PROGRESS REPORT: Creating and Visualizing VO2 Bulk Polymorphs

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VANADIUM DIOXIDE (VO2)

Vanadium dioxide (VO2) has become a focal point of research due to its notable **phase transition**, referred to as the **Metal-Insulator Transition (MIT).** This transition, occurring around 68 degrees Celsius, transforms VO2 **from an insulator to a conductor**, resulting in significant changes to its electrical and optical properties. This unique behavior has led to the widespread study of VO2 for its applications in electric and optical devices, smart windows, sensors, and actuators.

VO2 POLYMORPHS PARAMETERS

Table 1. Common synthetic environment, crystallography data and corresponding comments of VO_2 polymorphs.

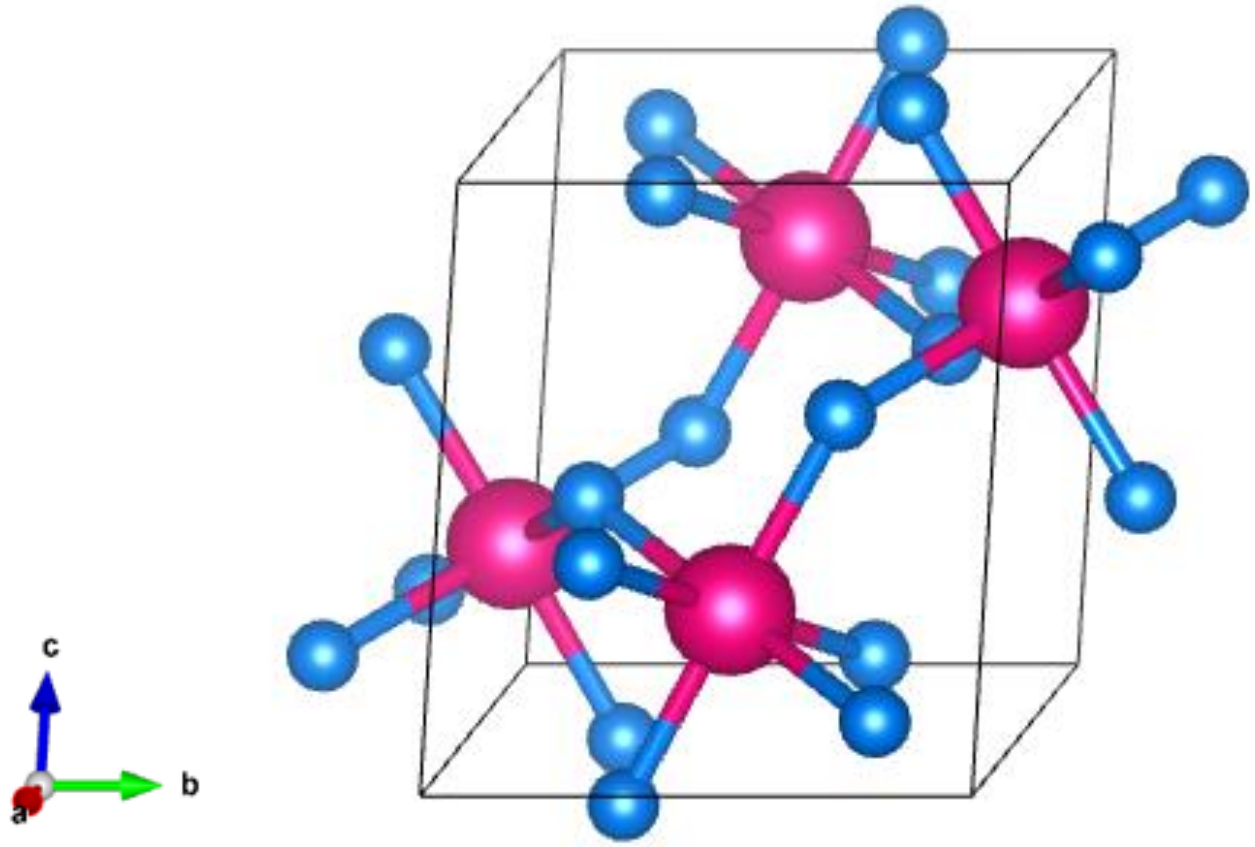
Polymorphs		Space Group	Unit Cell Parameters				Common Reaction Conditions	Comment	Reference
			a	b	c	αβγ			
VO_2 (M)	VO_2 (M1)	$P\,2_1/c$	5.715	4.554	5.385	β = 122.6°	V source: V_2O_5, VH_4VO_3 Reductant:	Most of the research and applications are based on the MIT of VO_2 (M).	[21]
	VO_2 (M2)	$C\,2/m$	9.067	5.797	4.526	β = 91.88°			
VO_2 (R)		$P\,4_2/mnm$	4.554	4.554	2.85	α = β = γ = 90°	$H_2C_2O_4$, N_2H_4 Surfacant:	The high-temperature rutile phase of VO_2.	[22]
VO_2 (A)		$P\,4_2/nmc$	8.434	8.434	7.678	α = β = γ = 90°	polyvinylpyrrolidone (PVP), polyethylene glycol (PEG)	Another phase with MIT Behaviour with T_c = 435 K	[27,29]
VO_2 (B)		$C\,2/m$	12.03	3.693	6.42	β = 106.6°	Temperature: ~150–260 °C	It has layer structure, which suitable for electrode materials and thermal sensitive materials of batteries.	[24,30]

