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Does the real ReN_2 have the MoS_2 structure?

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Table.S1 Lattice parameters and atomic coordinates (fractional) for the investigated crystal structures

structure	lattice parameters				atomic coordinates (fractional)			
	a (Å)	*b* (Å)	*c* (Å)	*β* (°)	atoms	*x*	*y*	*z*
$P6_3/mmc$[1]	2.866		10.076		Re(2c)	0.333	0.667	0.25
					N(4f)	0.333	0.667	0.632
$P6_3/mmc$[2]	2.857		7.957		Re(2a)	0	0	0
					N(4f)	0.667	0.333	0.164
$C2/m$[3]	6.817	2.835	9.363	142.40	Re(4i)	0.406	0.5	0.231
					N1(41)	0.009	0.5	0.136
					N2(4i)	0.432	0	0.53
$P4/mbm$[3]	4.390		2.644		Re(2b)	0	0	0.5
					N(4g)	0.617	0.117	0
$P2_1/m$[3]	4.233	2.884	5.182	64.71	Re(2e)	0.01	0.75	0.283
					N1(2e)	0.357	0.25	0.296
					N2(2e)	0.721	0.25	0.17
Pc [3]	4.813	4.813	5.613	149.00	Re(2a)	0.869	0.25	0.365
					N1(2a)	0.506	0.545	0.297
					N2(2a)	0.095	0.045	0.797
$Pnma$[3]	9.579	2.846	4.151		Re(4c)	0.109	0.75	0.1
					N1(4c)	0.174	0.25	0.455
					N2(4c)	0.094	0.25	0.741
Cm[3]	4.964	2.871	9.573	107.49	Re1(2a)	0.001	0	0.064
					Re2(2a)	0.251	0	0.495
					N1(2a)	0.248	0.5	0.202
					N2(2a)	0.338	0.5	0.357
					N3(2a)	0.492	0.5	0.624
					N4(2a)	0.093	0.5	0.935
Pm[3]	4.860	2.826	4.085	80.51	Re1(1b)	0.201	0.5	0.575
					Re2(1a)	0.778	1	0.972
					N1(1a)	0.353	1	0.195
					N2(1a)	0.192	1	0.936
					N3(1b)	0.825	0.5	0.346
					N4(1b)	0.622	0.5	0.641
$Immm$[3]	13.016	3.734	2.806		Re(4e)	0.158	0	0
					N1(4f)	0.051	0	0.5
					N2(4f)	0.292	0	0.5
$Pca2_1$[3]	4.957	2.901	7.857		Re(4a)	0.25	0.297	0.08
					N1(4a)	0.08	0.792	0.242
					N2(4a)	0.08	0.792	0.418
$P2/c$[3]	4.241	2.947	4.977	65.92	Re(2f)	0.5	0.191	0.25
					N(4g)	0.179	0.698	0.191
$Cmmm$[3]	7.704	5.701	2.827		Re(8d)	0.25	0.25	0
					N1(8e)	0.31	0	0.5
					N2(8f)	0	0.117	0
$P4_2/mnm$[4]	4.851		2.820		Re(2a)	0	0	0
					N(4f)	0.296	0.296	0

