029	15.496035431	10.994420722
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C	18.195968717	13.801813788	5.408709445
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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

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
H	13.695129736	13.493393402	7.785405139
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

H	12.777210861	3.663325483	4.895980789
H	13.000319431	11.048790059	10.454048071
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
C	5.236948963	8.826169316	-0.005394117
C	2.384704639	1.314707503	3.578306778
C	9.652295189	8.827688441	-0.015144906
C	12.558034545	3.890129771	0.039171200
C	5.264096990	2.925313782	8.262998379
C	7.446171154	9.184348165	4.787308975
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
H	13.323583282	5.014953103	2.233597195
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
C	17.767325026	6.136196812	0.975422929
C	17.528357018	14.170532575	6.412484670
C	8.722109237	8.008179891	6.420306860
C	15.613576034	12.217965816	0.968416269

C	14.243041453	5.069304066	11.118826238
C	21.145512781	8.749391034	5.285974701
C	11.228535343	7.253421471	1.017905493
C	18.509154843	3.365711482	6.470658373
C	11.643048654	13.812095068	5.140003859
C	18.338512706	9.656250717	11.099664350
C	12.064017569	4.280609239	12.042051889
C	7.507346103	6.775601341	8.214351977
C	7.499828549	10.074839079	3.521733386
C	17.801233684	4.285525201	12.064986722
C	9.812424227	8.108342944	12.075086549
C	12.600706407	1.290524241	3.547727652
C	9.729809667	2.953056294	8.209937737
C	12.699009555	13.050952710	12.013382463
C	2.418333070	1.297662030	3.511526341
C	17.110759592	13.084265396	12.018225412
C	19.986569543	8.131836409	12.105981590
C	5.330258492	2.922090194	8.164331408
C	7.502567732	9.168277885	4.698511684
C	16.316722583	4.333992631	12.095743871
C	13.548440736	4.331622861	12.083812292
C	7.506797410	7.579151399	6.964932977
C	10.421790574	2.554551795	6.961050307
C	4.628392842	7.490029206	-0.106268536
C	3.204872846	5.105570686	-0.023703636
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
O	10.072466174	12.989467062	3.089117877
O	19.756556761	7.330730363	11.135791316

O	16.936139400	15.908600706	11.176001034
O	22.349823279	6.571991143	11.214605628
O	22.338130926	12.806691110	2.406362533
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
H	13.908123566	11.667809818	10.195751240
H	13.629289232	10.001763128	9.665908972

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CELL_PARAMETERS (angstrom)

14.881046027	0.037715652	0.044796762
7.407059878	12.855254644	0.016778581
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
H	18.221132602	8.195900789	1.510679297
H	11.898492605	8.668196733	10.534364112
H	18.067346553	12.813242507	4.760528542
H	16.985117300	3.636764751	4.943965329
H	16.994958279	11.082802861	10.157987103
H	12.848873397	3.647652009	4.807261819
N	13.442764166	10.782759997	10.245499154
H	16.914989018	6.025371904	1.607986025
H	16.787498116	13.537527745	6.831671647
H	9.668296237	7.732606148	6.897313472
H	16.268264783	11.673401096	1.606890640
H	13.587861579	5.635264838	10.399577359
H	20.242362379	9.038721224	4.768749803
H	11.315597646	7.998760905	1.797046763
H	18.319656475	4.297976702	6.995950354
H	11.873650716	12.886598718	4.575840292
H	18.310151586	8.918783103	10.255193966

