

Proton ordering in cubic ice and hexagonal ice; a potential new ice phase — Xlc

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The following structures are relaxed configurations for cubic ice obtained using CP2K/PBE

24							
N=1, SG 109 (I41md), Cell	params	8.776	4.385	6.219	90.000	90.000	90.000
O	-0.0000000003	0.0000000025			-0.0776150808		
O	2.1847581972	2.1925806577			3.0322884996		
O	0.0000000021	2.1926433507			1.4746624481		
O	2.1845897480	0.0000000380			4.5839608510		
O	4.3691721513	0.0000000026			-0.0775991496		
O	6.5590960899	2.1925980395			3.0274589445		
O	4.3691745412	2.1925947892			1.4747244575		
O	6.5560475171	0.0000000411			4.5849241987		
H	0.0000000006	-0.8040876658			0.5257605776		
H	0.0000000006	0.8040876733			0.5257605725		
H	7.3646058116	0.0000001407			5.1800088829		
H	1.3813198025	0.0000000446			5.1883906097		
H	0.8033984280	2.1926051430			2.0789152335		
H	3.5667629711	2.1925889086			2.0802886635		
H	2.1845496663	1.3884493852			3.6356129756		
H	2.1845477859	2.9967104780			3.6356175970		
H	4.3684872382	-0.8040529554			0.5258692313		
H	4.3684872380	0.8040529624			0.5258692268		
H	2.9881776772	0.0000000447			5.1879476818		
H	5.7559898774	0.0000000484			5.1935728512		
H	5.1742413782	2.1926011203			2.0769169699		
H	-0.8033984236	2.1926051430			2.0789152339		
H	6.5568480273	1.3894936763			3.6310676153		
H	6.5568600258	2.9956398829			3.6311398690		
24							
N=2, SG 92 (P4121), Cell	params	8.773	4.382	6.236	89.999	89.980	90.000
O	8.8095753604	4.4517124894			0.0007160050		
O	2.1833560098	2.1901791930			3.1214661094		
O	-0.0066388467	2.1929493564			1.5586131429		
O	2.2256257403	-0.0021951735			4.6994604038		
O	4.4389407140	4.4522573037			-0.0002547424		
O	6.5539564607	2.12174446186			3.1185392246		
O	4.3696431314	2.2622915462			1.5587966657		
O	6.6277653713	-0.0691834679			4.6764399359		
H	8.7838985081	3.6310330797			0.5812128356		
H	0.0119464382	1.3592317024			0.9981009986		
H	7.9845550342	4.4026657945			-0.5725000193		
H	1.3901337175	0.0101596533			5.2572486354		
H	0.8223560316	2.1805483273			2.1257945934		
H	3.0115464813	2.2215023281			2.5529299249		
H	2.1986442493	0.8236024704			4.1286419931		
H	2.2027543496	3.0167094167			3.6914632041		
H	4.4107618992	3.6295622533			0.5773605823		
H	4.3922463446	1.4387259225			0.9827553120		
H	3.6048462559	4.4221132547			-0.5599444934		
H	5.8013318131	-0.0202435210			5.2472378132		
H	5.1948649307	2.2132945292			2.1315767402		
H	7.3784050856	2.1709599106			2.5445014240		

