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Structure and Properties of Some Layered U₂O₅ phases: a Density Functional Theory Study

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Supporting Information

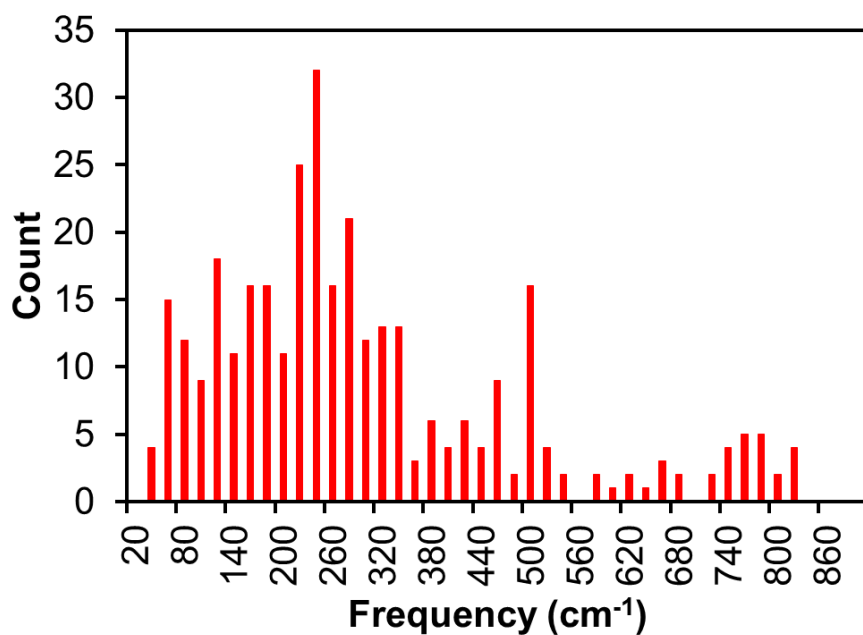


Figure S1. Histogram of the vibrational frequency distribution for δ - U_2O_5 structure¹. The structure contains 16 U_2O_5 units for a total of 336 modes. The 3 translational modes are not displayed.

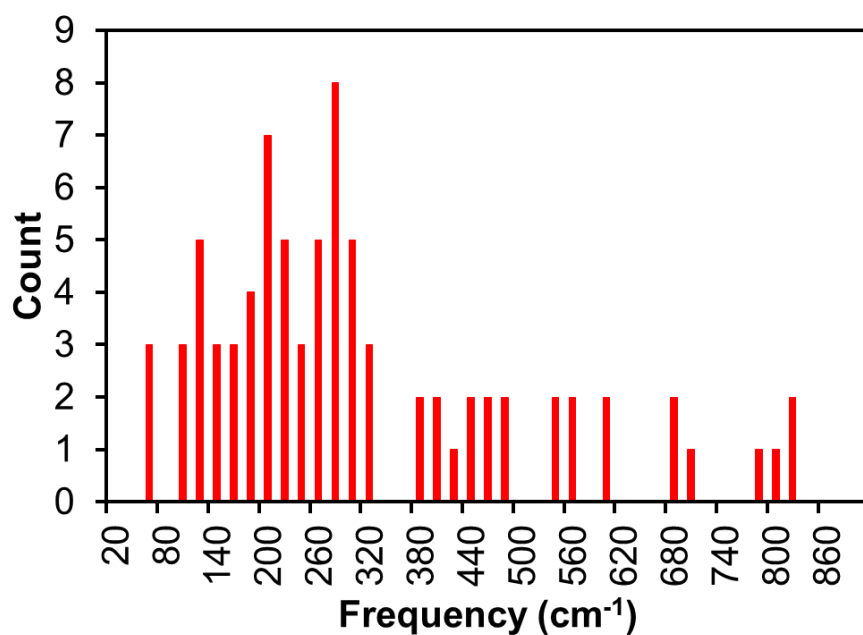


Figure S2. Histogram of the vibrational frequency distribution for the U_2O_5 in the Np_2O_5 ² structure. The structure contains 4 U_2O_5 units for a total of 84 modes. The 3 translational modes are not displayed.