H	22.369797220	12.824525044	3.353252265
H	26.985130791	15.467154373	10.828531395
H	17.745596994	15.431870144	10.838062924
H	22.386910540	7.499774674	10.872369459
C	8.724531673	8.818347712	5.269640445
C	15.598707063	5.156198442	11.072686583
C	14.276249069	12.187109365	0.941238890
C	21.186926858	7.947998398	6.392410430
C	11.385203049	3.410889990	6.392936399
C	18.458334753	7.352942032	0.856521127
C	11.669191592	9.500956126	11.206270704
C	18.247793564	13.776525098	5.244105330
C	11.969147682	6.050737250	1.084800608
C	12.434493429	14.172254910	6.236608630
C	17.799575970	3.021804127	5.331753976
C	17.651885424	10.839745705	10.995604415
C	12.082297189	3.015901283	5.262695714
C	12.416527961	10.689135555	11.143150648
C	17.744366577	6.174217244	0.913938614
C	17.551059961	14.171638526	6.374620620
C	8.736689583	8.019037097	6.402215303
C	15.655284572	12.235685735	0.897397681
C	14.195340522	5.084977641	11.125062925
C	21.174790671	8.747598872	5.259641132
C	11.232407866	7.246022267	1.007600650
C	18.531082928	3.377905437	6.444892765
C	11.668991370	13.817978937	5.112619995
C	18.372271794	9.664993006	11.051272483
C	12.065375136	4.253002767	12.042319926
C	7.532346796	6.772044205	8.194142163
C	7.493913957	10.080249985	3.509720060
C	17.802343220	4.322444886	12.010874600
C	9.827111713	8.106892760	12.058140313
C	12.613989367	1.313684417	3.526056391
C	9.737606179	2.943944180	8.197825007
C	12.703665332	13.055574025	11.995977850
C	2.413988103	1.299395535	3.506528337
C	17.110688185	13.071158032	11.997214419
C	20.024007373	8.143580784	12.054557028
C	5.336853648	2.933529753	8.143545184
C	7.502699589	9.172437782	4.685446207
C	16.333872036	4.391901503	12.026044178
C	13.549529165	4.315201438	12.077489224
C	7.526395539	7.576906630	6.946155185
C	10.429173849	2.552653779	6.946052833
C	12.035610216	11.749106399	12.015162343
C	10.615463186	9.362722049	12.094384842
C	11.818414347	1.766333977	4.692460405
C	19.240531021	9.382347734	12.120829558
C	4.683197609	2.524143621	6.896038908
C	3.226728803	1.768315660	4.653995381
C	17.807016138	11.762815413	12.042955718
O	8.638069219	10.448864593	3.076403471
O	18.414204848	4.954424800	11.064253607

O	11.500213682	12.154782076	0.848756390
O	21.270092845	6.498330811	8.714512259
O	10.053215371	4.078741942	8.691301827
O	19.840019656	9.692705793	0.814426428
O	10.107432717	7.291219505	11.114217814
O	19.763415778	13.000022000	3.097976613
O	13.504606254	3.701655608	0.863087335
O	13.590454378	14.961398120	8.677919047
O	16.392839647	2.134934501	3.126430016
O	16.299003463	13.254266603	11.025194306
O	13.501635831	2.124446848	3.095007857
O	13.575382540	13.259419151	11.067183232
O	16.403746488	3.747778704	0.880136453
O	16.320608315	14.951382243	8.698004195
O	8.674787242	6.488000988	8.690867505
O	18.382097415	12.221626336	0.815362751
O	11.493761121	4.888110409	11.090548704
O	21.231805094	10.466680950	3.104542131
O	10.001423743	9.651152742	0.802030792
O	19.886507227	4.096079896	8.699641827
O	10.077708970	12.983377635	3.081806376
O	19.805775973	7.348198491	11.075919338
O	16.951976421	15.891994887	11.156548661
O	22.394279846	6.578857082	11.180424216
O	22.365096376	12.816299101	2.382153004
O	27.772866776	15.923638446	11.166481183
O	13.421836214	0.862520590	0.506342868
O	7.502472802	11.004668011	0.496382647
O	7.529257824	4.218731419	10.047513250
O	1.665118327	0.837395924	0.491019148
Zr	9.319417461	11.743956882	1.349612490
Zr	20.587263558	5.289699050	10.504701771
Zr	9.340964884	5.261498566	10.491031251
Zr	20.546154029	11.770582771	1.363735135
Zr	14.973841270	2.051062933	1.367974274
Zr	14.932871618	14.986664643	10.498938193
N	13.462190433	13.365176080	6.621738917
H	13.898560225	13.575646604	7.520132202
H	13.566325640	12.460402806	6.177087470
N	12.760682024	5.828150364	2.168757506
H	13.350036984	4.994156965	2.154045381
H	12.861367497	6.552505227	2.868603622
H	14.031136239	11.614939643	10.309297306
H	13.813420376	9.921465652	9.858328103
H	15.620747808	6.349672315	9.399610231
H	17.207453610	5.889279188	10.058987391

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CELL_PARAMETERS (angstrom)

14.868703703	0.023301641	0.035796216
7.388424546	12.847816055	0.026411940
7.383954154	4.261076989	12.125241255

ATOMIC_POSITIONS (angstrom)

