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Supporting information for article:

Meta-generalized gradient approximation time-dependent densityfunctional theory study of electron trapping in Hf- and Zr-doped lutetium oxide: influencing the oxygen vacancy

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# Meta-GGA TD-DFT study on electron trapping in Hf and Zr doped lutetium oxide: influencing the oxygen vacancy

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# Supplementary information

### **Geometry optimization**

Quantum Espresso 6.5, 6.6 and 7.1 (QE, <u>https://www.quantum-espresso.org/</u>) module pw.x (total energy calculations and geometry optimization) was used with mostly default settings. Perdew-Zunger local density approximation (LDA) functional (<u>10.1103/PhysRevB.23.5048</u>) was used. Crucial settings are shown in Table S1. The results should be reproducible with either of codes.

14010	e it e ereeted settings used m	Quantum Depresso curculune	,1101
Section &CONTROL		Section & ELE	CTRONS
calculation	'vc-relax'	electron_maxstep	200
etot_conv_thr	1E-5	conv_thr	1.0D-7
forc_conv_thr	0.0001	diago_thr_init	1.0E-4
nstep	700	startingpot	'atomic'
		mixing_mode	'plain'
Section	Section &SYSTEM		0.5
ecutwfc	40	mixing_ndim	8
ecutrho	400	diagonalization	'david'
occupations	'smearing'	Section &I	IONS
smearing	'gaussian'	ion_dynamics	'bfgs'
degauss	0.001		
nspin	1 or 2 *	Section & C	CELL
tot_charge	2 / 1 / 0 / -1 / -2 *	cell_dynamics	'bfgs'

Table S1. Selected settings used in Quantum Espresso calculations.

\* tot\_charge is total charge on the system, while nspin controls spin polarization (1 for unpolarized and 2 for polarized); spinpolarization was used for systems with odd tot\_charge.

#### **Pseudopotentials**

The pseudopotentials (PPs) used were ultrasoft (USPP), generated by the Vanderbilt code version 7.3.6. oxygen PP recipe (PP generation input file) from GBRV The group (10.1016/j.commatsci.2013.08.053), version 1.2 was used. The Lu USPP recipe was kindly provided by co-author of the GBRV set, Kevin F. Garrity. The potential had the 4f electrons in core; the valence electrons were effectively of a *d*-element, not an *f*-element. Hf<sup>4+</sup> USPP was used. Zr default (general purpose) GBRV USPP was used. For test purposes, custom Zr<sup>4+</sup> USPP (analogous to the Hf<sup>4+</sup> USPP) was prepared, but the respective results are only shown Table S5 below.

#### Initial geometry of Lu<sub>2</sub>O<sub>3</sub> cell

Initial geometry (in the from of fractional coordinates of atoms) was generated by Spacegroup code shipped with Elk code version 4.3.6 (*http://elk.sourceforge.net/*), using space group Ia-3, all cell angles of 90.0 degrees and the following fractional coordinates of atoms (*10.3390/ma7107059*):

Lu1: 0.25, 0.25, 0.25

Lu2: 0.46685, 0.0, 0.25

O: 0.39159, 0.15282, 0.38011

Positions of the rest of the atoms were generated by the symmetry operations respective to the space group. Note that Lu1 and Lu2 here are site labels, not to be confused with the atom labels used below. The geometry from Spacegroup code was optimized using QE and shown in Table S2. Cell dimension was 19.432845 bohr.

Table S2. The initial geometry used in the calculations (fractional coordinates).

Atom label	fc1	fc2	fc3	Atom label	fc1	fc2	fc3
Lu1	0.2499998	0.2499998	0.2499998	O41	0.3912785	0.8476405	0.1200032
Lu2	0.7500002	0.7500002	0.7500002	O42	0.8912793	0.3476402	0.6200032
Lu3	0.7500004	0.2500000	0.2499994	O43	0.6087215	0.1523595	0.8799968
Lu4	0.2499996	0.7500000	0.7500006	O44	0.1087207	0.6523598	0.3799968
Lu5	0.2499994	0.7500004	0.2500000	O45	0.6087213	0.6523598	0.1200033
Lu6	0.7500006	0.2499996	0.7500000	O46	0.1087210	0.1523596	0.6200034
Lu7	0.7500000	0.7500006	0.2499996	O47	0.3912787	0.3476402	0.8799967
Lu8	0.2500000	0.2499994	0.7500004	O48	0.8912790	0.8476404	0.3799966
Lu9	0.4664097	0.0000001	0.2499996	O49	0.3799966	0.3912785	0.1523596
Lu10	0.9664106	0.4999998	0.7500001	O50	0.8799967	0.8912790	0.6523597
Lu11	0.5335903	-0.0000001	0.7500004	O51	0.6200034	0.6087215	0.8476404
Lu12	0.0335894	0.5000002	0.2499999	O52	0.1200033	0.1087210	0.3476403
Lu13	0.5335896	0.5000000	0.2500000	O53	0.3799966	0.6087216	0.3476403
Lu14	0.0335890	0.0000003	0.7500004	O54	0.8799966	0.1087207	0.8476408
Lu15	0.4664104	0.5000000	0.7500000	O55	0.6200034	0.3912784	0.6523597
Lu16	0.9664110	-0.0000003	0.2499996	O56	0.1200034	0.8912793	0.1523592
Lu17	0.2499996	0.4664097	0.0000001	O57	0.1200032	0.3912785	0.8476405
Lu18	0.7500001	0.9664106	0.4999998	O58	0.6200032	0.8912793	0.3476402
Lu19	0.7500004	0.5335903	-0.0000001	O59	0.8799968	0.6087215	0.1523595
Lu20	0.2499999	0.0335894	0.5000002	O60	0.3799968	0.1087207	0.6523598
Lu21	0.2500000	0.5335896	0.5000000	O61	0.1200033	0.6087213	0.6523598
Lu22	0.7500004	0.0335890	0.0000003	O62	0.6200034	0.1087210	0.1523596
Lu23	0.7500000	0.4664104	0.5000000	O63	0.8799967	0.3912787	0.3476402
Lu24	0.2499996	0.9664110	-0.0000003	O64	0.3799966	0.8912790	0.8476404
Lu25	0.0000001	0.2499996	0.4664097	O65	0.1523596	0.3799966	0.3912785
Lu26	0.4999998	0.7500001	0.9664106	O66	0.6523597	0.8799967	0.8912790
Lu27	-0.0000001	0.7500004	0.5335903	O67	0.8476404	0.6200034	0.6087215
Lu28	0.5000002	0.2499999	0.0335894	O68	0.3476403	0.1200033	0.1087210
Lu29	0.5000000	0.2500000	0.5335896	O69	0.3476403	0.3799966	0.6087216
Lu30	0.000003	0.7500004	0.0335890	O70	0.8476408	0.8799966	0.1087207
Lu31	0.5000000	0.7500000	0.4664104	O71	0.6523597	0.6200034	0.3912784
Lu32	-0.0000003	0.2499996	0.9664110	072	0.1523592	0.1200034	0.8912793
<b>O</b> 33	0.3912785	0.1523596	0.3799966	O73	0.8476405	0.1200032	0.3912785
O34	0.8912790	0.6523597	0.8799967	074	0.3476402	0.6200032	0.8912793
O35	0.6087215	0.8476404	0.6200034	O75	0.1523595	0.8799968	0.6087215
O36	0.1087210	0.3476403	0.1200033	O76	0.6523598	0.3799968	0.1087207
O37	0.6087216	0.3476403	0.3799966	077	0.6523598	0.1200033	0.6087213
O38	0.1087207	0.8476408	0.8799966	O78	0.1523596	0.6200034	0.1087210
O39	0.3912784	0.6523597	0.6200034	O79	0.3476402	0.8799967	0.3912787
O40	0.8912793	0.1523592	0.1200034	O80	0.8476404	0.3799966	0.8912790