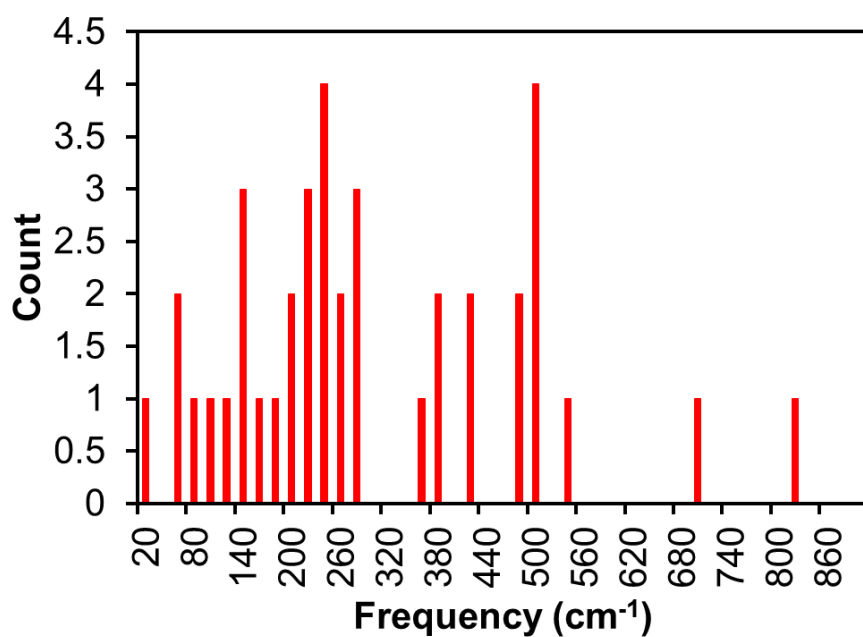


Figure S3. Histogram of the vibrational frequency distribution for the U₂O₅ in the R-Nb₂O₅ ³ structure. The structure contains 2 U₂O₅ units for a total of 42 modes. The 3 translational modes are not displayed.

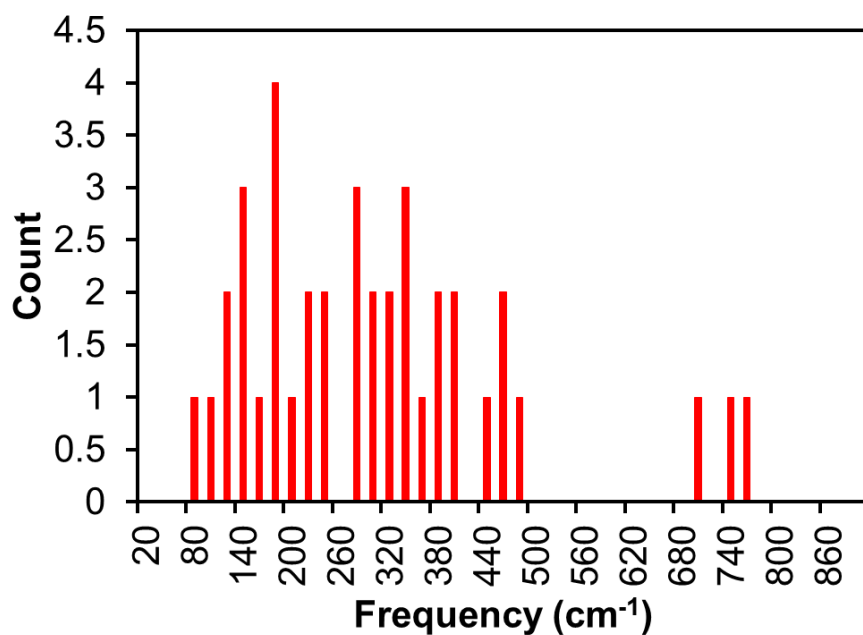


Figure S4. Histogram of the vibrational frequency distribution for the U₂O₅ in the Z-Nb₂O₅ ⁴ structure. The structure contains 2 U₂O₅ units for a total of 42 modes. The 3 translational modes are not displayed.

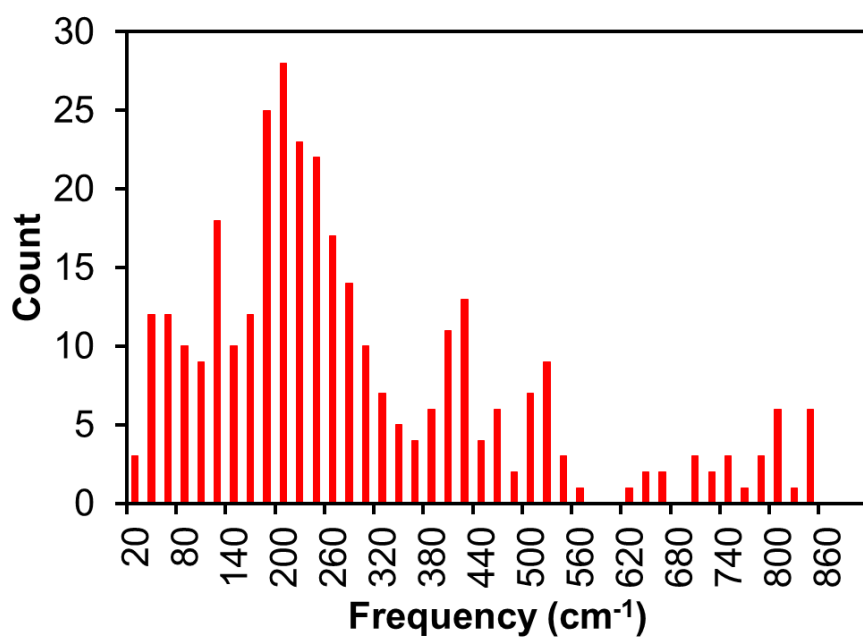


Figure S5. Histogram of the vibrational frequency distribution for the U_2O_5 in the $\text{N-Nb}_2\text{O}_5$ ⁵ structure. The structure contains 16 U_2O_5 units for a total of 336 modes. The 3 translational modes are not displayed.

