

!BIOSYM archive 3

PBC=ON

SiO2 Stishovite (P42/MNM #136)

!DATE

PBC	4.1576	4.1576	2.6910	90.0000	90.0000	90.0000 (P42/MNM)			
O	2.893226212		1.264339361	-0.000000000	CORE 1	O	O	0.000	
Si	2.078782787		2.078782787	1.345516667	CORE 7	Si	Si	0.000	

end

end

!BIOSYM archive 3

PBC=ON

SiO2 Anatase (I41/AMD #141)

!DATE

PBC	3.4392	3.4392	8.5112	90.0000	90.0000	90.0000 (I41/AMD)			
O	0.000000000		-1.719605125	3.912797438	CORE 1	O	O	0.000	
Si	-1.719605125		0.000000000	6.383400395	CORE 7	Si	Si	0.000	

end

end

!BIOSYM archive 3

PBC=ON

TiO2 rutile (P42/MNM, #136)

!DATE

PBC	4.6578	4.6578	2.9693	90.0000	90.0000	90.0000 (P42/MNM)			
O	1.422313607		1.422313607	0.000000000	CORE 1	O	O	0.000	
Ti	0.000000000		0.000000000	0.000000000	CORE 5	Ti	Ti	0.000	

end

end

!BIOSYM archive 3

PBC=ON

TiO2 pyrite (PA-3, #205)

!DATE

PBC	4.9042	4.9042	4.9042	90.0000	90.0000	90.0000 (PA-3)			
O	3.236839201		0.784739201	1.667360799	CORE 1	O	O	0.000	
Ti	2.452100000		2.452100000	2.452100000	CORE 9	Ti	Ti	0.000	

end

end

!BIOSYM archive 3

PBC=ON

TiO2 MI (P21/C, #14)

```

!DATE
PBC    4.8828    4.9175    5.1481    90.0000    100.5899    90.0000 (P21/C)
O      -0.526770609    1.555074740    4.354278627 CORE 1    O      O      0.000
O      1.319857231    3.734187069    4.795888282 CORE 2    O      O      0.000
Ti      0.655738479    0.294074369    3.640902957 CORE 9    Ti      Ti      0.000
end
end

```

!BIOSYM archive 3

PBC=ON

TiO2 II (PBCN, #60)

```

!DATE
PBC    4.5898    5.5988    4.9341    90.0000    90.0000    90.0000 (PBCN)
O      3.344146258    7.724832312    2.865960294 CORE 1    O      O      0.000
Ti      2.294900000    7.400345755    1.233525000 CORE 9    Ti      Ti      0.000
end
end

```

!BIOSYM archive 3

PBC=ON

TiO2 anatase (I41/AMD, #141)

```

!DATE
PBC    3.7998    3.7998    9.7817    90.0000    90.0000    90.0000 (I41/AMD)
O      1.899900786    1.899900786    2.880686526 CORE 1    O      O      0.000
Ti      1.899900786    -0.000000000    7.336291461 CORE 5    Ti      Ti      0.000
end
end

```

!BIOSYM archive 3

PBC=ON

TiO2 #88 (I41/A, #88)

```

!DATE
PBC    4.7666    4.7666    10.9629    90.0000    90.0000    90.0000 (I41/A)
O      -1.206985532    0.941275173    1.916571720 CORE 1    O      O      0.000
Ti      0.000000000    0.000000000    3.020391013 CORE 9    Ti      Ti      0.000
end
end

```