#### Anionic and cationic voids

The crystal properties of the voids are similar to those of the anions and cations. There are namely 8 cationic voids of  $C_{3i}$  symmetry and 24 cationic voids of  $C_2$  symmetry, generated by the cell symmetry operations from position fc. 0, 0, 0 and 0, 0.25, 0.25, respectively. The anionic voids were generated from a position fc. 0.375, 0.375, 0.375. The list is given below, in Table S3.

Site label	fc1	fc2	fc3	Site symmetry
Oi1	0.375	0.375	0.375	$C_1$
Oi2	0.875	0.875	0.875	$C_1$
Oi3	0.625	0.625	0.625	$C_1$
Oi4	0.125	0.125	0.125	$C_1$
Oi5	0.625	0.125	0.375	$C_1$
Oi6	0.125	0.625	0.875	$C_1$
Oi7	0.375	0.875	0.625	$C_1$
Oi8	0.875	0.375	0.125	C <sub>1</sub>
Oi9	0.375	0.625	0.125	$C_1$
Oi10	0.875	0.125	0.625	$C_1$
Oi11	0.625	0.375	0.875	$C_1$
Oi12	0.125	0.875	0.375	$C_1$
Oi13	0.625	0.875	0.125	$C_1$
0i14	0.125	0.375	0.625	$C_1$
Oi15	0.375	0.125	0.875	$C_1$
Qi16	0.875	0.625	0.375	C.
CV/1	0	0		
		U O F		$C_{3i}$
CV2	0.5	0.5	0.5	$C_{3i}$
	0	0.5	0	$C_{3i}$
CV4	0.5	0	0.5	C <sub>3i</sub>
CV5	0	0	0.5	C <sub>3i</sub>
CV6	0.5	0.5	0	C <sub>3i</sub>
CV7	0	0.5	0.5	C <sub>3i</sub>
CV8	0.5	0	0	C <sub>3i</sub>
CV9	0	0.25	0.25	$C_2$
CV10	0.5	0.75	0.75	C <sub>2</sub>
CV11	0	0.75	0.75	$C_2$
CV12	0.5	0.25	0.25	$C_2$
CV13	0	0.75	0.25	$C_2$
CV14	0.5	0.25	0.75	$C_2$
CV15	0	0.25	0.75	$C_2$
CV16	0.5	0.75	0.25	$C_2$
CV17	0.25	0	0.25	$C_2$
CV18	0.75	0.5	0.75	$C_2$
CV19	0.75	0	0.75	$C_2$
CV20	0.25	0.5	0.25	$C_2$
CV21	0.25	0	0.75	$C_2$
CV22	0.75	0.5	0.25	$C_2$
CV23	0.75	0	0.25	$C_2$
CV24	0.25	0.5	0.75	$C_2$
CV25	0.25	0.25	0	$C_2$
CV26	0.75	0.75	0.5	$C_2$
CV27	0.75	0.75	0	$C_2$
CV28	0.25	0.25	0.5	$C_2$
CV29	0.75	0.25	0	$C_2$
CV30	0.25	0.75	0.5	$C_2$
CV31	0.25	0.75	0	$C_2$
CV32	0.75	0.25	0.5	$C_2$

#### **FP-LAPW calculations**

Calculations with Elk 7.0.12 or 8.5.02 used species files provided with the code. Only oxygen species file was modified – the local orbital with lorbl = 0 and lorbord = 3 was removed, resulting in total of two local orbitals with fixed linearization energies for oxygen. The muffin-tin radius for Lu was 2.0 bohr (2.3 bohr in some of the latter cases), and 1.45 bohr for O. Other non-default options are specified in Table S4. Note that, due to the use of atomic units, electron charge in elk is +1, while proton charge is –1. Consequently, e.g. "*chgexs* -2" means two additional holes in the system, while "*chgexs* 1" means one additional electron. The value of *rgkmax* (defines maximum | **G**+**k** for APW functions) was 7.9-8.3, depending on the system. The value of *qmaxvr* (maximum | **G** for potential and density) was 17. Smoothing operations to the exchange-correlation potentials were applied using msmooth value 4. Fixed spin magnetization (FSM) was used via *fsmtype* 1 and *msmooth* 0. 0. *X*, where *X* was the total cell magnetization(i.e. the number of unpaired electrons), directed up along *z* axis. In the calculation without FSM, Broyden mixing (default) was used, but the mixing parameters set via *broydpm* were reduced. The k-point grid was 3×3×3. Convergence threshold was twofold: root mean square change from last three iterations in Kohn-Sham potential was required to be lower than  $1 \cdot 10^{-6}$  a.u., change in total energy was required to be lower than 1·10<sup>-4</sup> a.u..

Table S4. Selected settings used in Elk code.							
Variable name	Value	Variable name	Value				
tasks	0, 10	chgexs	-2 / -1 / 0 / 1 / 2				
xctype	100 209 9	fsmtype	1				
gmaxvr	17	momfix	0. 0. 1. or 0. 0. 2.				
rgkmax	7.9 - 8.3	ngridk	333				
msmooth	4	spinpol	f / t				
isgkmax	-2	lradstp	2				
broydpm	0.2 0.075 (or 0.1 0.0375)	dosmsum	t				

The *xctype* option selects Räsänen, Pittalis and Proetto mGGA for exchange (209) and PZ correlation (9) from libxc (100).

## Dopant, vacancy and interstitial sites

The sites for the impurities were selected so that different structures had something in common. Hf/Zr initial  $C_{3i}$  site was [0.75, 0.75, 0.75]. Hf/Zr initial  $C_2$  site was [0.4664104, 0.5, 0.75].