Zhang, Y.; Xiong, W.; Chen, W.; Zheng, Y. Recent Progress on Vanadium Dioxide Nanostructures and Devices: Fabrication, Properties, Applications and Perspectives. Nanomaterials 2021, 11, 338. https:// doi.org/10.3390/nano11020338

Monoclinic Phase of Vanadium Dioxide (VO2 (M1))

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ cat VO2_M1.poscar
Monoclinic phase (M1) of VO2
1.0
5.715 0.0 0.0
0.0 4.554 0.0
-2.901 0.0 4.537
V O
4 8
Direct
0.254816 0.504216 0.750833
0.245184 0.004216 0.249167
0.745184 0.495784 0.249167
0.754816 0.995784 0.750833
0.599060 0.298315 0.899845
0.900400 0.798315 0.100155
0.400940 0.701685 0.100155
0.099060 0.201685 0.899845
0.399050 0.798629 0.599194
0.100950 0.298629 0.400806
0.600950 0.201371 0.400806
0.899050 0.701371 0.599194
```

Monoclinic Phase of Vanadium Dioxide (VO2 (M1))



Lattice parameters

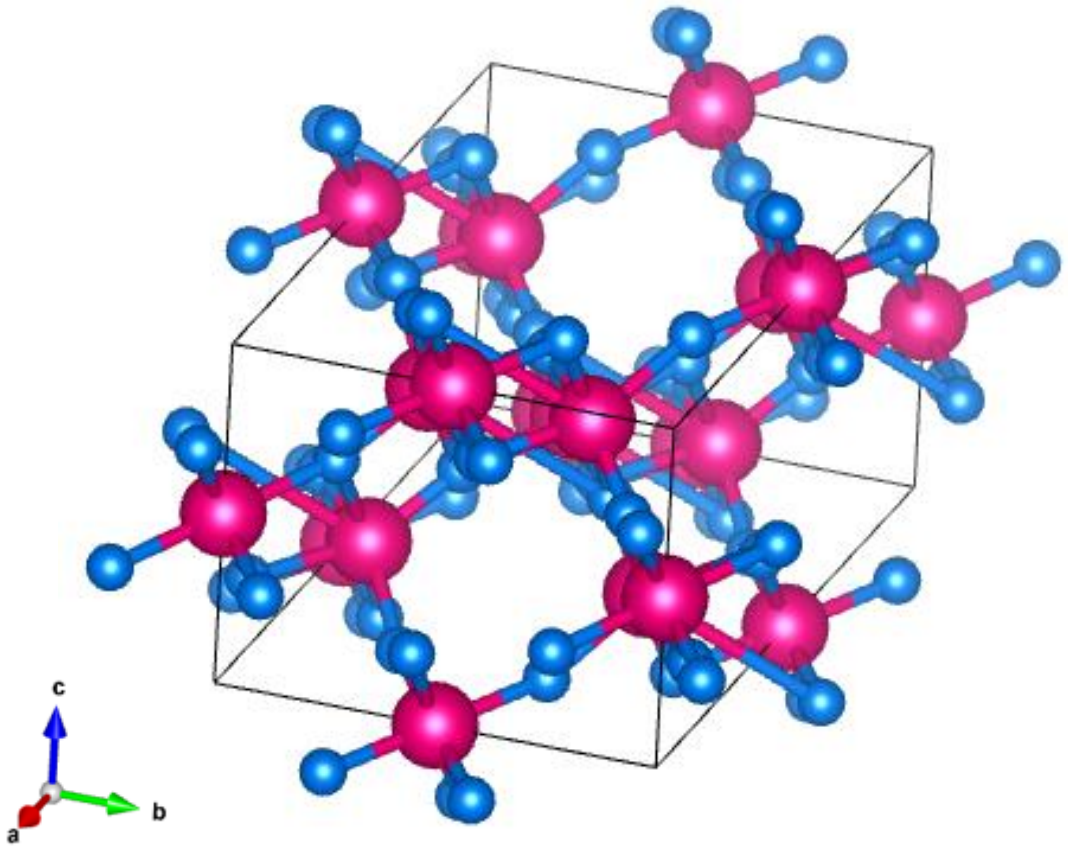
a	b	c	alpha	beta	gamma
5.71500	4.55400	5.38518	90.0000	122.5952	90.0000

Unit-cell volume = 118.080454 Å^3

Monoclinic Phase of Vanadium Dioxide (VO2 (M2))