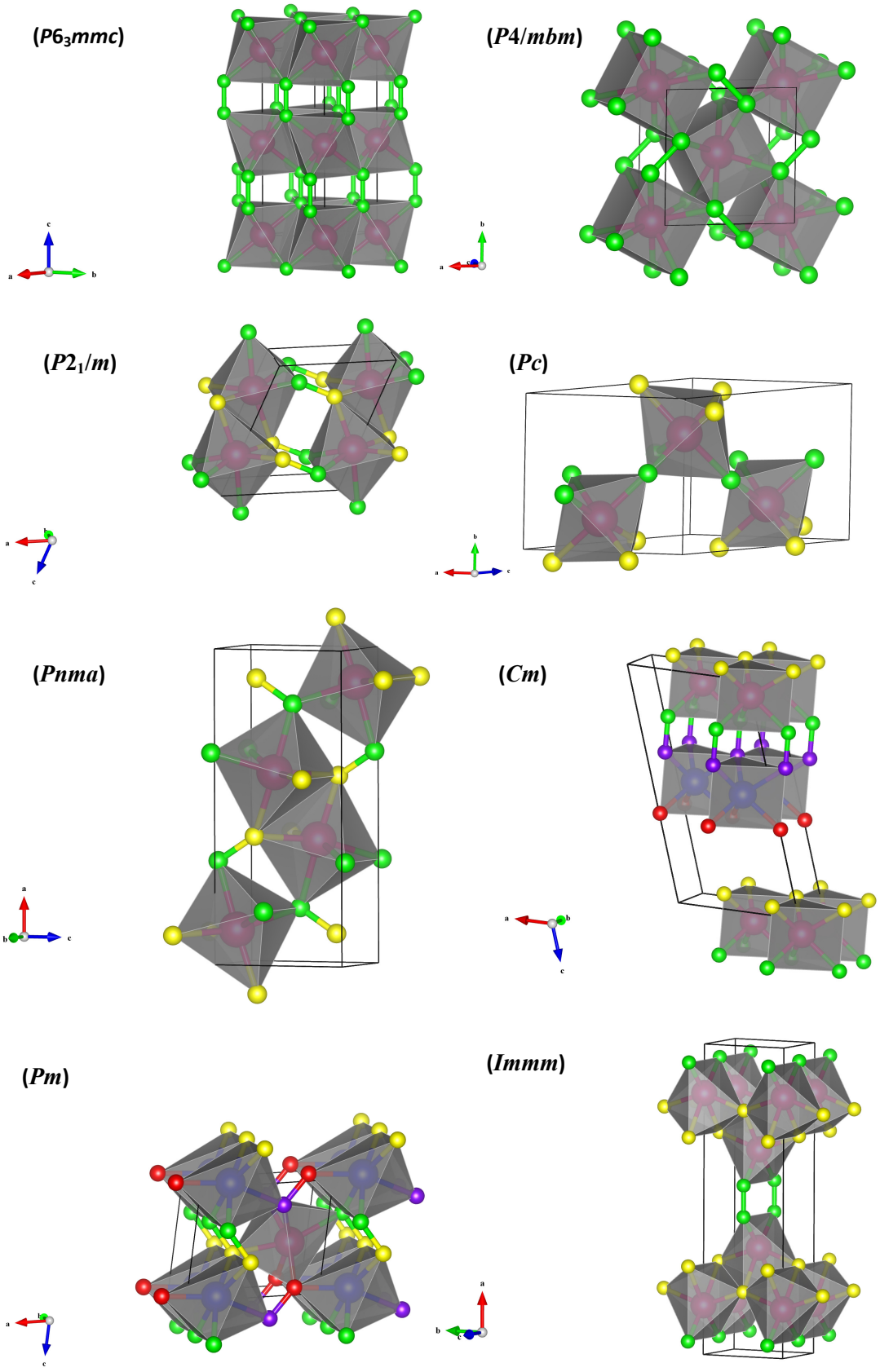
[1]F. Kawamura, H. Yusa, T. Taniguchi, Appl. Phys. Lett. 100, 251910 (2012)

[2] Particle swarm searched structure in the same space group with reference 1

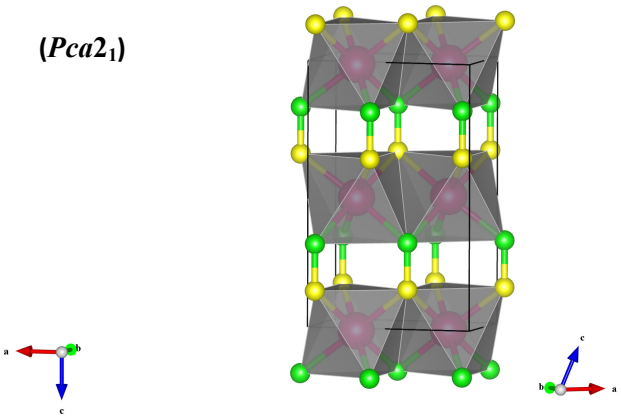
[3]Other particle swarm searched structure, wherein *C*2/*m* is the most energetically favorable structure, and *P*4/*mbm* is the high pressure phase of *C*2/*m*

[4]E. Zhao, Z. Wu, Comput. Mater. Sci. 44, 531 (2008)

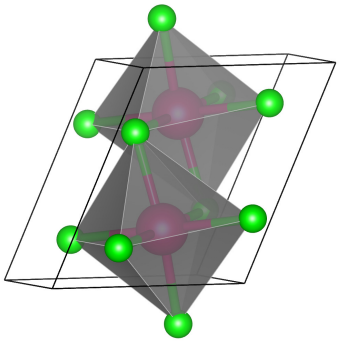
Figure. S1 Features of the studied crystal structures



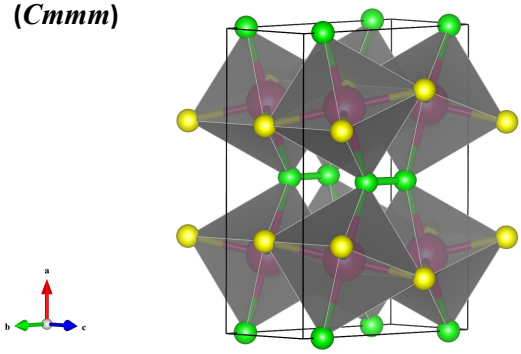
($Pca2_1$)



($P2/c$)



($Cmmm$)



($P4_2/mnm$)