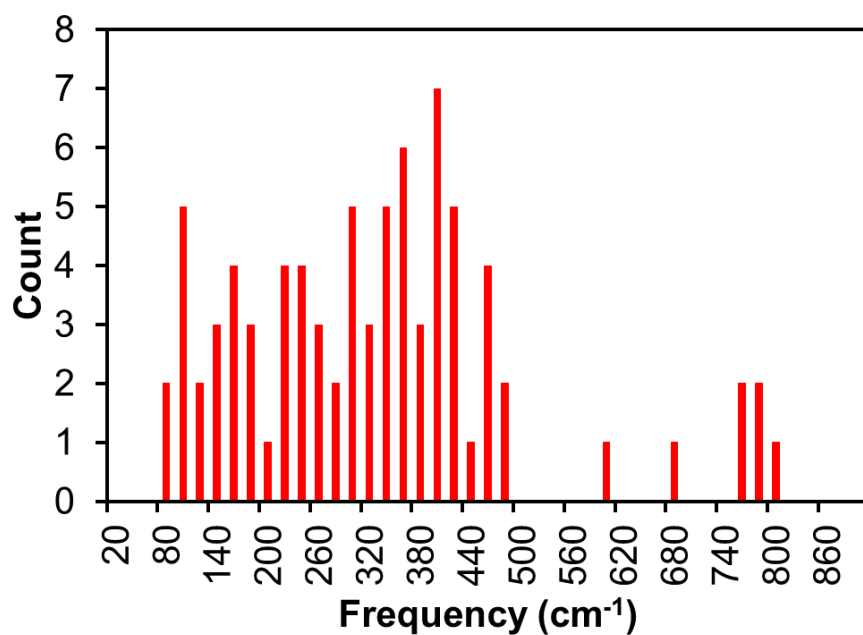


Figure S6. Histogram of the vibrational frequency distribution for the U_2O_5 in the $\text{B-Ta}_2\text{O}_5$ ⁶ structure. The structure contains 4 U_2O_5 units for a total of 84 modes. The 3 translational modes are not displayed.

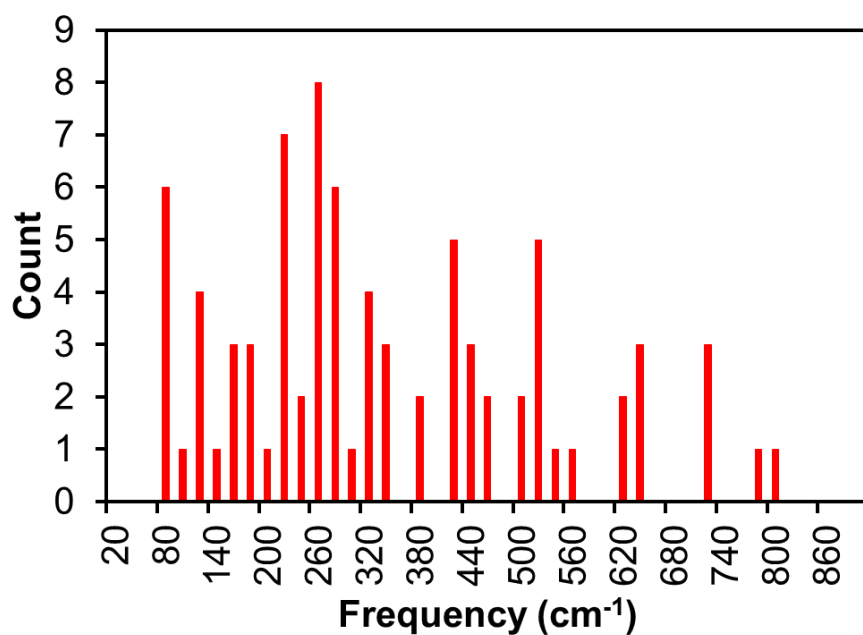


Figure S7. Histogram of the vibrational frequency distribution for the U₂O₅ in the β -V₂O₅ ⁷ structure. The structure contains 4 U₂O₅ units for a total of 84 modes. The 3 translational modes are not displayed.