```
Monoclinic phase (M2) of VO2
1.0
0.000 9.067 0.000
5.797 0.000 0.000
0.000 -0.148 -4.524
V O
12 24
direct
0.2380310000000000    0.6853095000000000    0.2488645000000000
0.7619690000000000    0.6853095000000000    0.7511355000000000
0.2380310000000000    0.3146905000000000    0.2488645000000000
0.7619690000000000    0.3146905000000000    0.7511355000000000
0.5000000000000000    0.0000000000000000    0.0000000000000000
0.5000000000000000    0.5000000000000000    0.5000000000000000
0.7380309999999999    0.1853095000000000    0.2488645000000000
0.2619690000000000    0.1853095000000000    0.7511355000000000
0.7380309999999999    0.8146905000000000    0.2488645000000000
0.2619690000000000    0.8146905000000000    0.7511355000000000
0.0000000000000000    0.5000000000000000    0.0000000000000000
0.0000000000000000    0.0000000000000000    0.5000000000000000
0.8861320000000000    0.5000000000000000    0.6950194999999999
0.3837690000000000    0.5000000000000000    0.2144354999999999
0.6162310000000000    0.5000000000000000    0.7855645000000001
0.1138680000000000    0.5000000000000000    0.3049805000000001
0.3581665000000001    0.1674359999999999    0.0621584999999999
0.3583399999999999    0.6698885000000000    0.5837655000000000
0.3581665000000001    0.8325640000000001    0.0621584999999999
0.3583399999999999    0.3301115000000000    0.5837655000000000
0.6416600000000001    0.3301115000000000    0.4162345000000000
0.6418334999999999    0.8325640000000001    0.9378415000000001