H	9.623008582	9.232329552	4.839884115
N	16.153801387	5.911472147	10.089515778
H	13.710695415	11.639761071	1.721223483
H	20.245426450	7.541472842	6.841789582
N	11.658263551	4.727616721	6.777643668
H	18.133118127	8.227598607	1.417235190
H	11.959989208	8.613058688	10.663883927
H	18.081023603	12.720290497	4.907759313
H	16.940536522	3.610339460	4.950576703
H	16.942810836	11.072328545	10.183599685
H	12.758145170	3.628419188	4.656479857
N	13.518098494	10.723610170	10.377741870
H	16.826310420	6.056926850	1.531968101
H	16.880182334	13.534953978	6.986317975
H	9.656601257	7.793733695	6.933515347
H	16.244145102	11.707389410	1.628585849
H	13.553299872	5.608817004	10.376184503
H	20.212074076	8.983789590	4.751792596
H	11.315949619	7.999881256	1.789137507
H	18.280004618	4.282370506	6.996262429
H	11.846345351	12.884104116	4.592358573
H	18.240591876	8.898258020	10.289895811
H	22.315698362	12.792192814	3.352820955
H	26.939549645	15.452503269	10.821129711
H	17.710147707	15.446351409	10.850455204
H	22.349309762	7.502113959	10.892974206
C	8.705373904	8.840009027	5.285929032
C	15.565467599	5.141277557	11.049853943
C	14.249715677	12.212305391	0.963904055
C	21.164146758	7.926042816	6.392937759
C	11.371073369	3.474886614	6.320635856
C	18.403934236	7.360682758	0.809500877
C	11.697604590	9.468691821	11.293496689
C	18.250350391	13.714291131	5.326481531
C	11.952897199	6.044042485	1.085402613
C	12.406902024	14.174486521	6.250988378
C	17.760757632	3.001437639	5.335100205
C	17.602039464	10.830513428	11.019558090
C	12.028244424	2.998585930	5.173655816
C	12.445780532	10.656367784	11.222779681
C	17.690011556	6.182298685	0.876510747
C	17.600520112	14.163393376	6.456506500
C	8.723338536	8.054627303	6.427201693
C	15.628032299	12.254332481	0.909823694
C	14.163097666	5.075762353	11.112303592
C	21.145640115	8.713191054	5.251287193
C	11.223194379	7.241894434	1.005170666
C	18.494339372	3.363072096	6.445456021
C	11.638674990	13.814874712	5.128605349
C	18.313983441	9.650262498	11.079736106
C	12.037685004	4.271776796	12.061072990
C	7.525897396	6.798997573	8.218715485

C	7.468364469	10.059573151	3.503597222
C	17.770186303	4.314695421	11.990885485
C	9.803308570	8.112122224	12.092192001
C	12.573195005	1.265209746	3.514793080
C	9.747551921	2.965481148	8.195066294
C	12.677800367	13.055105214	11.997817660
C	2.394618469	1.291958729	3.519033688
C	17.079656233	13.072628468	12.008844720
C	19.977282080	8.133771136	12.071972135
C	5.330387982	2.953022748	8.139284616
C	7.482127362	9.165286341	4.689103618
C	16.302991225	4.396975863	12.016143219
C	13.520977554	4.331670538	12.087726049
C	7.517532319	7.596057196	6.966727428
C	10.453830902	2.594557794	6.963858554
C	12.017061794	11.745955387	12.032768952
C	10.599527561	9.362094391	12.131837842
C	11.788582890	1.725246946	4.686401739
C	19.190268851	9.372082039	12.143294240
C	4.667483259	2.532597623	6.901148587
C	3.207781551	1.764959314	4.664822204
C	17.771973867	11.761844978	12.057319316
O	8.613587697	10.432391823	3.074571184
O	18.381125040	4.941156602	11.039810533
O	11.474284370	12.157981923	0.866400845
O	21.251417991	6.514158772	8.731260703
O	10.021191110	4.117314173	8.709817662
O	19.803392792	9.677470570	0.784946779
O	10.082727804	7.300098439	11.145215313
O	19.704959124	12.943887110	3.096981687
O	13.482746566	3.690059686	0.864268336
O	13.576662921	14.981765137	8.676640744
O	16.357267941	2.109765941	3.132478777
O	16.269569794	13.256228600	11.036271085
O	13.458721142	2.075372272	3.075606472
O	13.553846408	13.255241806	11.073496051
O	16.379308640	3.733455857	0.889153689
O	16.315485224	14.965323877	8.715464547
O	8.669185127	6.515930785	8.716983306
O	18.347667211	12.194891852	0.789181224
O	11.463148048	4.911444731	11.114117958
O	21.195462668	10.416543488	3.078674192
O	9.988439595	9.646150911	0.803523806
O	19.866373553	4.102699526	8.684799572
O	10.043058444	12.969736996	3.101619810
O	19.756656833	7.339610017	11.094780090
O	16.916096431	15.899223178	11.178370143
O	22.352462725	6.579271195	11.194952352
O	22.318678655	12.781823291	2.381594697
O	27.728121354	15.908756587	11.157621195
O	13.399018854	0.845790077	0.491948089
O	7.482692981	11.001610174	0.489831892
O	7.508529101	4.235008924	10.059073128
O	1.654457486	0.840639357	0.507701889