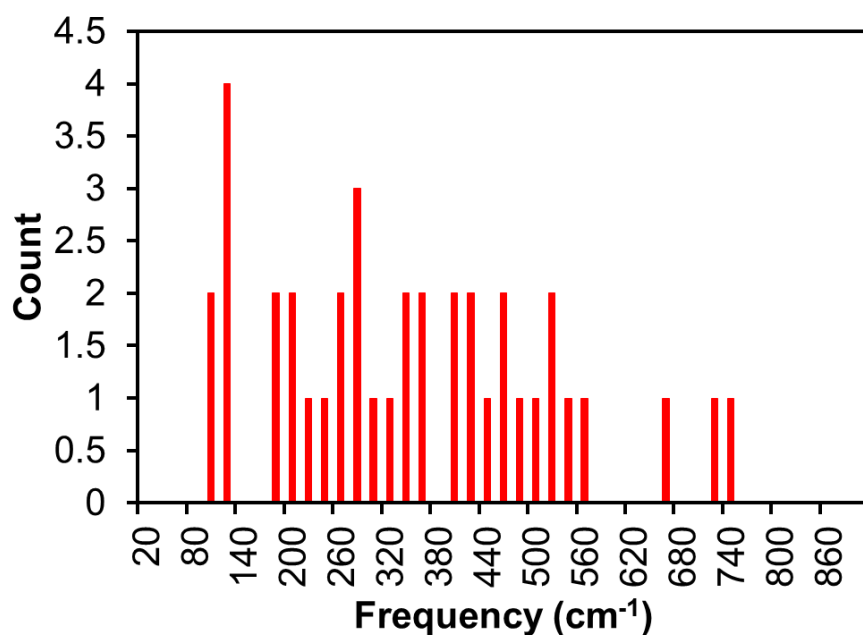


Figure S8. Histogram of the vibrational frequency distribution for the U₂O₅ in the α -V₂O₅ ⁸ structure. The structure contains 2 U₂O₅ units for a total of 42 modes. The 3 translational modes are not displayed.

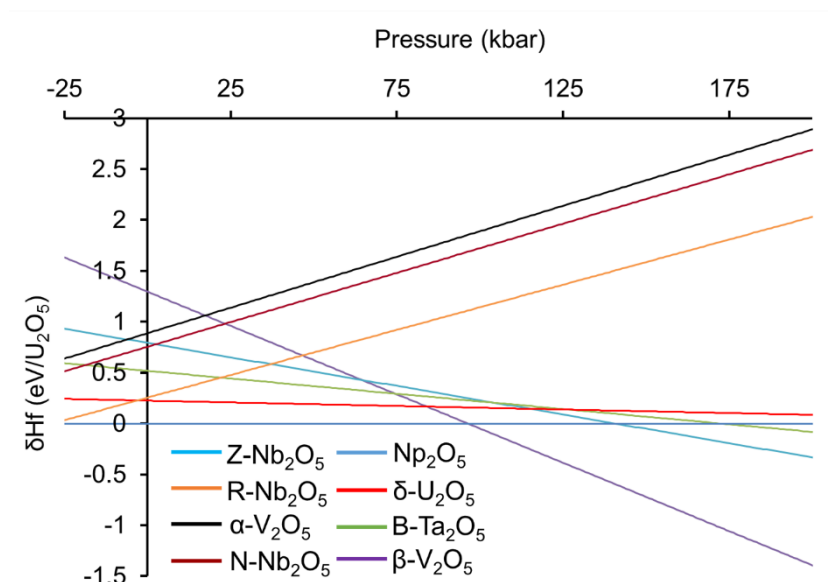


Figure S9. Calculated enthalpies of formation per U_2O_5 unit as a function of pressure, relative to Np_2O_5 (the most stable phase without considering entropy), for all the U_2O_5 phases.

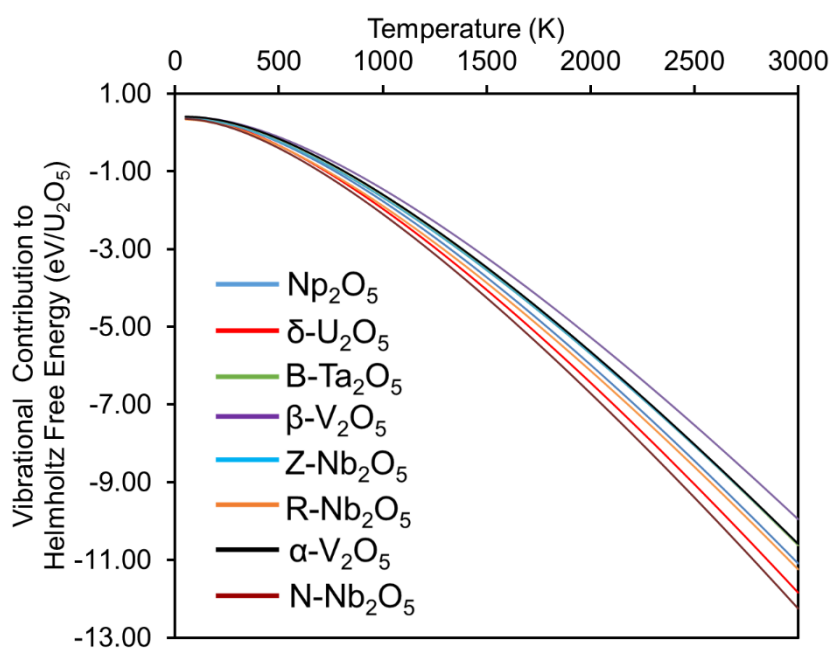


Figure S10. Vibrational contribution to the Helmholtz free energy per U_2O_5 unit as a function of temperature for all the U_2O_5 phases.