0.6416600000000001    0.6698885000000000    0.4162345000000000
0.6418334999999999    0.1674359999999999    0.9378415000000001
0.3861320000000000    0.0000000000000000    0.6950194999999999
0.8837690000000000    0.0000000000000000    0.2144354999999999
0.1162310000000000    0.0000000000000000    0.7855645000000001
0.6138680000000001    0.0000000000000000    0.3049805000000001
0.8581665000000001    0.6674359999999999    0.0621584999999999
0.8583399999999999    0.1698885000000000    0.5837655000000000
0.8581665000000001    0.3325640000000001    0.0621584999999999
0.8583399999999999    0.8301115000000001    0.5837655000000000
0.1416600000000001    0.8301115000000001    0.4162345000000000
0.1418334999999999    0.3325640000000001    0.9378415000000001
0.1416600000000001    0.1698885000000000    0.4162345000000000
0.1418334999999999    0.6674359999999999    0.9378415000000001
```

Monoclinic Phase of Vanadium Dioxide (VO2 (M2))



Lattice parameters

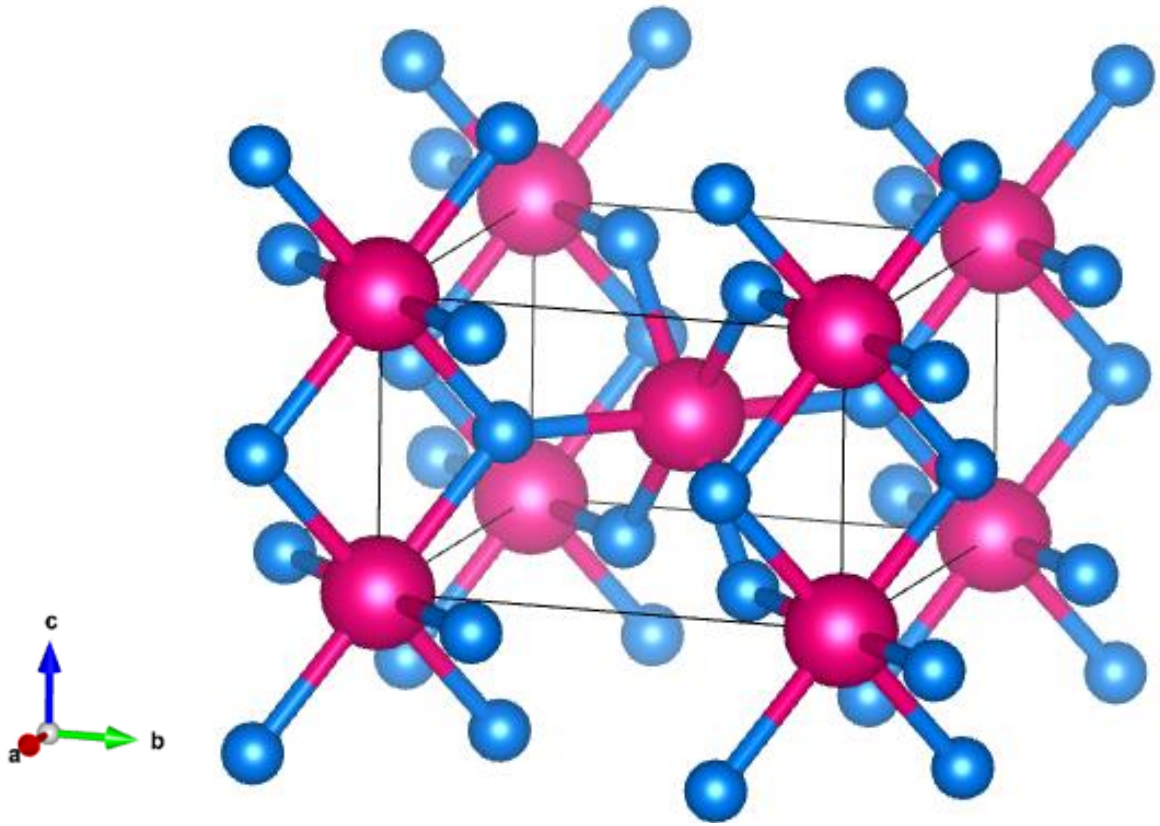
a	b	c	alpha	beta	gamma
9.06700	5.79700	4.52642	90.0000	91.8737	90.0000

Unit-cell volume = 237.787772 Å^3

Rutile Phase of Vanadium Dioxide (VO2 (R))

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ cat VO2_R.poscar
Tetragonal Rutile (R) Structure of VO2
1.0
4.554 0.0 0.0
0.0 4.554 0.0
0.0 0.0 2.85
V O
2 4
Direct
0.00000 0.00000 0.00000
0.50000 0.50000 0.50000
0.29964 0.29964 0.00000
0.70036 0.70036 0.00000
0.20036 0.79964 0.50000
0.79964 0.20036 0.50000
```