Table S5.	Defect positions,	file names,	defect-defect	distances	(Angstrom,	optimized	cells)	and	cell
			charge	S					

He nameO/Vo initial positionO, initial positionO, initial positionO, initial positionP(H-C)P(V-O)O LangeLHTurc1[0.620397, 0.620034, 0.39127844.0504.131LHTurc1[0.1200033, 0.0607213, 0.62325964.5856.724.131LHTurc1[0.1200033, 0.108721, 0.3476403]6.7236.7011LHTurc1[0.1200033, 0.108721, 0.3476403]6.7236.7011LHTurc1[0.1200033, 0.108721, 0.3476403]6.7236.7211LHTurc1[0.3799966, 0.891279, 0.8476404]4.194.132.084.42-1LHTurc1[0.625, 0.625, 0.625]4.142.084.42-1LHTurc2[0.627, 0.375, 0.375]4.142.084.42-1LHTurc1[0.620034, 0.6087215, 0.8476404]4.194.132.084.42-1LHTurc1H[0.620034, 0.6087215, 0.8476404]2.154.142.084.23-1LTurc1h4[0.520037, 0.20034, 0.6087215, 0.8476404]2.194.142.074.142.10LTurc1h4[0.520037, 0.20034, 0.6087215, 0.8476404]2.194.1211LTurc1h4[0.620033, 0.108721, 0.3476404]2.186.7311LTurc1h4[0.620033, 0.108721, 0.3476404]2.184.344.000.001LHT2h4[0.620033, 0.108721, 0.3476404]2.184.344.1411LTurc1h4[0.620033, 0.108721, 0.3476404]2.18 <th></th> <th></th> <th>CI.</th> <th>luiges</th> <th></th> <th></th> <th></th> <th></th>			CI.	luiges				
LHIve1(0.620034, 0.6087215, 0.8476404)2.2152.191LHI1cc1(0.020033, 0.6087213, 0.620239, 0.3999664.5854.131LHHbe1(0.00073, 0.108721, 0.3476403)6.7236.701LHHw1(0.1200033, 0.108721, 0.3476403)6.7234.131LHHw1(0.1200033, 0.108721, 0.3476403)6.7234.131LHHw1(0.3799966, 0.891279, 0.3476404)4.194.132.074.400LHI1wAc-1(0.3799966, 0.891279, 0.3476404)4.194.142.084.421LHI1wAc-1(0.3799966, 0.891279, 0.3476404)4.194.142.094.442LHI1wBc-1(0.620034, 0.6087215, 0.8476404)2.194.142.094.442LHI1wBc-1(0.620034, 0.6087215, 0.8476404)2.194.142.094.442LZ1wc1h4(0.620034, 0.6087215, 0.8476404)2.194.142.094.442LZ1wc1h4(0.620034, 0.6087215, 0.8476404)2.194.142.024.390LZ1wc1h4(0.620034, 0.6087215, 0.8476404)2.194.145.437.480LZ1wc1h4(0.620034, 0.6087215, 0.8476403)2.19(0.875, 0.375, 0.12)4.145.437.480LZ1wc1h4(0.620034, 0.6087215, 0.8476403)6.784.7490.0011LHZawc1(0.620034, 0.6087215, 0.8476403)6.784.347.48001LHZawc1(0.620034, 0.6087215, 0.8476403)6.78<	File name	O/V <sub>o</sub> initial position		$O_{\rm i}\xspace$ initial position	$R(Hf-V_0)$	R(Hf-O <sub>i</sub> )	$R(V_0-O_i)$	Charge
Inflect(0.522357, 0.620034, 0.3912784)4.0504.311I.HInci(0.0007215, 0.1523595, 0.8793968)4.5854.131I.HInci(0.1200033, 0.108721, 0.3476403)6.725.701I.Hifuxi(0.1200033, 0.108721, 0.3476404)6.724.131I.Hifuxi(0.1200033, 0.108721, 0.3476404)6.724.131I.Hifuxi(0.3799966, 0.891279, 0.9476404)4.142.094.442I.Hifuxic(0.3799966, 0.891279, 0.9476404)4.194.142.094.442I.Hifuxic(0.3799966, 0.891279, 0.9476404)4.194.142.094.442I.Hifuxic(0.3799966, 0.891279, 0.9476404)2.104.142.094.442I.Hifuxic(0.620034, 0.6087215, 0.8476404)2.104.165.457.531I.Zriuxihi(0.400034, 0.6087215, 0.8476404)2.104.122.024.300I.Zriuxihi(0.3799966, 0.891279, 0.9476404)2.104.122.024.300I.Zriuxihi(0.620034, 0.6087215, 0.8476404)2.104.122.024.300I.Hif2xc1(0.620034, 0.6087215, 0.8476404)2.165.386.000.001I.Hif2xc1(0.620034, 0.6087215, 0.8476404)2.164.334.650.000.001I.Hif2xc1(0.620034, 0.6087215, 0.8476404)2.164.344.650.000.001I.Hif2xc1(0.620034, 0.6087215, 0.8476404)2.16 <td< td=""><td>LHf1vc1</td><td>[0.6200034, 0.6087215, 0.8476404]</td><td>2.215</td><td></td><td>2.19</td><td></td><td></td><td>1</td></td<>	LHf1vc1	[0.6200034, 0.6087215, 0.8476404]	2.215		2.19			1
Inflac10.1200033, 0.6087213, 0.65235984.1954.131LHfluc10.06067215, 0.1523595, 0.037999684.5856.701LHfluc10.1200033, 0.108721, 0.34764036.236.701LHfluc1H4.131LHfluc4H4.132.074.400LHfluc4H0.1999966, 0.691279, 0.64764044.142.084.42-1LHflux6H0.1999966, 0.691279, 0.64764044.194.132.094.42-1LHflux6L10.1999966, 0.691279, 0.64764044.194.142.094.44-2LHflux6L10.3999966, 0.691279, 0.64764044.194.155.447.53-1LHflux6L10.6200034, 0.6087215, 0.14764042.212.2311LZrlux1140.6200034, 0.6087215, 0.14764042.162.22.101LZrlux1140.6200034, 0.6087215, 0.14764042.104.122.004.001LZrlux1140.6200034, 0.6087215, 0.14764042.101.122.024.390LZrlux1140.6200034, 0.6087215, 0.14764042.101.122.024.390LH2x110.62500123, 0.6235913.663.390.000.001LH2x120.62500123, 0.6235913.663.390.000.001LH2x110.120003, 0.6087213, 0.6235913.663.390.000.001LH2x120.65250.6254.122.024.312.04.410	LHf1cc1	[0.6523597, 0.6200034, 0.3912784]	4.050		4.31			1
LHfluc1[0.6087215, 0.1523395, 0.879968]4.5854.321LHfluc1[0.1200033, 0.108721, 0.3476403]6.7236.701LHfluc1[0.1200033, 0.108721, 0.3476403]6.7236.701LHfluc414.132.074.400LHfluc4[0.3799966, 0.891279, 0.8476404]4.142.084.42-1LHflux6-1H11.03799966, 0.891279, 0.8476404]4.142.084.42-1LHflux6-24.142.094.44-2-1LHflux6-1H1.1411480-1H2.094.44-2-1LHflux6-11.141148-1H2.094.44-2-1LHflux6-11.141148-1H2.142.477.53-1LHflux6-11.141148-1H2.142.477.57-2LZrluc1h1.0529066, 0.891279, 0.84764042.162.2311LZrlux1h1.03799966, 0.891279, 0.84764042.1802.184.122.024.390LHflux110.6200034, 0.6087215, 0.84764042.1802.380.000.001LHflux110.200033, 0.08721, 0.323953.863.990.000.001LHflux110.20033, 0.108721, 0.34764036.726.490.000.001LHflux110.20033, 0.108721, 0.34764036.726.490.000.001LHflux110.20033, 0.108721, 0.34764036.726.490.000.001LHflux110.20033, 0.108721, 0.	LHf1ac1	[0.1200033, 0.6087213, 0.6523598]	4.195		4.13			1