H	6.6021501498	0.7511320679	4.0953381885
H	6.5803700478	2.9421971300	3.6992123015
24			
N=3, SG 33 (Pna21), Cell	params	8.778 4.381 6.232	90.005 89.995 90.007
O	8.8167413025	4.4503269337	0.0025670652
O	2.2518386537	2.1896663810	3.1145060152
O	8.8172966231	2.2596861161	1.5550539645
O	2.2443090669	-0.0020090077	4.6810310295
O	4.4455398077	4.4516034196	0.0018549280
O	6.6329103527	2.1209751558	3.1182812763
O	4.4467690455	2.2611776009	1.5557929687
O	6.6331609322	-0.0695956349	4.6713147869
H	8.7948356332	3.6285217581	0.5821005643
H	8.7952226240	1.4379073622	0.9755090039
H	7.9924078435	4.4011237102	-0.5700149944
H	1.4117788919	0.0110246236	5.2420830750
H	1.4195103297	2.2022526201	2.5530537167
H	3.6190997990	2.2304180200	2.1240560947
H	2.2170674814	0.8270541507	4.1137848122
H	2.2209088356	3.0178671951	3.6829314327
H	4.4203003685	3.6266233998	0.5766519911
H	4.4202931864	1.4360492674	0.9814618320
H	3.6156576206	4.4208608646	-0.5628300720
H	5.8079301465	-0.0200945115	5.2423713221
H	5.8081312290	2.1706301500	2.5465160630
H	7.9931920461	2.2103670996	2.1279622890
H	6.6114300173	0.7518562970	4.0912766652
H	6.6110731474	2.9424598657	3.6982384722
24			
N=4, SG 33 (Pna21), Cell	params	8.774 4.389 6.229	89.946 89.978 90.003
O	8.8108156676	4.4610366783	0.0003673496
O	2.1828631004	2.1946995874	3.1185464648
O	-0.0054388424	2.1954288526	1.5567989408
O	2.2245371382	4.3829168505	4.6980744314
O	4.4398254980	-0.0720508682	-0.0006582226
O	6.5538578573	2.1262270921	3.1145773541
O	4.3690145968	2.1226494979	1.5573455137
O	6.6291461372	-0.0672800450	4.6712078298
H	8.7873550471	3.6376327859	0.5763812113
H	0.0106560187	1.3677031927	0.9878387272
H	7.9853234168	4.4129281089	-0.5722821236
H	1.3884312754	4.3610720759	5.2551693205
H	0.8221021399	2.1660779874	2.1258987491
H	3.0109551891	2.1646122944	2.5493200599
H	2.2052090250	1.3705119390	3.6907865199
H	2.1995008644	3.5611379075	4.1220273630
H	4.3995923483	2.9490012495	0.9867029531
H	4.4127647198	0.7541887467	0.5709461520
H	3.6037441577	-0.0480823012	-0.5582966546
H	5.8014201098	-0.0401733064	5.2417446966
H	5.1956031294	2.1502193235	2.1296490646
H	7.3788167653	2.1735717521	2.5411135472
H	6.5950839217	0.7554609480	4.0951379720
H	6.5777681651	2.9499590189	3.6899049168
24			
N=5, SG 31 (Pmn21), Cell	params	8.787 4.393 6.217	89.975 90.000 90.000
O	-0.0000000000	0.0018023392	-0.0761435458
O	2.1589698944	2.2314959642	3.0723332374
O	-0.0000000000	2.1972575993	1.4737249405
O	2.2275385902	4.4310038079	4.6310586934
O	4.4012699843	4.4322489333	6.2506871572
O	6.6326658679	2.2709848946	3.1080332280
O	4.4105392782	2.2351906245	1.5872525071

O	6.5649478983	4.4682479479	4.6633778996
H	-0.0000000000	-0.8012995526	0.5282026364
H	-0.0000000000	0.8048394835	0.5292392568
H	7.3934606517	4.4435007220	5.2324962981
H	1.3968161415	4.4068049428	5.1963826328
H	0.8033350784	2.1998367888	2.0776547775
H	2.9958821979	2.2183062838	2.5170464904
H	2.1902294225	1.4037543295	3.6417827790
H	2.1982167887	3.6026964556	4.0639198291
H	4.4066920455	3.0390250482	0.9833942560
H	4.4082662286	1.4342715259	0.9807789853
H	3.6003013678	4.4230017793	5.6453013332
H	5.2056658877	4.4346322590	5.6474322691
H	5.8035227812	2.2451724836	2.5400460469
H	-0.8033350784	2.1998367888	2.0776547774
H	6.6026637201	1.4440492948	3.6782690706
H	6.5957484336	3.6412246446	4.0934578261
24			
N=6, SG 29 (Pca21), Cell params 8.771 4.383 6.231 90.007 89.956 89.995			
O	8.8098679721	4.4540819298	0.0019784739
O	2.2249191394	2.1929740081	3.0938125830
O	8.8112665236	2.2624678639	1.5555474782
O	2.2481051997	4.3812308198	4.6758090953
O	4.4417275252	-0.0726146255	0.0003314406
O	6.6291403460	2.1197735162	3.1175370810
O	4.4418288817	2.1189510296	1.5570942449
O	6.6310281065	-0.0719696451	4.6716758164
H	8.7918341473	3.6302468779	0.5779387631
H	8.7924414125	1.4387872281	0.9794496289
H	7.9850518828	4.4050347954	-0.5702347678
H	1.4174833673	4.3567718360	5.2395949476
H	1.3915932641	2.1659218375	2.5325059428
H	3.6073878922	2.1479865907	2.1156531376
H	2.2027002672	1.3706287905	3.6688872573
H	2.2144048007	3.5599421486	4.0983822993
H	4.4209689704	2.9456166867	0.9855467764
H	4.4186761195	0.7546696219	0.5708536575
H	3.6126370508	-0.0440386630	-0.5662087425
H	5.8045604622	-0.0444077457	5.2428857727
H	5.8015862299	2.1472256650	2.5482821817
H	7.9865415550	2.2134190558	2.1278955454
H	6.6023906951	0.7527320856	4.0974533076
H	6.6017107477	2.9445336865	3.6919171115
24			
N=7, SG 18 (P2121), Cell params 8.785 4.392 6.221 90.000 90.000 89.979			
O	-0.0000007430	0.0000045639	-0.0761004416
O	2.1600156727	2.2235762582	3.0740839422
O	0.0008006044	2.1960244374	1.4748940077
O	2.2286875136	4.4228214780	4.6341404521
O	4.4021969898	4.3568949639	6.2543292604
O	6.6323444447	2.1244872753	3.1098976767
O	4.4101880963	2.1615998820	1.5881883020
O	6.5642219044	-0.0713585133	4.6663687904
H	0.0020318740	-0.8028965759	0.5289515204
H	-0.0020364893	0.8028962089	0.5289640325
H	7.3903125695	-0.0346515635	5.2377196488
H	1.3983169024	4.3982326634	5.1999261502
H	0.8040418024	2.1931520381	2.0790284352
H	2.9952796951	2.1910050977	2.5168464519
H	2.1852222846	1.3991968891	3.6488707409
H	2.1972154864	3.5977449124	4.0624770153
H	4.4107646554	2.9623826652	0.9809385846
H	4.4043882488	1.3580099553	0.9847676957