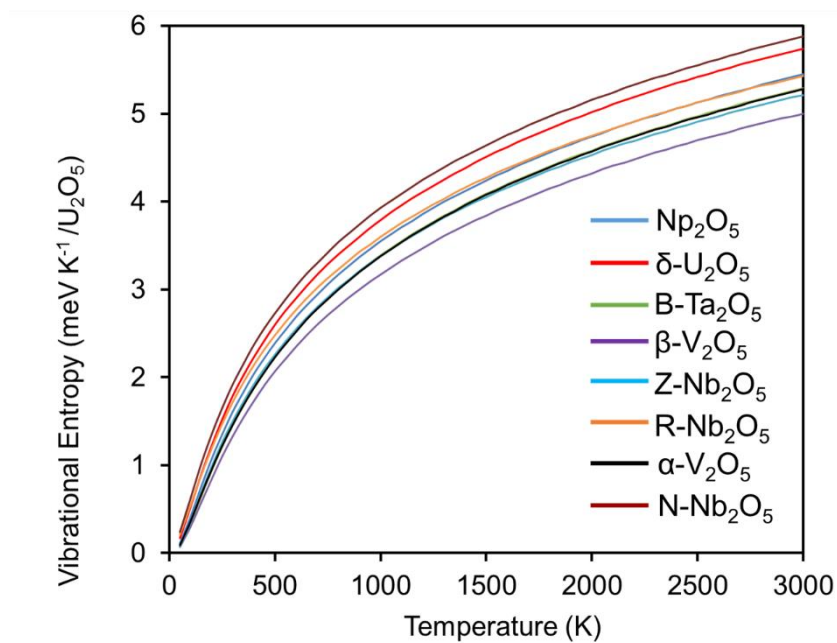


Figure S11. Vibrational Entropy per U₂O₅ unit as a function of temperature for all the U₂O₅ phases.

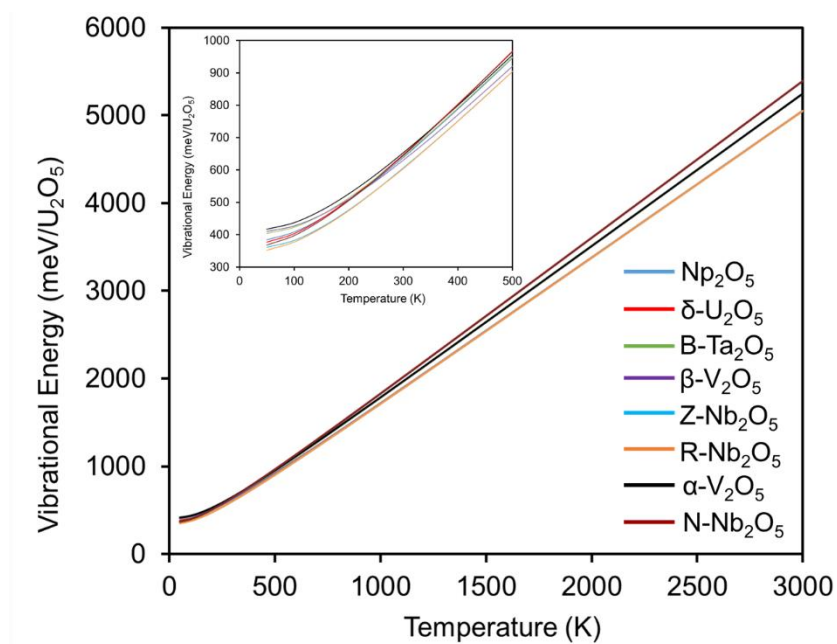


Figure S12. Vibrational Energy per U₂O₅ unit as a function of temperature for all the U₂O₅ phases.