Zr	9.293614968	11.733966401	1.360005907
Zr	20.552935862	5.287144125	10.502058475
Zr	9.309436151	5.277324710	10.523601449
Zr	20.508607333	11.742507711	1.349424027
Zr	14.943460258	2.032037301	1.370584352
Zr	14.906538339	14.990267336	10.501025577
N	13.429402158	13.368452302	6.639179460
H	13.939406576	13.623533299	7.484553186
H	13.635529158	12.529434191	6.110242250
N	12.750997749	5.822215027	2.170993498
H	13.380590912	5.019412784	2.106554768
H	12.964159945	6.608374489	2.775260924
H	14.090521587	11.567692649	10.428404879
H	13.928330726	9.850897339	10.061884651
H	15.583585370	6.246116236	9.320895915
H	17.168231933	5.827596416	10.000538390
H	12.161329287	5.359896092	6.165036997
H	11.093955167	5.073966601	7.555225220

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CELL_PARAMETERS (angstrom)

14.854373498	0.014004327	0.045214523
7.373336365	12.848084167	0.020557063
7.381832030	4.248130713	12.134515092

ATOMIC_POSITIONS (angstrom)

H	9.580520044	9.262006465	4.764060790
N	16.138004213	5.890714086	10.087963553
H	13.703450026	11.650515186	1.735400027
H	20.301282174	7.475424979	6.877348013
N	11.640584701	4.716522581	6.769493291
H	18.091054136	8.224530649	1.397273037
H	11.987301125	8.584477279	10.701438737
H	18.079690746	12.684268454	4.933014095
H	16.915669731	3.588832519	4.970160618
H	16.914813963	11.042609403	10.201038027
H	12.740138904	3.607975314	4.656870314
N	13.531385737	10.702603927	10.405364256
H	16.799679323	6.045584270	1.525711104
H	16.906144494	13.490819375	7.031024806
N	10.027801392	7.838809217	6.935212170
H	16.236837615	11.730790329	1.634286830
H	13.536837998	5.571995618	10.380576202
H	20.157548002	8.929424716	4.807252130
H	11.305705305	7.998005017	1.784872364
H	18.261021644	4.264486979	7.010629780
H	11.827847051	12.878213694	4.588648683
H	18.224805238	8.876778581	10.302042151
H	22.271703108	12.773404261	3.355213966
H	26.908559166	15.442442145	10.817946212
H	17.694361889	15.421145663	10.865840530
H	22.351639070	7.472254642	10.904193096

C	8.680932772	8.859014898	5.239376424
C	15.553025321	5.124343598	11.054804426
C	14.237844713	12.219465732	0.971810079
C	21.196125623	7.884980096	6.401867565
C	11.366497062	3.450636201	6.329848881
C	18.371577166	7.353443706	0.799667133
C	11.708804373	9.446490834	11.315362653
C	18.246633008	13.680270991	5.347663604
C	11.947547624	6.044162200	1.081103568
C	12.385223507	14.165074856	6.250386287
C	17.737936358	2.981711414	5.352379598
C	17.580956477	10.806056628	11.033350006
C	12.018402387	2.974555628	5.180971926
C	12.448799339	10.638476846	11.237973780
C	17.666554391	6.170566238	0.874169690
C	17.610565916	14.125319951	6.487251035
C	8.783216336	8.079730034	6.400614955
C	15.615224415	12.268092262	0.913186685
C	14.151603916	5.050969687	11.121096305
C	21.111857688	8.673809889	5.272255480
C	11.212688757	7.238765553	1.002370730
C	18.473452583	3.343526799	6.461613848
C	11.619015251	13.808362315	5.126279504
C	18.299777122	9.629862668	11.090704512
C	12.034276849	4.243898557	12.082939360
C	7.556465226	6.797296466	8.209518664
C	7.426024053	10.051140800	3.491606052
C	17.762540583	4.308951981	11.994597843
C	9.812476875	8.087420825	12.107214442
C	12.554218109	1.247150527	3.516921409
C	9.760594167	2.937080616	8.218076808
C	12.655130760	13.046485388	11.988817796
C	2.385799986	1.281902420	3.526316963
C	17.054306945	13.048801851	12.020991669
C	19.975629763	8.121390652	12.078393845
C	5.332352311	2.947354434	8.139573073
C	7.449725455	9.155620436	4.676585606
C	16.295790028	4.391699851	12.025153628
C	13.516531280	4.311917303	12.106004094
C	7.577136351	7.576753177	6.962959359
C	10.470344613	2.562332608	6.990024410
C	12.002024974	11.733889825	12.029865271
C	10.602750484	9.341093188	12.143641597
C	11.782880600	1.698807872	4.699175093
C	19.183719839	9.357036106	12.150091216
C	4.661660817	2.522971070	6.906595581
C	3.201142994	1.755962356	4.670336725
C	17.751814572	11.740449204	12.067821389
O	8.570810273	10.427428172	3.060467560
O	18.374052484	4.938064720	11.045823801
O	11.458239364	12.145921930	0.875211778
O	21.269280566	6.494254884	8.730813047
O	10.029820854	4.089745336	8.731169927
O	19.766595500	9.672489819	0.773882376