Rutile Phase of Vanadium Dioxide (VO2 (R))



Lattice parameters

a	b	c	alpha	beta	gamma
4.55400	4.55400	2.85000	90.0000	90.0000	90.0000

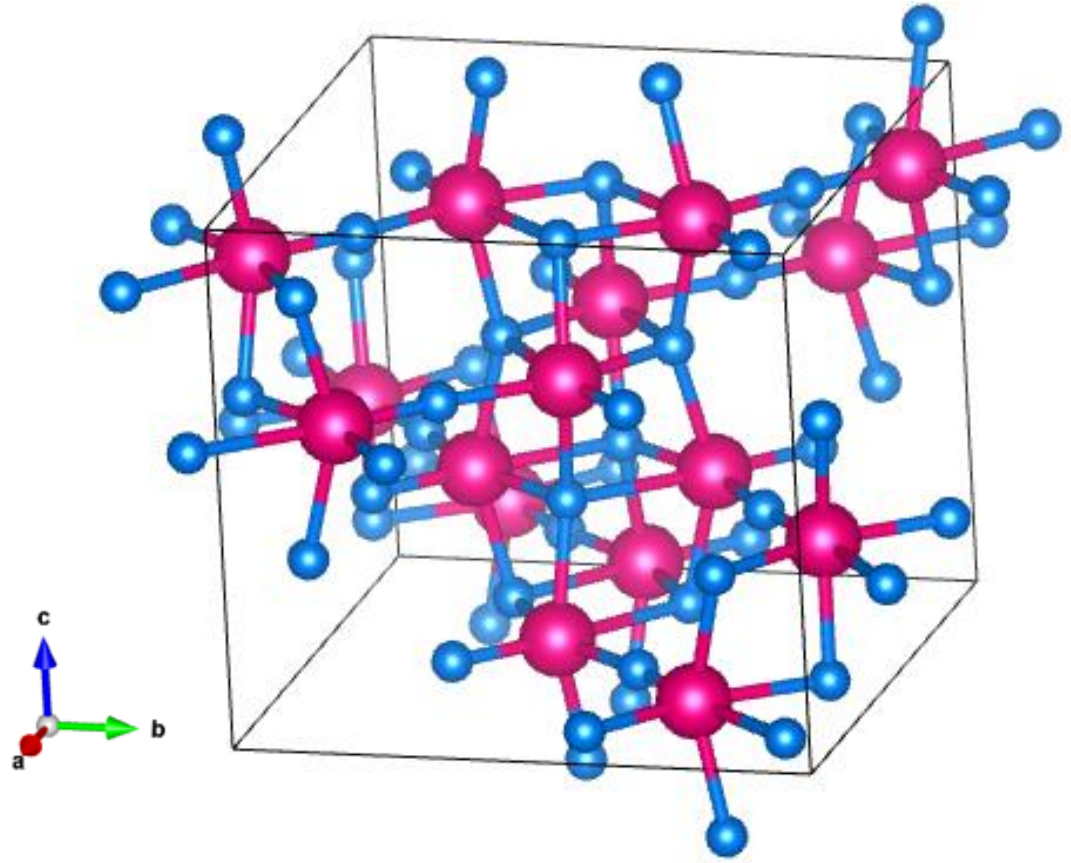
Unit-cell volume = 59.105906 Å^3

A Phase of Vanadium Dioxide (VO2 (A))

```
VO2 (A)
1.0
8.434 0.000 0.000
0.000 8.434 0.000
0.000 0.000 7.678
V O
16 32
direct
0.2016740000000000    0.9817060000000000    0.8753649999999998
0.9817060000000000    0.2016740000000000    0.6246350000000002
0.9817060000000000    0.7983260000000000    0.1246350000000002
0.2983260000000000    0.5182940000000000    0.1246350000000002
0.0182940000000000    0.7983260000000000    0.6246350000000002
0.2016740000000000    0.0182940000000000    0.3753649999999999
0.2983260000000000    0.4817060000000000    0.6246350000000002
0.0182940000000000    0.2016740000000000    0.1246350000000002
0.5182940000000000    0.7016740000000000    0.8753649999999998
0.4817060000000000    0.7016740000000000    0.3753649999999999
0.7983260000000000    0.0182940000000000    0.8753649999999998
0.7016740000000000    0.5182940000000000    0.6246350000000002
0.5182940000000000    0.2983260000000000    0.3753649999999999
0.7016740000000000    0.4817060000000000    0.1246350000000002
0.4817060000000000    0.2983260000000000    0.8753649999999998
0.7983260000000000    0.9817060000000000    0.3753649999999999
0.8498080000000000    0.9951820000000000    0.1252499999999999
0.5048180000000000    0.3498079999999999    0.1252499999999999
0.6501920000000000    0.5048180000000000    0.8747500000000000
0.6604620000000000    0.8391010000000000    0.8747529999999999
0.4951820000000000    0.3498079999999999    0.6252500000000000
0.3391009999999999    0.1604619999999999    0.3747529999999999
0.3395380000000000    0.1608990000000000    0.8747529999999999