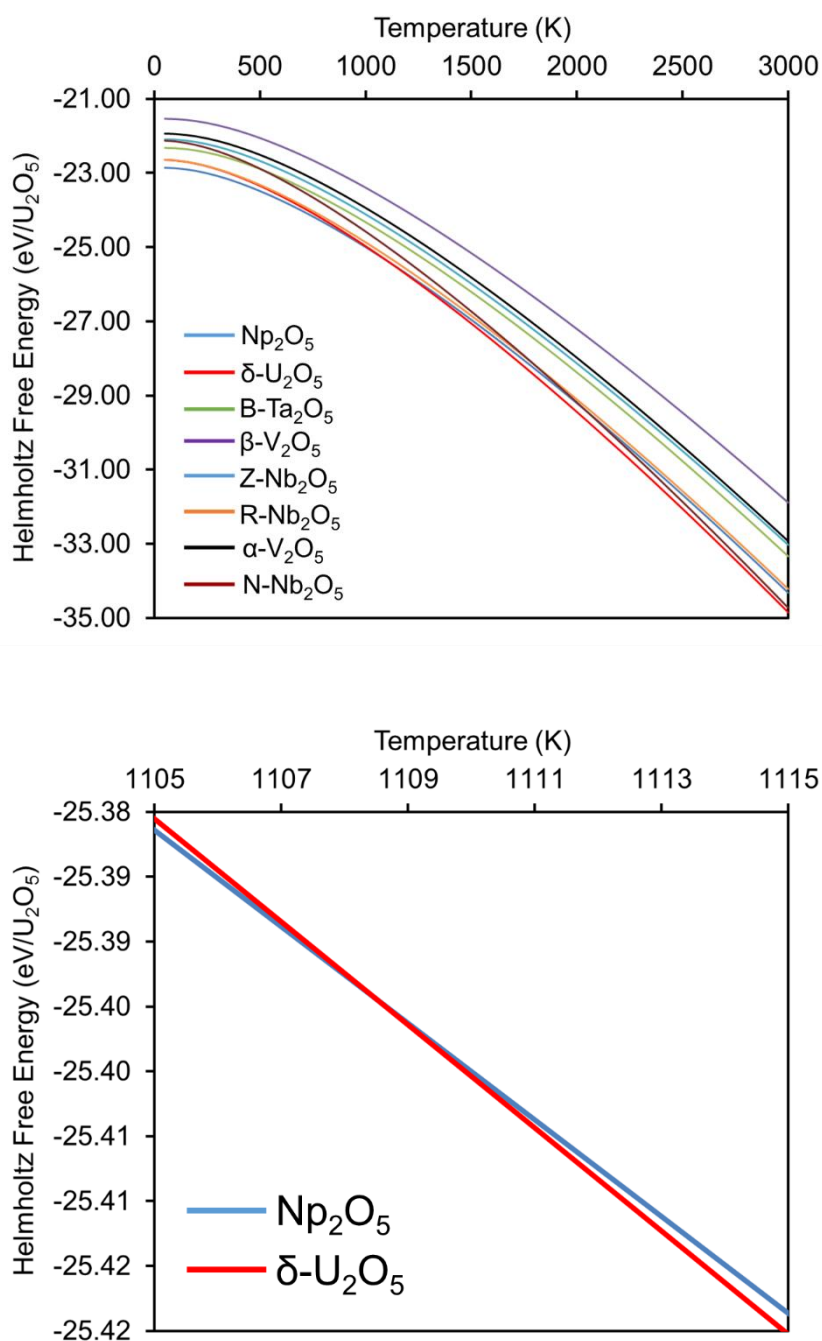


Figure S13. Helmholtz free energy per U₂O₅ unit as a function of temperature for all the U₂O₅ phases (above). Helmholtz free energy per U₂O₅ unit as a function of temperature for all the two most stable phase U₂O₅ phases (below).

Table S1. Predicted independent elastic constants for the DFT relaxed U_2O_5 structures in GPa. The values for $\delta\text{-U}_2\text{O}_5$ are consistent with our previous work⁹.

		C11	C12	C13	C14	C15	C16	C22	C23	C24	C25	C26	C33	C34	C35	C36	C44	C45	C46	C55	C56	C66
<i>Pcma</i> (55)	$\delta\text{-U}_2\text{O}_5$ ¹	271.4	29.5	148.0				513.6	27.9				246.5				27.7			27.1		60.6
<i>I2/a</i> (15)	Np_2O_5 ²	218.7	130.4	-3.7		-0.1		280.9	21.5		0.0		398.7		-0.2		59.1		0.3	26.8		24.0
<i>Pm</i> (6)	$\text{R-Nb}_2\text{O}_5$ ³	452.5	24.8	34.1		0.9		208.6	132.1		-9.4		295.9		19.3		23.4		0.5	15.2		27.9
<i>P1</i> (1)	$\text{Z-Nb}_2\text{O}_5$ ⁴	120.5	72.8	65.3	-0.7	0.9	7.0	194.3	60.4	0.1	1.9	-20.4	80.0	-0.7	0.6	22.6	98.9	-41.0	-0.6	68.9	-0.2	61.9
<i>P1</i> (1)	$\text{N-Nb}_2\text{O}_5$ ⁵	251.6	51.6	25.9	1.1	0.9	-6.5	218.2	39.0	1.4	0.2	-0.4	268.1	1.5	-0.6	9.6	13.6	-0.8	0.1	13.7	-0.1	21.9
<i>P-1</i> (2)	$\text{B-Ta}_2\text{O}_5$ ⁶	162.2	33.2	14.7	0.2	0.4	0.4	86.0	46.2	-0.3	-0.2	-18.1	80.3	1.0	-0.8	-32.5	29.6	-22.0	0.6	89.6	0.0	26.5
<i>P2₁</i> (4)	$\alpha\text{-V}_2\text{O}_5$ ⁸	191.1	65.3	63.9		14.6		174.2	29.8		7.7		58.5		8.0		10.3		4.0	14.4		13.9
<i>Pm</i> (6)	$\beta\text{-V}_2\text{O}_5$ ⁷	298.2	132.8	128.8		7.2		253.8	87.3		1.2		330.1		-0.1		51.1		-0.4	64.9		33.5