Lhfluc1       [0.1200033, 0.108721, 0.3476403]       6.723       6.70       1         LHfluc1       LHfluc1       4.13       1         LHfluc1       4.12       1         LHfluc1       4.13       2.07       4.00       0         LHfluc1       4.13       2.07       4.00       0         LHfluc2       4.13       2.07       4.00       0         LHfluc2       4.13       2.07       4.00       0         LHfluc2       4.14       2.09       4.44       -1         LHfluc2       4.14       2.09       4.44       -2         LHfluc2       4.15       5.44       7.53       -1         LHfluc2       4.16       5.45       7.53       -1         LHfluc2       1       2.23       1       1         LZrive1h4       1       0.6200034, 0.6087215, 0.8476404       4.19       -1       -1         LZrive1h4       1       0.6200034, 0.6087215, 0.8476404       4.19       -1       -1         LZrive1h4       1       0.620033, 0.6087213, 0.6523981       3.866       3.99       0.00 <t< td=""><td>LHf1bc1</td><td>[0.6087215, 0.1523595, 0.8799968]</td><td>4.585</td><td></td><td>4.32</td><td></td><td></td><td>1</td></t<>	LHf1bc1	[0.6087215, 0.1523595, 0.8799968]	4.585		4.32			1
LHflwc1 LHflwc1H LHflwc1H LHflwc1H LHflwc1H LHflwc1H LHflwc40 LHflwc40+ LLflwc40+ LZrlwc1h LHZwc1 LHZwc1 LHZwc1 LHZwc1 LHZwc1 LHZwc1 LHZwc1 LHZwc1 LHZwc1 LLZrwc1h LZrlwc1h LZrlwc1h LZrlwc1h LZrlwc1h LZrlwc1h LZrlwc1h LZrlwc1h LZrlwc1h LZrlwc1h LZrlwc1h LZrlwc1h LZrlwc1h LZrlwc1h LZrlwc1h LZrlwc1h LZrlwc1h LZrlwc1h LZrlwc1h LHZwc1 LHZwc1 LHZwc1 LHZwc1 LLZrwc1h LHZwc1 LHZwc1 LLZrwc1h LHZwc1 LLZrwc1h L	LHf1uc1	[0.1200033, 0.108721, 0.3476403]	6.723		6.70			1
LH1wcH LH1wAc0 LH1wAc1 LH1wAc-1 LH1wAc-1 LH1wAc-1 LH1wAc-1 LH1wAc-1 LH1wAc-1 LH1wAc-1 LH1wAc-1 LH1wB04.132.074.400LH1wAc-1 LH1wB010.3799966, 0.891279, 0.8476404 LH1wBc-14.194.142.094.44-2LH1wBc-1 LH1wBc-1H04.142.094.44-2LH1wBc-1 LH1wBc-1H04.165.467.54-1LH1wBc-1H0.6200034, 0.6087215, 0.8476404 LZrlwc1h2.2152.23-1LZrlwc1h4 LZrlwc1h40.3799966, 0.891279, 0.8476404 LZrlwc1h42.1094.12-1LZrlwc1h4 LZrlwc1h0.3799966, 0.891279, 0.8476404 LZrlwc1h42.1004.12-1LZrlwc1h4 LH2wc10.6200034, 0.6087215, 0.84764044 LZrlwc1h42.1004.12-1LH2wc1 LH2wc10.6020034, 0.6087215, 0.8476404 LL1wc1h42.1004.145.437.480LH2wc1 LH2wc10.602013, 0.1632759, 0.820986 LL1w2wc13.6663.990.001LH2wc1 LH2wc10.602013, 0.1632713, 0.6323598 LH2wc14.640.000.001LH2wc1 LH2wc10.1200033, 0.168721, 0.3476403 LH2wc16.7824.040.000.001LH2wc1 LH2wc10.1200033, 0.168721, 0.3476404 LH2wc14.040.000.001LH2wc1 LH2wc10.3799966, 0.891279, 0.8476404 LH2wc14.040.000.001LH2wc1 LH2wc10.6620034, 0.6087215, 0.8476404 LH2wc14.040.000.00	LHf1wc1				4.13			1
LHfiwAc0       4.13       2.07       4.40       0         LHfiwAc-11       [0.625, 0.625, 0.625]       4.14       2.08       4.42       -1         LHfiwAc-12       4.195       4.19       4.11       2.09       4.42       -1         LHfiwAc-11       LHfiwAc-11       4.11       2.09       4.42       -1         LHfiwAc-11       LHfiwBc-1       4.11       2.09       4.42       -1         LHfiwBc-1       4.16       5.46       7.54       -1         LHfiwBc-2       4.16       5.46       7.54       -1         LHfiwBc-1       1.0.6200034, 0.6087215, 0.8476404]       2.215       2.23       1       1         LZrtwc1h4       1.0.3799966, 0.891279, 0.8476404]       2.101       4.12       1       1         LZrtwc1h4       1.0.3799966, 0.891279, 0.8476404]       2.180       1.866       3.99       0.00       0.00       1         LH2avc1       10.620034, 0.6087215, 0.637518       3.866       3.99       0.00       0.00       1         LH2avc1       10.6620337, 0.620034, 0.6087215, 0.8799968]       4.08       4.36       0.00       0.01	LHf1wc1H				4.12			1
LHftwAc-1 LHftwAc-1H LHftwAc-2H LHftwBc-10.3799966, 0.891279, 0.84764040.625, 0.62	LHf1wAc0				4.13	2.07	4.40	0
LHfiwAc-1H       [0.3799966, 0.891279, 0.8476404]       4.19       4.13       2.08       4.42       -1         LHfiwBc0       4.14       2.09       4.44       -2         LHfiwBc0       4.15       5.44       7.49       0         LHfiwBc-1H	LHf1wAc-1				4.14	2.08	4.42	-1
LHfuwAc-2       (0.3793906, 0.391279, 0.347600)       4.195       4.14       2.09       4.44       -2         LHfuwBc-1	LHf1wAc-1H	[0.2700066 0.901270 0.9476404]		[0.625, 0.625, 0.625]	4.13	2.08	4.42	-1
LHfiwBc04.155.447.490LHfiwBc-10.875, 0.375, 0.125]4.165.467.54-1LHfiwBc-14.165.467.53-1LHfiwBc-14.215.477.57-2LTrivch40.600034, 0.6007215, 0.84764042.2152.231LZrivcth42.2311LZrivcth44.121LZrivcth40.3799966, 0.891279, 0.84764044.1954.121LZrivcth40.3799966, 0.891279, 0.84764042.1802.380.000.001LHrivc110.6200034, 0.6087213, 0.65235983.8663.990.000.001LHrivc110.6200034, 0.6087213, 0.65235983.8663.990.000.001LHrivc110.1200033, 0.6087213, 0.65235983.8663.990.000.001LHrivc110.1200033, 0.6087213, 0.65235983.8663.990.000.001LHrivc110.1200033, 0.108721, 0.34764036.7826.490.000.001LHrivc110.1200033, 0.108721, 0.34764036.7826.490.000.001LHrivc110.1200033, 0.108721, 0.34764044.344.450.000.001LHrivc110.1200033, 0.108721, 0.34764044.214.040.000.001LHrivc110.1200034, 0.6087215, 0.84764044.214.040.001LHrivc110.1200034, 0.6087215, 0.84764044.214.035.887.541	LHf1wAc-2	[0.3/99966, 0.8912/9, 0.84/6404]			4.14	2.09	4.44	-2