0.6501920000000000    0.4951820000000000    0.3747500000000000
0.8395380000000000    0.3391009999999999    0.6252470000000001
0.6604620000000000    0.1608990000000000    0.3747529999999999
0.1604619999999999    0.3391009999999999    0.1252470000000001
0.1501920000000000    0.0048180000000000    0.1252499999999999
0.3498079999999999    0.5048180000000000    0.3747500000000000
0.0048180000000000    0.8498080000000000    0.8747500000000000
0.1604619999999999    0.6608990000000000    0.6252470000000001
0.1608990000000000    0.6604620000000000    0.1252470000000001
0.3395380000000000    0.8391010000000000    0.3747529999999999
0.5048180000000000    0.6501920000000000    0.6252500000000000
0.0048180000000000    0.1501920000000000    0.3747500000000000
0.9951820000000000    0.1501920000000000    0.8747500000000000
```

```
0.8391010000000000    0.6604620000000000    0.6252470000000001
0.8498080000000000    0.0048180000000000    0.6252500000000000
0.1501920000000000    0.9951820000000000    0.6252500000000000
0.4951820000000000    0.6501920000000000    0.1252499999999999
0.6608990000000000    0.1604619999999999    0.8747529999999999
0.8395380000000000    0.6608990000000000    0.1252470000000001
0.9951820000000000    0.8498080000000000    0.3747500000000000
0.8391010000000000    0.3395380000000000    0.1252470000000001
0.1608990000000000    0.3395380000000000    0.6252470000000001
0.3391009999999999    0.8395380000000000    0.8747529999999999
0.6608990000000000    0.8395380000000000    0.3747529999999999
0.3498079999999999    0.4951820000000000    0.8747500000000000
```

A Phase of Vanadium Dioxide (VO2 (A))



Lattice parameters

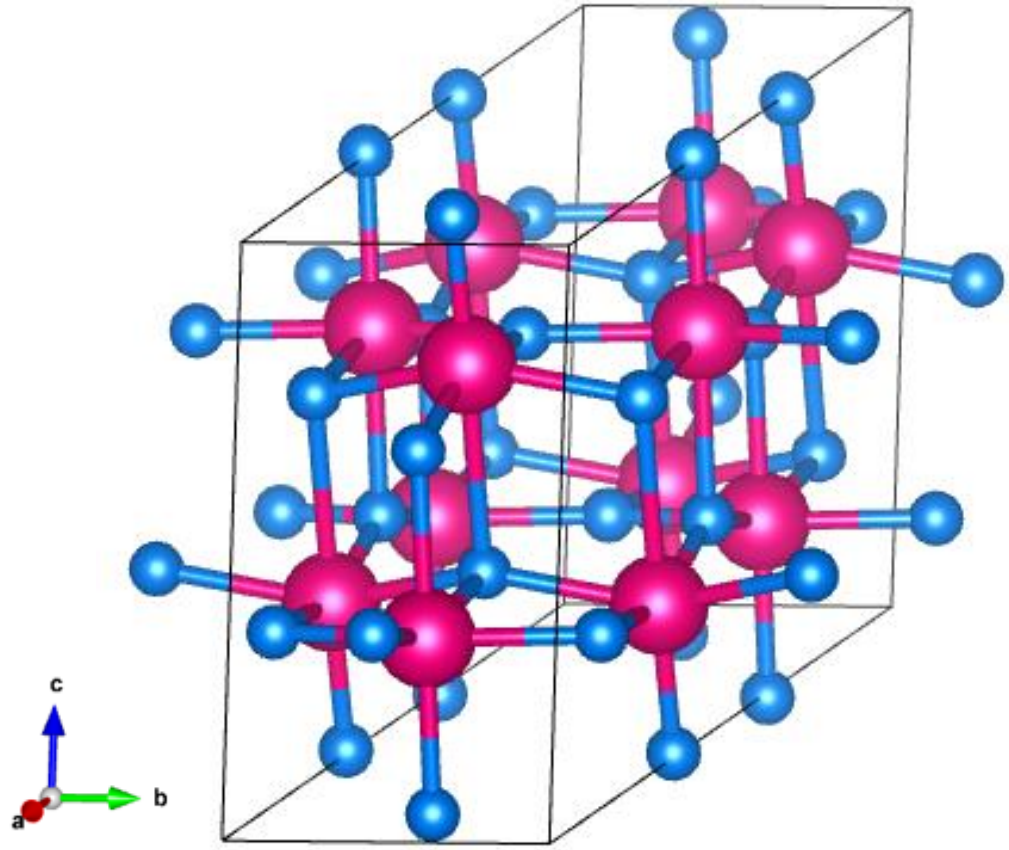
a	b	c	alpha	beta	gamma
8.43400	8.43400	7.67800	90.0000	90.0000	90.0000