H	3.6011131701	4.3660538978	5.6492255471
H	5.2063949115	4.3572153005	5.6505856892
H	5.8031404270	2.1513772469	2.5421758476
H	-0.8024499129	2.1988965423	2.0790259675
H	6.5925344624	0.7534008975	4.0926928092
H	6.6012092904	2.9486892694	3.6839573515
24			
N=8, SG 7 (Pc), cell params 8.781 4.389 6.222 90.035 89.930 89.982			
O	-0.0008997686	0.0008767089	-0.0775442538
O	2.1601649725	2.2277509132	3.0728841501
O	0.0015982506	2.1939514585	1.4748862562
O	2.2292019696	4.4211852265	4.6296142280
O	4.4076777822	4.4620230758	-0.0270151665
O	6.5968001999	2.2309038435	3.0737443467
O	4.3720127167	2.2653892128	1.5505849524
O	6.6007762052	0.0351984458	4.6267867572
H	0.0006992578	-0.8028972662	0.5259716098
H	-0.0005778470	0.8041279560	0.5273531301
H	7.4015657795	0.0363435377	5.2345447224
H	1.4001504412	4.3958599531	5.1972990982
H	0.8048103545	2.1954277211	2.0791308264
H	2.9974921764	2.2155384806	2.5160898845
H	2.1906281511	1.3986638533	3.6394207754
H	2.1997600010	3.5938824869	4.0596581575
H	4.3866557320	3.6388557710	0.5463241423
H	4.3960809745	1.4447653478	0.9724159513
H	3.5820370163	4.4248014475	-0.5995646619
H	5.7923842398	0.0375596169	5.2231779700
H	5.2006014021	2.2365325899	2.1180119487
H	-0.8021018078	2.1958663595	2.0785182909
H	6.5983447854	1.4275343763	3.6774614173
H	6.5994223554	3.0343259652	3.6779039842
24			
N=9, SG 7 (Pc), Cell params 8.782 4.387 6.221 89.990 89.988 89.998			
O	8.8212240822	4.4587707831	0.0019026241
O	2.2510079763	2.2661877070	3.1019741387
O	8.8216076374	2.2654099681	1.5528995830
O	2.2603733098	4.4609068531	4.6642512088
O	4.4493378353	4.4589770197	0.0015306792
O	6.6367401477	2.1249474302	3.1128638266
O	4.4496946029	2.2653800303	1.5530858811
O	6.6370871195	-0.0684644426	4.6627628155
H	8.8032643312	3.6343904907	0.5770714579
H	8.8033460071	1.4409914598	0.9778337561
H	7.9960945306	4.4106313071	-0.5698361362
H	1.4244977959	4.4288171524	5.2219653649
H	1.4250241805	2.2310455807	2.5328419333
H	3.6209019267	2.2387123405	2.1200487324
H	2.2290520468	1.4412607327	3.6756966423
H	2.2365547528	3.6381053877	4.0888204509
H	4.4215983535	3.6337930774	0.5751397216
H	4.4221840024	1.4403130504	0.9790882296
H	3.6217727875	4.4320993189	-0.5677086812
H	5.8124160023	-0.0180610864	5.2349129150
H	5.8119512535	2.1750588797	2.5410276193
H	7.9966139628	2.2175152230	2.1248284037
H	6.6155207026	0.7528993484	4.0827241837
H	6.6153718107	2.9464075639	3.6928255359
24			
N=10, SG 4 (P21), Cell params 8.780 4.387 6.228 89.963 89.937 90.018			
O	-0.0009338879	0.0002617731	-0.0774927630
O	2.1583114688	2.2244905248	3.0764104304
O	0.0000557391	2.1943203915	1.4763947887