LH1wBe-1 LH1wBe-1H $0.875, 0.375, 0.125$ $4.16$ $4.16$ $5.46$ $5.45$ $7.53$ $-1$ $4.16$ LH1wBe-2 $4.16$ $5.47$ $7.57$ $-2$ LZrlve1h4 LZrlve1h4 $0.600034, 0.6007215, 0.84764001$ LZrlve1h4 $2.215$ $2.23$ $1$ LZrlve1h4 LZrlve1h4 $0.3799966, 0.891279, 0.84764001$ LZrlve2h4 $4.12$ $1$ LZrlve1h4 LZrlve2h1 $0.3799966, 0.891279, 0.84764001$ $1.1271wSc0h$ $4.12$ $2.02$ $4.39$ $0$ LZrlve2h4 LH2ve1 $0.600034, 0.6087215, 0.87640401$ $1.01200033, 0.6087213, 0.652539813.6863.690.000.001LH2ve1LH2ve110.620034, 0.6087213, 0.652359813.6863.990.000.001LH2ve1LH2ve110.6007315, 0.125359, 0.879996814.0884.0884.364.0000.001LH2ve1LH2ve1LH2ve110.20033, 0.108721, 0.347640311.020033, 0.108721, 0.347640311.3346.7826.490.000.001LH2ve1LH2ve1LH2ve10.3799966, 0.891279, 0.84764041LH2ve24.334.344.450.000.001LH2ve2LH2we20.3799966, 0.891279, 0.84764041LH2ve34.2410.875, 0.375, 0.12514.034.042.104.044.454.062.114.454.544.072.104.042.104.042.104.042.104.042.104.042.104.042.104.042.104.042.104.042.$	LHf1wBc0				4.15	5.44	7.49	0
LHftwBc-1H       (0.057, 0.375, 0.120)       4.16       5.45       7.53       -1         LHftwBc-2       4.21       5.47       7.57       -2         LZrtw1h4       [0.6200034, 0.6087215, 0.8476404]       2.215       2.23       1         LZrtw1h4       [0.6200034, 0.6087215, 0.8476404]       2.215       4.12       1         LZrtw1h4       [0.3799966, 0.891279, 0.8476404]       4.19       4.12       1         LZrtw1k0h       [0.6200034, 0.6087215, 0.8476404]       2.180       4.14       5.43       7.48       0         LH12vc1       [0.6200034, 0.6087215, 0.8476404]       2.180       3.866       3.99       0.00       0.00       1         LH12vc1       [0.6200033, 0.6087215, 0.325398]       3.866       3.99       0.00       0.00       1         LH12vc1       [0.6200033, 0.6087215, 0.3476404]       4.33       4.45       0.00       0.00       1         LH12vc1       [0.620033, 0.108721, 0.3476403]       6.34       0.00       0.00       1         LH12vc1       [0.620033, 0.108721, 0.3476403]       6.34       0.00       0.00       1         LH12vc1       [0.620033, 0.108721, 0.34	LHf1wBc-1			[0 97E 0 27E 0 12E]	4.16	5.46	7.54	-1
LHfuwbe-2       421       5.47       7.57       -2         LZrtvcth4       [0.6200034, 0.6087215, 0.8476404]       2.215       2.23       1         LZrtvcth4       [0.3799966, 0.891279, 0.8476404]       4.195       4.12       1         LZrtwch4       [0.3799966, 0.891279, 0.8476404]       4.195       4.12       2.02       4.39       0         LZrtwBc0h       [0.6200034, 0.6087215, 0.8476404]       2.180       4.12       2.02       4.39       0         LHf2vc1       [0.6200034, 0.6087215, 0.8476404]       2.180       3.38       0.00       0.00       1         LHf2vc1       [0.6200034, 0.6087215, 0.8476404]       2.180       3.38       0.00       0.00       1         LHf2vc1       [0.6200034, 0.6087215, 0.8476404]       2.180       4.36       0.00       0.00       1         LHf2vc1       [0.6007315, 0.625996, 0.891279, 0.8476404]       6.782       6.49       0.00       0.00       1         LHf2wAc1       [0.1200033, 0.108721, 0.3476403]       6.782       6.49       0.00       0.00       1         LHf2wAc2       [0.3799966, 0.891279, 0.8476404]       4.241       4.04       6.00	LHf1wBc-1H			[0.0/5, 0.5/5, 0.125]	4.16	5.45	7.53	-1
LZrivch4       0.6200034, 0.6087215, 0.8476404       2.215       2.23       1         LZrivch4       2.23       1         LZrivch4       4.12       1         LZrivch4       4.12       1         LZrivch4       4.12       1         LZrivch4       6.3799966, 0.891279, 0.8476404       1.415       4.12       1         LZrivkc0h       0.6200034, 0.6087215, 0.8476404       2.180       2.38       0.00       0.00       1         LH72vc1       0.6200034, 0.6087215, 0.879986       3.866       3.99       0.00       0.00       1         LH72vc1       0.6200034, 0.6087215, 0.879986       4.088       4.36       0.00       0.00       1         LH72vc1       0.6200034, 0.3912780       4.334       4.45       0.00       0.00       1         LH72vc1       0.6523597, 0.620034, 0.3912784       4.334       4.45       0.00       0.00       1         LH72vc1       0.120033, 0.108721, 0.3476403       6.782       6.49       0.00       0.00       1         LH72wc1       0.1200033, 0.108721, 0.3476403       6.782       6.49       0.00       0.00       1	LHf1wBc-2				4.21	5.47	7.57	-2
LZrivchh       10.0000034, 0.0007215, 0.8476404]       2.213       2.23       1         LZrivchh       4.12       1	LZr1vc1h4		2.215		2.23			1