Unit-cell volume = 546.154229 Å^3

B Phase of Vanadium Dioxide (VO2 (B))

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ cat VO2_B.poscar
VO2 (B)
1.0
0.000000 12.030000 0.000000
3.693000 0.000000 0.000000
0.000000 -1.834119 -6.152431
V O
8 16
direct
0.8035356700000000    0.5000000000000000    0.7207595800000001
0.6964643300000000    0.0000000000000000    0.2792404199999999
0.8998421200000000    0.5000000000000000    0.3015058500000001
0.6001578800000000    0.0000000000000000    0.6984941499999999
0.3035356700000000    0.0000000000000000    0.7207595800000001
0.1964643300000000    0.5000000000000000    0.2792404199999999
0.3998421200000000    0.0000000000000000    0.3015058500000001
0.1001578800000000    0.5000000000000000    0.6984941499999999
0.8623664650000000    0.5000000000000000    0.9922722400000002
0.6376335350000000    0.0000000000000000    0.0077277599999998
0.7324424750000000    0.5000000000000000    0.3457944900000001
0.7675575250000000    0.0000000000000000    0.6542055099999999
0.9406924350000000    0.5000000000000000    0.6306869700000001
0.5593075650000000    0.0000000000000000    0.3693130299999999
0.6345345600000001    0.5000000000000000    0.7047645100000001
0.8654654399999999    0.0000000000000000    0.2952354899999999
0.3623664650000000    0.0000000000000000    0.9922722400000002
0.1376335350000000    0.5000000000000000    0.0077277599999998
0.2324424750000000    0.0000000000000000    0.3457944900000001