O	2.2248367241	4.4184414952	4.6330218153
O	4.4075978847	-0.0655891306	-0.0265738874
O	6.5943109202	2.1630702590	3.0764109303
O	4.3705353850	2.1262564706	1.5502416431
O	6.5998333072	-0.0304214210	4.6309828691
H	0.0011401461	-0.8023998885	0.5276848517
H	-0.0010285097	0.8042589431	0.5261427078
H	7.4002804201	-0.0073242656	5.2385406777
H	1.3963867280	4.3922747411	5.2014064038
H	0.8029926251	2.1941588960	2.0810494031
H	2.9935939446	2.1909373430	2.5178355135
H	2.1815963623	1.3978348184	3.6477930252
H	2.1939975751	3.5935256324	4.0593838970
H	4.3957597272	2.9473163549	0.9724348261
H	4.3863368816	0.7577949824	0.5470854931
H	3.5816056131	-0.0303079758	-0.5979768585
H	5.7915598201	-0.0298678312	5.2275841472
H	5.1978900591	2.1569607835	2.1194505231
H	-0.8037354321	2.1955754016	2.0798863717
H	6.5979548547	1.3565359066	3.6763870251
H	6.5946652328	2.9628882144	3.6847419334

24

N=11, SG 4 (Pc), Cell params 8.761 4.386 6.239 90.015 90.065 90.008

O	8.7978297981	4.4571608258	0.0002562686
O	2.1722135078	2.2656371744	3.1144614675
O	-0.0280009868	2.2305062251	1.5318997456
O	2.2469822622	4.4559373081	4.6790818449
O	4.4362453099	4.4570851495	0.0003836567
O	6.5395261878	2.1228191630	3.1208287356
O	4.3593408945	2.2641236496	1.5586885993
O	6.6118669209	-0.0700847016	4.6784526025
H	8.7732074062	3.6334644407	0.5758870697
H	0.0047589863	1.4012290009	0.9657380153
H	7.9730156073	4.4105705455	-0.5740151214
H	1.4118026303	4.4238500132	5.2371292148
H	0.7963361621	2.2130634440	2.1051102508
H	2.9989663802	2.2395137272	2.5426093916
H	2.2052777034	1.4417419434	3.6872544852
H	2.2206271502	3.6328906040	4.1026215526
H	4.4022100065	3.6340018692	0.5760870245
H	4.3845954900	1.4406046694	0.9829618463
H	3.6094990386	4.4300346273	-0.5718263352
H	5.7874295848	-0.0203659910	5.2527573792
H	5.1831364416	2.2171094273	2.1338593159
H	7.3630480427	2.1732255190	2.5455692517
H	6.5855919424	0.7500480401	4.0973913313
H	6.5655819552	2.9429561346	3.7017871099

The following structures are relaxed configurations for hexagonal ice obtained using CP2K/PBE

24

N=1, SG 36 (Cmc21), Cell params 4.369 7.641 7.184 90.000 90.000 90.000

O	0.0000000379	5.1229894503	0.4491168724
O	0.0000004435	2.5174409400	4.0411823145
O	2.1845654330	1.3027864667	0.4491192874
O	2.1845658367	6.3376439235	4.0411847294
O	2.1845559041	6.4140428096	6.7346690396
O	2.1845555010	1.2263885763	3.1426035934
O	0.0000007712	2.5938316942	6.7346739224
O	0.0000003661	5.0465996916	3.1426084762
H	0.0000000110	4.1672977472	0.1377779765
H	0.0000001501	5.0904260819	1.4528759836
H	0.0000004158	3.4731326152	3.7298433321