O	10.094374341	7.274555854	11.160200075
O	19.665902666	12.929593185	3.087414415
O	13.478468215	3.688220674	0.865366849
O	13.569127326	14.979883117	8.666043515
O	16.332457304	2.089112338	3.150445367
O	16.242433746	13.231211011	11.049921427
O	13.434371439	2.060960813	3.073665200
O	13.527295850	13.246704590	11.061034268
O	16.377802451	3.711154895	0.904447544
O	16.310160945	14.937126840	8.729713512
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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CELL_PARAMETERS (angstrom)

14.845583769	0.038072374	0.070580895
7.389678592	12.855551993	0.056057464
7.404968607	4.280244852	12.166969742

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

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

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

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

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

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

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

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

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

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

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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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

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
C	2.414969446	3.845553471	-0.035934741
C	9.815394223	2.974725124	8.270650951
C	5.261043737	8.837462873	-0.188875222
C	2.366019738	1.269526017	3.570246497
C	9.702776321	8.811158507	-0.066045041
C	12.651670707	3.861193275	-0.003714511
C	5.409205809	2.929941352	8.166943135
C	7.370556471	9.141036516	4.687943263
C	8.930775744	0.110612676	-0.159982993
C	6.137026418	0.050781881	-0.016671348
C	7.519471174	7.567756274	6.995742054
C	10.515062555	2.613967451	7.009427954
C	4.536199666	7.541309345	-0.213216258
C	3.155526913	5.130170084	-0.062216782
C	11.812098219	1.703094056	4.715593298
C	11.866170082	5.123407709	0.086514294
C	4.727625246	2.505741604	6.912100506
C	3.189396525	1.736001671	4.713861169
C	10.404010206	7.502333063	-0.007447201
O	4.089962193	-0.694462905	0.900578333
O	2.681005039	3.041897187	-0.992645106
O	1.460957239	2.068856175	3.158972555
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
Zr	1.888327952	-1.129576860	1.369036739
Zr	-1.691227169	1.003294277	-1.654617076
Zr	1.933351472	1.006837012	-1.583398537
Zr	-1.758780639	-1.128387024	1.274626134
Zr	0.080704231	2.008178563	1.359483205
Zr	0.150310060	-2.141796057	-1.649310474
Br	6.717825248	0.407305998	6.349878406
Br	13.264216310	6.021592198	2.538788994
Br	8.829001552	1.720476276	-2.638291210
O	6.405560749	6.482906746	8.743367322
O	8.691108074	6.500277414	8.747672068
O	6.291004575	10.403486270	3.010710205
O	8.566625216	10.411079698	3.107197253
O	9.006126121	2.104772980	8.739719281
O	10.101968049	4.100107271	8.790958433
O	4.907756004	9.657711713	0.726467635
O	6.163800474	9.015052065	-1.065547227
O	8.910849632	8.993185271	-1.048072804
O	9.985345949	9.641788876	0.862185973
O	12.390881857	3.084129339	-0.983612114
O	13.539860709	3.681334435	0.889532796
O	5.072406261	4.066748500	8.641115693
O	6.225549948	2.100282801	8.680934333
C	10.419776365	0.042579200	-0.159525273
C	12.579314201	1.239088203	3.533294169
O	10.957973965	-0.653897291	0.765964817
O	11.029768162	0.664764052	-1.087623274
O	12.308486292	0.074509308	3.086861300
O	13.462069452	2.049711495	3.098991916