0.2675575250000000    0.5000000000000000    0.6542055099999999
0.4406924350000000    0.0000000000000000    0.6306869700000001
0.0593075650000000    0.5000000000000000    0.3693130299999999
0.1345345600000001    0.0000000000000000    0.7047645100000001
0.3654654399999999    0.5000000000000000    0.2952354899999999
```

B Phase of Vanadium Dioxide (VO2 (B))

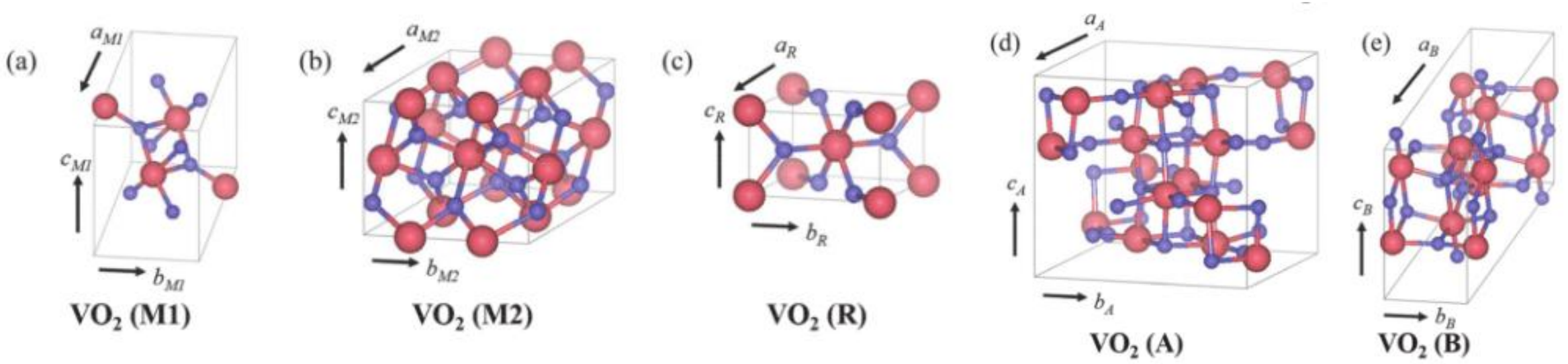


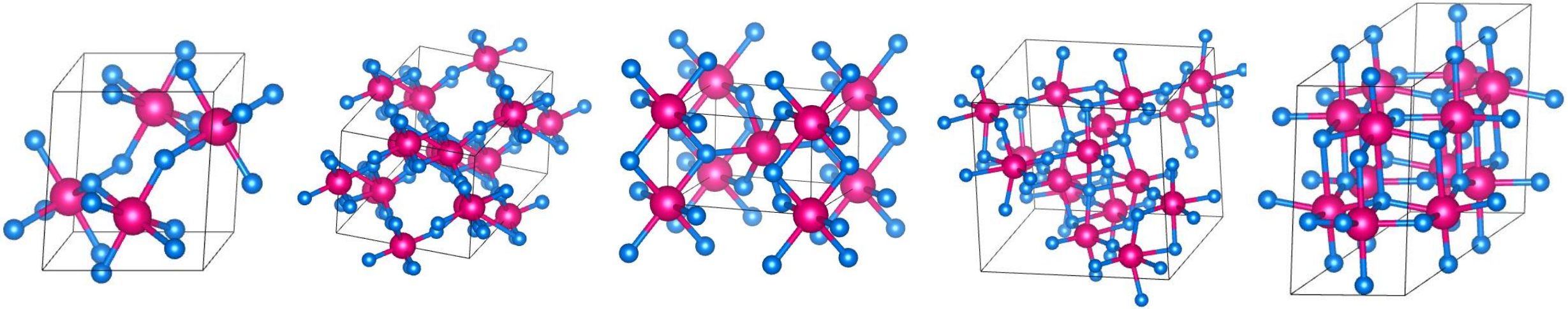
Lattice parameters

a	b	c	alpha	beta	gamma
12.03000	3.69300	6.42000	90.0000	106.6000	90.0000

Unit-cell volume = 273.332762 Å^3

COMPARISON


(a)
a_{M1}
c_{M1}
b_{M1}
VO_2 (M1)
(b)
a_{M2}
c_{M2}
b_{M2}
VO_2 (M2)
(c)
a_R
c_R
b_R
VO_2 (R)
(d)
a_A
c_A
b_A
VO_2 (A)
(e)
a_B
c_B
b_B
VO_2 (B)



References

- Zhang, Y.; Xiong, W.; Chen, W.; Zheng, Y. Recent Progress on Vanadium Dioxide Nanostructures and Devices: Fabrication, Properties, Applications and Perspectives. Nanomaterials 2021, 11, 338. https:// doi.org/10.3390/nano11020338
- https://next-gen.materialsproject.org/materials/mp-1102963?_skip=15&_sort_fields=-symmetry.symbol&formula=VO2
- https://next-gen.materialsproject.org/materials/mp-1100908?_sort_fields=symmetry.symbol&formula=VO2
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- https://next-gen.materialsproject.org/materials/mp-1178787?_skip=15&_sort_fields=-symmetry.symbol&formula=VO2
- *https://next-gen.materialsproject.org/materials/mp-541404?_sort_fields=symmetry.symbol&formula=VO2*