LZrlwclh4       4.12       1         LZrlwchh       10.3799966, 0.891279, 0.8476404]       4.195       4.195       4.12       1         LZrlwAc0h       10.3799966, 0.891279, 0.8476404]       2.180       2.02       4.39       0         LZrlwBc0h       10.875, 0.375, 0.125]       4.14       5.43       7.48       0         LHf2vc1       10.6020034, 0.6087215, 0.8476404]       2.180       2.38       0.00       0.00       1         LHf2vc1       10.6087215, 0.1523595, 0.8799968       4.088       4.36       0.00       0.00       1         LHf2vc1       10.6087215, 0.1523595, 0.8799968       4.088       4.36       0.00       0.00       1         LHf2vc1       10.6087215, 0.1523595, 0.8799968       4.088       4.36       0.00       0.00       1         LHf2vc1       10.6087215, 0.1523595, 0.8799968       4.088       4.36       0.00       0.00       1         LHf2vc1       10.6087215, 0.1523596, 0.891279, 0.8476403       6.782       6.49       0.00       0.00       1         LHf2wC1       10.3799966, 0.891279, 0.8476404]       4.241       10.625, 0.625, 0.625       4.03       2.10 <td< td=""><td>LZr1vc1h</td><td>[0.6200034, 0.608/215, 0.84/6404]</td><td>2.215</td><td></td><td>2.23</td><td></td><td></td><td>1</td></td<>	LZr1vc1h	[0.6200034, 0.608/215, 0.84/6404]	2.215		2.23			1
LZriwcih       [0.3799966, 0.891279, 0.8476404]       4.195       4.195       4.12       1         LZriwAc0h       [0.625, 0.625, 0.625]       4.12       2.02       4.39       0         LZriwBc0h       [0.625, 0.625, 0.625]       4.14       5.43       7.48       0         LHf2vc1       [0.620034, 0.6087215, 0.8476404]       2.180       2.38       0.00       0.00       1         LHf2vc1       [0.6087215, 0.1523595, 0.8799968]       4.088       4.36       0.00       0.00       1         LHf2vc1       [0.6087215, 0.1523595, 0.8799968]       4.088       4.36       0.00       0.00       1         LHf2vc1       [0.6087215, 0.1523595, 0.8799968]       4.088       4.36       0.00       0.00       1         LHf2vc1       [0.6087215, 0.1523597, 0.620034, 0.3912784]       4.334       4.45       0.00       0.00       1         LHf2wc1       [0.1200033, 0.108721, 0.3476403]       6.782       6.49       0.00       0.00       1         LHf2wAc0       [0.625, 0.625, 0.625]       4.01       2.09       4.41       0         LHf2wAc1       [0.627, 0.375, 0.152]       4.05       5.88       <	LZr1wc1h4				4.12			1
LZr1wAc0h       10.3799966, 0.891279, 0.8476404]       4.195       [0.625, 0.625]       4.12       2.02       4.39       0         LZr1wBc0h       [0.620034, 0.6087215, 0.8476404]       2.180       2.38       0.00       0.00       1         LHf2vc1       [0.6087215, 0.1523595, 0.8799968]       3.866       3.99       0.00       0.00       1         LHf2vc1       [0.6087215, 0.1523595, 0.8799968]       4.088       4.36       0.00       0.00       1         LHf2vc1       [0.6087215, 0.523597, 0.6200034, 0.3912784]       4.334       4.45       0.00       0.00       1         LHf2vc1       [0.1200033, 0.108721, 0.3476403]       6.782       6.49       0.00       0.00       1         LHf2wc1       [0.1200033, 0.108721, 0.3476403]       6.782       6.49       0.00       0.00       1         LHf2wc1       [0.1200033, 0.108721, 0.3476404]       4.03       2.10       4.43       -1         LHf2wAc0       [0.625, 0.625, 0.625, 0.625]       4.03       2.10       4.44       -1         LHf2wAc-1       [0.627, 0.6375, 0.151]       4.05       5.88       7.49       0         LHf2wBc0       [0.379	LZr1wc1h	-	4.195		4.12			1
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	LZr1wAc0h	[0.3799966, 0.891279, 0.8476404]		[0.625, 0.625, 0.625]	4.12	2.02	4.39	0
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	LZr1wBc0h			[0.875, 0.375, 0.125]	4.14	5.43	7.48	0
LHf2ac1     [0.1200033, 0.6087213, 0.6523598]     3.866     3.99     0.00     0.00     1       LHf2bc1     [0.6087215, 0.1523595, 0.8799968]     4.088     4.36     0.00     0.00     1       LHf2cc1     [0.6523597, 0.6200034, 0.3912784]     4.334     4.45     0.00     0.00     1       LHf2uc1     [0.1200033, 0.108721, 0.3476403]     6.782     6.49     0.00     0.00     1       LHf2wc1     [0.1200033, 0.108721, 0.3476403]     6.782     6.49     0.00     0.00     1       LHf2wc1     [0.1200033, 0.108721, 0.3476403]     6.782     6.49     0.00     0.00     1       LHf2wc1     [0.1200033, 0.108721, 0.3476404]     6.782     4.01     2.09     4.41     0       LHf2wAc-1     [0.625, 0.625, 0.625, 0.625]     4.03     2.10     4.43     -1       LHf2wAc-2     [0.3799966, 0.891279, 0.8476404]     4.241     [0.625, 0.625, 0.625]     4.05     5.88     7.49     0       LHf2wBc-1     [0.6200034, 0.6087215, 0.8476404]     2.180     [0.875, 0.375, 0.125]     4.04     0.00     10       LHf2wBc-2     [0.6200034, 0.6087215, 0.8476404]     2.180 <td< td=""><td>LHf2vc1</td><td>[0.6200034, 0.6087215, 0.8476404]</td><td>2.180</td><td></td><td>2.38</td><td>0.00</td><td>0.00</td><td>1</td></td<>	LHf2vc1	[0.6200034, 0.6087215, 0.8476404]	2.180		2.38	0.00	0.00	1