δ -U₂O₅¹

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U 0.755961030 0.500001705 0.974218150

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U 0.752750785 0.500001416 0.841407065

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O	0.879853279	0.499990849	0.773007849
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O	0.427645130	0.499923878	0.965506249

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O	0.500105762	0.860295563	0.250038254
O	0.499876974	0.139648116	0.749894242
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O	0.702875583	0.446653039	0.241437877
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O	0.202734041	0.053376890	0.241448418
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O	0.621443447	0.220791526	0.484055797
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O	0.878360863	0.279179707	0.015932418
O	0.121132297	0.279238142	0.484062985
O	0.121483486	0.720961166	0.984029467
O	0.878062060	0.720879534	0.514772041

R-Nb₂O₅³

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U	0.000113880	0.114408811	0.148014160
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U	0.000034466	0.806262901	0.352035763
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O	0.000106904	0.655595644	0.191325179
O	0.999964339	0.273307350	0.808720100

O	0.500103726	0.116233950	0.148239314
O	0.499953559	0.813712775	0.851830135
O	0.499930464	0.124260960	0.648127862
O	0.499969982	0.802623511	0.351815665
O	0.999975013	0.964572396	0.499972864
O	0.000018331	0.964567493	0.999995711

Z-Nb₂O₅⁴

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U	0.831680012	0.989600081	0.786082921		
U	0.670720040	0.489973155	0.216786034		
U	0.170412429	0.414119152	0.715835527		
O	0.101417927	0.148368348	0.006993884		
O	0.701402079	0.290273694	0.892339771		
O	0.799081900	0.789596890	0.109672919		
O	0.396884871	0.647830189	0.994288302		
O	0.200439095	0.619664252	0.382546443		

O	0.000788847	0.699179718	0.745534540
O	0.495294628	0.199477228	0.246325159
O	0.300470445	0.120267107	0.618417746
O	0.895576864	0.248673858	0.498735021
O	0.605982207	0.752683584	0.502056598

N-Nb₂O₅⁵

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U	0.656952656	0.012048739	0.098849883
U	0.342288689	0.986200873	0.903244667
U	0.288897263	0.490975440	0.094419644
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O	0.922390762	0.496084006	0.903210603
O	0.586678693	0.013891084	0.103327788
O	0.412232647	0.986583326	0.898072999
O	0.132249638	0.980459506	0.073181845
O	0.871545093	0.997618811	0.922181593
O	0.633006058	0.512338040	0.075451349
O	0.365833071	0.485821931	0.926131822
O	0.270843946	0.991153360	0.054951183
O	0.728158578	0.007773056	0.948154629
O	0.771336799	0.507194913	0.056974669
O	0.228446074	0.491087455	0.946119189
O	0.398587876	0.988850311	0.041359529

O	0.600127383	0.014569410	0.960146254
O	0.902429782	0.496045854	0.047994949
O	0.100030361	0.484711620	0.958767962
O	0.022046004	0.488721195	0.367960559
O	0.976929133	0.496600008	0.633520086
O	0.521549497	0.990715016	0.366456146
O	0.476785416	0.989700456	0.634013210
O	0.176309939	0.477417358	0.365129821
O	0.825800168	0.497390607	0.636144153
O	0.676289302	0.005560909	0.366720033
O	0.322266167	0.979750351	0.635328359
O	0.228410151	0.976782843	0.362910241
O	0.772164086	0.998011829	0.635995814
O	0.728619464	0.504810368	0.364418376
O	0.269967012	0.480377844	0.637385477
O	0.383895538	0.986125047	0.361879311
O	0.614131744	0.991963412	0.637479730

O	0.884179485	0.497181263	0.362434542
O	0.114892221	0.489846004	0.639077078
O	0.224259567	0.490824821	0.097838607
O	0.771017487	0.507839188	0.899165298
O	0.724131688	0.009884419	0.099682788
O	0.274630412	0.990905855	0.902534550
O	0.351660902	0.491942484	0.090073640
O	0.647103596	0.512546718	0.911388618
O	0.850907058	0.003268637	0.086662239
O	0.147791526	0.990069145	0.912088872
O	0.478745356	0.491579418	0.049054261
O	0.519754020	0.514510343	0.951802330
O	0.979234510	0.992328172	0.046110744
O	0.018180741	0.987876077	0.948666276
O	0.103651486	0.977985522	0.237201205
O	0.896405240	0.995702740	0.771642995
O	0.603643849	0.510532046	0.237879888

O	0.394908764	0.480800640	0.762730577
O	0.200210550	0.474819997	0.226683038
O	0.798711171	0.496659422	0.766979849
O	0.700783456	0.008022595	0.229789280
O	0.298229127	0.982311862	0.772945728
O	0.339674542	0.485967877	0.237030290
O	0.657576903	0.492533411	0.762344914
O	0.840302282	0.998882368	0.236765883
O	0.158933692	0.989797434	0.764139126
O	0.479247747	0.491007668	0.227488384
O	0.519804020	0.492706998	0.773651611
O	0.979920931	0.986373666	0.229714231
O	0.021135572	0.996336527	0.772543845
O	0.088153631	0.987129710	0.376004325
O	0.912195511	0.997616356	0.629420018
O	0.587784069	0.491397014	0.375857516
O	0.411063476	0.489585567	0.625207815