LHf2bc1       [0.6087215, 0.1523595, 0.8799968]       4.088       4.36       0.00       0.00       1         LHf2cc1       [0.5523597, 0.6200034, 0.3912784]       4.334       4.45       0.00       0.00       1         LHf2uc1       [0.1200033, 0.108721, 0.3476403]       6.782       6.49       0.00       0.00       1         LHf2wc1       [0.1200033, 0.108721, 0.3476403]       6.782       6.49       0.00       0.00       1         LHf2wc1       [0.1200033, 0.108721, 0.3476403]       6.782       4.04       0.00       0.00       1         LHf2wc1       [0.4799966, 0.891279, 0.8476404]       6.782       4.01       2.09       4.41       0         LHf2wRc-1       [0.3799966, 0.891279, 0.8476404]       4.241       [0.625, 0.625, 0.625]       4.03       2.10       4.44       -1         LHf2wBc-1       [0.875, 0.375, 0.125]       4.05       5.88       7.49       0         LHf2wBc-2       [0.875, 0.375, 0.125]       4.07       5.90       7.54       -1         LHf2wBc-2       [0.620034, 0.6087215, 0.8476404]       2.180       2.42       0.00       0.00       1         LZr2vc1h4	LHf2ac1	[0.1200033, 0.6087213, 0.6523598]	3.866		3.99	0.00	0.00	1
LHf2cc1     [0.6523597, 0.6200034, 0.3912784]     4.334     4.45     0.00     0.00     1       LHf2uc1     [0.1200033, 0.108721, 0.3476403]     6.782     6.49     0.00     0.00     1       LHf2uc1     [0.1200033, 0.108721, 0.3476403]     6.782     4.04     0.00     0.00     1       LHf2wc1	LHf2bc1	[0.6087215, 0.1523595, 0.8799968]	4.088		4.36	0.00	0.00	1
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	LHf2cc1	[0.6523597, 0.6200034, 0.3912784]	4.334		4.45	0.00	0.00	1
LH2wc1     4.04     0.00     0.00     1       LHf2wAc0     4.01     2.09     4.41     0       LHf2wAc-1H     [0.625, 0.625, 0.625]     4.03     2.10     4.43     -1       LHf2wAc-1H     [0.625, 0.625, 0.625]     4.04     2.10     4.44     -1       LHf2wAc-2     [0.3799966, 0.891279, 0.8476404]     4.241     4.06     2.11     4.45     -2       LHf2wBc0     4.05     5.88     7.49     0     0     0     1       LHf2wBc-1H     0     0.875, 0.375, 0.125]     4.07     5.90     7.54     -1       LHf2wBc-2     4.00     5.99     7.54     -1     1       LHf2wBc-2     4.10     5.92     7.59     -2       LZr2vc1h4     [0.6200034, 0.6087215, 0.8476404]     2.180     2.42     0.00     0.00     1       LZr2vc1h4     [0.3799966, 0.891279, 0.8476404]     2.180     4.04     0.00     0.00     1       LZr2wc1h4     [0.3799966, 0.891279, 0.8476404]     4.241     [0.625, 0.625, 0.625]     4.01     2.03     4.40     0       LZr2wc1h4     [0.3799966, 0.891279, 0.8	LHf2uc1	[0.1200033, 0.108721, 0.3476403]	6.782		6.49	0.00	0.00	1
LH12wAc0     4.01     2.09     4.41     0       LHf2wAc-1     [0.625, 0.625, 0.625]     4.03     2.10     4.43     -1       LHf2wAc-1H     [0.625, 0.625, 0.625]     4.04     2.10     4.44     -1       LHf2wAc-2     [0.3799966, 0.891279, 0.8476404]     4.241     4.06     2.11     4.45     -2       LHf2wBc0     4.05     5.88     7.49     0     0     0     1       LHf2wBc-1H     6.05     5.89     7.54     -1     1 <td>LHf2wc1</td> <td></td> <td></td> <td></td> <td>4.04</td> <td>0.00</td> <td>0.00</td> <td>1</td>	LHf2wc1				4.04	0.00	0.00	1
LHf2wAc-1     [0.625, 0.625, 0.625]     4.03     2.10     4.43     -1       LHf2wAc-1H     [0.625, 0.625, 0.625]     4.04     2.10     4.44     -1       LHf2wAc-2     [0.3799966, 0.891279, 0.8476404]     4.241     4.06     2.11     4.45     -2       LHf2wBc0     4.05     5.88     7.49     0       LHf2wBc-1     [0.875, 0.375, 0.125]     4.07     5.90     7.54     -1       LHf2wBc-2     1     4.08     5.89     7.54     -1       LHf2wBc-2     1     4.00     5.92     7.59     -2       LZr2vc1h4     [0.6200034, 0.6087215, 0.8476404]     2.180     2.42     0.00     0.00     1       LZr2vc1h4     [0.6200034, 0.6087215, 0.8476404]     2.180     2.42     0.00     0.00     1       LZr2vc1h4     [0.3799966, 0.891279, 0.8476404]     2.180     4.04     0.00     0.00     1       LZr2wc1h4     [0.3799966, 0.891279, 0.8476404]     4.241     [0.625, 0.625, 0.625]     4.01     2.03     4.40     0       LZr2wc1h     [0.3799966, 0.891279, 0.8476404]     [0.875, 0.375, 0.125]     4.05     5.88	LHf2wAc0				4.01	2.09	4.41	0
LHf2wAc-1H     4.04     2.10     4.44     -1       LHf2wAc-2     [0.3799966, 0.891279, 0.8476404]     4.241     4.06     2.11     4.45     -2       LHf2wBc0     4.05     5.88     7.49     0       LHf2wBc-1     [0.875, 0.375, 0.125]     4.07     5.90     7.54     -1       LHf2wBc-1H     [0.875, 0.375, 0.125]     4.08     5.89     7.54     -1       LHf2wBc-2     4.10     5.92     7.59     -2       LZr2vc1h4     [0.6200034, 0.6087215, 0.8476404]     2.180     2.42     0.00     0.00     1       LZr2vc1h4     [0.6200034, 0.6087215, 0.8476404]     2.180     4.04     0.00     0.00     1       LZr2vc1h4     [0.6200034, 0.6087215, 0.8476404]     2.180     4.04     0.00     0.00     1       LZr2wc1h4     [0.6200034, 0.6087215, 0.8476404]     4.241     [0.625, 0.625, 0.625]     4.04     0.00     0.00     1       LZr2wc1h4     [0.3799966, 0.891279, 0.8476404]     4.241     [0.625, 0.625]     4.01     2.03     4.40     0       LZr2wc1h4     [0.875, 0.375, 0.125]     4.05     5.88     7.48     <	LHf2wAc-1			[0.625, 0.625, 0.625]	4.03	2.10	4.43	-1