O	0.313999775	0.483987783	0.365395727
O	0.684027598	0.493548063	0.634962141
O	0.814652029	0.999442673	0.365227292
O	0.184450880	0.986769041	0.635435236
O	0.455787053	0.489768079	0.358588100
O	0.542088659	0.489879215	0.641098819
O	0.956177240	0.991353545	0.360309626
O	0.042320525	0.994125415	0.639863409
O	0.069350522	0.989800417	0.513220704
O	0.929465014	0.997134397	0.488655808
O	0.568439050	0.491533864	0.511894161
O	0.429605942	0.486480888	0.487316533
O	0.203035820	0.977321907	0.497215424
O	0.797353729	0.000316373	0.504224095
O	0.703277939	0.502574900	0.498163586
O	0.295695641	0.477180226	0.503492024

B-Ta₂O₅⁶

14.29459 5.29818 6.13991 90.00200 104.40209 90.00806

U 0.139827208 0.251310581 0.268201545

U 0.859543635 0.748526747 0.732185401

U 0.859476811 0.253458843 0.232070190

U 0.139886983 0.746421395 0.768222576

U 0.641277426 0.753479656 0.283452196

U 0.358127408 0.246596391 0.716777947

U 0.358137480 0.751454480 0.216847993

U 0.641222202 0.248479241 0.783363288

O 0.999491593 0.107391711 0.250245034

O 0.999898710 0.892342499 0.750599841

O 0.499856539 0.610157801 0.250575662

O 0.499588770 0.390025487 0.750175987

O 0.390322157 0.066931571 0.029717157

O 0.609038319 0.933062568 0.970448145

O 0.608951281 0.068614582 0.470462019

O 0.390302537 0.931372606 0.529663799

O	0.892115207	0.569256781	0.044921156
O	0.107346230	0.430604048	0.955622493
O	0.107267459	0.567255823	0.455510727
O	0.892073070	0.432683172	0.544860581
O	0.294214397	0.417504561	0.376895081
O	0.705151989	0.582738540	0.623406449
O	0.705153332	0.419537832	0.123278716
O	0.294246256	0.580422993	0.876929646
O	0.795516521	0.919262415	0.393190789
O	0.203799967	0.080899336	0.607124889
O	0.203801838	0.916690712	0.107247551
O	0.795444360	0.083118643	0.892829453

β -V₂O₅⁷

11.54247	4.36381	10.59769	90.01524	90.00353	89.97558
U	0.382993164	0.228328780	0.577671990		
U	0.585616319	0.727975559	0.407323994		
U	0.085782084	0.734550553	0.090215751		
U	0.883099038	0.234727804	0.919804071		

U	0.085672284	0.230927368	0.590150185
U	0.882967697	0.731077549	0.419738128
U	0.383118425	0.733133506	0.077626701
U	0.585754002	0.233009983	0.907213764
O	0.239262826	0.228127130	0.700760984
O	0.739219455	0.728232850	0.296761917
O	0.239389433	0.735464961	0.200753713
O	0.739397053	0.235472788	0.796745904
O	0.488893828	0.230781379	0.740088724
O	0.488906065	0.729717684	0.240110347
O	0.988679167	0.733476539	0.257058751
O	0.988719706	0.233295260	0.757052151
O	0.228383033	0.230062800	0.463776905
O	0.728308629	0.729952431	0.533724952
O	0.228460518	0.733335656	0.963798334
O	0.728410133	0.233180290	0.033681934
O	0.538785669	0.227761180	0.443780702

O	0.425441017	0.728203910	0.539380079
O	0.925531854	0.734674255	0.958039095
O	0.039035126	0.234614463	0.053512276
O	0.925364343	0.231382642	0.457990351
O	0.038963230	0.731244741	0.553455537
O	0.539010754	0.733023046	0.943769776
O	0.425552361	0.232912559	0.039290190

α -V₂O₅⁸

6.61250	4.02594	7.32035	89.99944	79.70602	90.00062
U	0.127958574	0.249998046	0.785071988		
U	0.861053139	0.749995116	0.215064685		
U	0.358855760	0.250000602	0.210074046		
U	0.638038185	0.750029519	0.784327184		
O	0.787424989	0.749979747	0.501051370		
O	0.267689986	0.249990458	0.475226225		
O	0.044669402	0.249998904	0.113053592		
O	0.943236828	0.749996388	0.899405311		

O	0.669964783	0.249992634	0.268027568
O	0.335245740	0.750003119	0.724489769
O	0.425796853	0.250007387	0.927244611
O	0.559795420	0.750000004	0.099659936
O	0.188456378	0.750000513	0.251150777
O	0.791813962	0.250007564	0.746152939

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