LHf2wAc-2     [0.3799966, 0.891279, 0.8476404]     4.241     4.06     2.11     4.45     -2       LHf2wBc0     4.05     5.88     7.49     0       LHf2wBc-1     [0.875, 0.375, 0.125]     4.07     5.90     7.54     -1       LHf2wBc-1H     [0.875, 0.375, 0.125]     4.08     5.89     7.54     -1       LHf2wBc-2     4.10     5.92     7.59     -2       LZr2vc1h4     [0.6200034, 0.6087215, 0.8476404]     2.180     2.42     0.00     0.00     1       LZr2vc1h4     [0.6200034, 0.6087215, 0.8476404]     2.180     2.41     0.00     0.00     1       LZr2vc1h4     [0.3799966, 0.891279, 0.8476404]     2.180     4.04     0.00     0.00     1       LZr2wc1h4     [0.3799966, 0.891279, 0.8476404]     4.241     [0.625, 0.625, 0.625]     4.01     2.03     4.40     0       LZr2wc1h4     [0.3799966, 0.891279, 0.8476404]     4.241     [0.625, 0.625, 0.625]     4.01     2.03     4.40     0       LZr2wAc0h     [0.3799966, 0.891279, 0.8476404]     [0.875, 0.375, 0.125]     4.05     5.88     7.48     0	LHf2wAc-1H				4.04	2.10	4.44	-1
LHf2wBc0     4.05     5.88     7.49     0       LHf2wBc-1     -1     4.07     5.90     7.54     -1       LHf2wBc-1H     -1     4.08     5.89     7.54     -1       LHf2wBc-2     4.10     5.92     7.59     -2       LZr2vc1h4     -0.6200034, 0.6087215, 0.8476404]     2.180     2.42     0.00     0.00     1       LZr2vc1h4     -1     2.41     0.00     0.00     1       LZr2vc1h4     -1     2.42     0.00     0.00     1       LZr2vc1h4     -1     -1     2.42     0.00     0.00     1       LZr2vc1h4     -1     -1     -1     -1     -1       LZr2vc1h4     -1     -1     -1     -1       LZr2wc1h4     -1     -1     -1     -1       LZr2wc1h4     -1     -1     -1     -1       LZr2wc1h4     -1     -1     -1     -1       LZr2wAc0h     -1     -1     -1     -1       LZr2wBc0h     -1     -1     -1     -1       LZr2wBc0h     -1	LHf2wAc-2	[0.3799966, 0.891279, 0.8476404]	4.241		4.06	2.11	4.45	-2
LHf2wBc-1     [0.875, 0.375, 0.125]     4.07     5.90     7.54     -1       LHf2wBc-1H     4.08     5.89     7.54     -1       LHf2wBc-2     4.10     5.92     7.59     -2       LZr2vc1h4     [0.6200034, 0.6087215, 0.8476404]     2.180     2.42     0.00     0.00     1       LZr2vc1h4     [0.6200034, 0.6087215, 0.8476404]     2.180     2.41     0.00     0.00     1       LZr2vc1h4     [0.6200034, 0.6087215, 0.8476404]     2.180     4.04     0.00     0.00     1       LZr2vc1h4     [0.6200034, 0.6087215, 0.8476404]     4.241     [0.625, 0.625, 0.625]     4.04     0.00     0.00     1       LZr2wc1h4     [0.3799966, 0.891279, 0.8476404]     4.241     [0.625, 0.625, 0.625]     4.01     2.03     4.40     0       LZr2wAc0h     [0.3799966, 0.891279, 0.8476404]     [0.875, 0.375, 0.125]     4.05     5.88     7.48     0	LHf2wBc0				4.05	5.88	7.49	0
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	LHf2wBc-1			[0,875,0375,0125]	4.07	5.90	7.54	-1
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	LHf2wBc-1H			[0.073, 0.373, 0.123]	4.08	5.89	7.54	-1
$ \begin{array}{c c} LZr2vc1h4 \\ \hline LZr2vc1h4 \\ \hline LZr2vc1h4 \\ \hline LZr2wc1h4 \\ \hline LZr2wAc0h \\ \hline LZr2wAc0h \\ \hline LZr2wBc0h \end{array} \begin{array}{c c} 2.42 & 0.00 & 0.00 & 1 \\ \hline 2.41 & 0.00 & 0.00 & 1 \\ \hline 4.04 & 0.00 & 0.00 & 1 \\ \hline 4.04 & 0.00 & 0.00 & 1 \\ \hline 4.04 & 0.00 & 0.00 & 1 \\ \hline 0.625, 0.625, 0.625 \\ \hline 0.875, 0.375, 0.125 \\ \hline 4.05 & 5.88 & 7.48 & 0 \\ \hline \end{array} $	LHf2wBc-2				4.10	5.92	7.59	-2
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	LZr2vc1h4		D 100		2.42	0.00	0.00	1
$ \begin{array}{c c} LZr2wc1h4 & \\ \hline LZr2wc1h & \\ \hline LZr2wAc0h & \\ LZr2wBc0h & \\ \end{array} \begin{array}{c c} 0.3799966, 0.891279, 0.8476404 \\ \hline LZr2wBc0h & \\ \end{array} \begin{array}{c c} 4.04 & 0.00 & 0.00 & 1 \\ \hline 4.04 & 0.00 & 0.00 & 1 \\ \hline 0.625, 0.625, 0.625 \\ \hline 0.875, 0.375, 0.125 \\ \hline 4.05 & 5.88 & 7.48 & 0 \\ \hline \end{array} $	LZr2vc1h	[0.6200034, 0.608/215, 0.84/6404]	2.180		2.41	0.00	0.00	1
LZr2wc1h       4.04       0.00       0.00       1         LZr2wAc0h       4.241       [0.625, 0.625]       4.01       2.03       4.40       0         LZr2wBc0h       [0.875, 0.375, 0.125]       4.05       5.88       7.48       0	LZr2wc1h4				4.04	0.00	0.00	1
LZr2wAc0h       [0.3799966, 0.891279, 0.8476404]       4.241       [0.625, 0.625]       4.01       2.03       4.40       0         LZr2wBc0h       [0.875, 0.375, 0.125]       4.05       5.88       7.48       0	LZr2wc1h				4.04	0.00	0.00	1
LZr2wBc0h [0.875, 0.375, 0.125] 4.05 5.88 7.48 0	LZr2wAc0h	[0.3799966, 0.891279, 0.8476404]	4.241	[0.625, 0.625, 0.625]	4.01	2.03	4.40	0
	LZr2wBc0h			[0.875, 0.375, 0.125]	4.05	5.88	7.48	0