H	0.0000005552	2.5500045197	5.0449414187
H	2.1845635463	1.2702201098	1.4528804303
H	2.1845621288	0.3470952290	0.1377784463
H	2.1845639495	6.3702104917	5.0449458654
H	2.1845625317	7.2933351333	3.7298438018
H	1.3827745905	5.9172871523	7.0814011289
H	2.9863343024	5.9172829366	7.0814080177
H	1.3827741902	1.7231442680	3.4893356478
H	2.9863338979	1.7231484821	3.4893425359
H	0.8017805051	2.0970745125	7.0814076577
H	-0.8017789412	2.0970744797	7.0814076916
H	0.8017800985	5.5433569061	3.4893421759
H	-0.8017793434	5.5433569405	3.4893422104
24			
N=2, SG 33 (Pna21), Cell params			
O	4.4179951523	5.1006676659	0.4522052052
O	4.4179952426	2.5187711985	4.0210527889
O	2.1730637485	1.2569523256	0.4212507719
O	2.1730638620	6.3624865128	3.9900982974
O	2.2093654705	6.3284989051	6.6854856985
O	2.2093654553	1.2909399924	3.1166381554
O	-0.0355723659	2.5527643767	6.7164385725
O	-0.0355724644	5.0666745133	3.1475909760
H	4.3987268614	4.1562060565	0.1102359053
H	3.5807125204	5.5426942261	0.1149145229
H	4.3987269783	3.4632328068	3.6790834862
H	3.5807126034	2.0767446584	3.6837621047
H	2.1922894092	1.2731104352	1.4257482043
H	3.0048029927	1.7324790127	0.1195986044
H	2.1922895201	6.3463284102	4.9945957280
H	3.0048031344	5.8869598651	3.6884461326
H	1.3720708206	5.8864826038	7.0227593823
H	2.1900963443	7.2729613348	7.0274591792
H	1.3720708076	1.7329562918	3.4539118495
H	2.1900963398	0.3464775613	3.4586116344
H	0.7961603983	2.0772320517	7.0180982554
H	-0.0163537709	2.5365883605	5.7119441679
H	-0.0163538787	5.0828505187	2.1430965693
H	0.7961602962	5.5422068493	3.4492506451
24			
N=3, SG 33 (Pna21), Cell params			
O	-0.0029980365	5.0975741366	0.4514896050
O	-0.0030048495	2.5189154784	4.0210173957
O	2.1762381451	1.2564796545	0.4217735798
O	2.1762315939	6.3600099590	3.9913013609
O	2.2046081346	6.3271843494	6.6875450713
O	2.2046146974	1.2893052250	3.1180172911
O	-0.0313544724	2.5517596355	6.7172838659
O	-0.0313476531	5.0647299465	3.1477560759
H	0.8337170964	5.5400906969	0.1134873310
H	0.0163595795	4.1532242484	0.1086718144
H	0.8337102790	2.0763988996	3.6830151318
H	0.0163528282	3.4632653672	3.6781996160
H	2.2075359262	1.2729952339	1.4260756516
H	3.0045487889	1.7338677889	0.1132743946
H	2.2075293677	6.3434943623	4.9956034332
H	3.0045422371	5.8826218193	3.6828021788
H	3.0413145876	5.8846578406	7.0255567080
H	2.2239571996	7.2715317459	7.0303737615
H	3.0413211602	1.7318317120	3.4560289280
H	2.2239637100	0.3449578268	3.4608459847
H	0.7969497404	2.0743653080	7.0257915208
H	-0.0000591462	2.5352326015	5.7129841636

H	-0.0000523290	5.0812569928	2.1434563741
H	0.7969565675	5.5421242588	3.4562637312
24			
N=4, SG 33 (Pbn21), Cell	params	4.423 7.540 7.188	90.000 90.000 90.000
O	-0.0003470958	5.0452927419	0.4493096800
O	4.4237015916	2.4947031869	4.0434312224
O	2.2120433845	1.2752702228	0.4493141761
O	2.2113632463	6.2646930240	4.0434312235
O	2.2099480189	6.2647692840	6.7390666203
O	2.2134616192	1.2751975165	3.1449472422
O	4.4251171193	2.4947794454	6.7390666300
O	-0.0017583087	5.0452158648	3.1449564490
H	0.8374897853	5.4768967649	0.0976842774
H	0.0095949054	4.1011635931	0.1084226641
H	4.4137555536	3.4388299400	3.7025348663
H	3.5858733089	2.0630848563	3.6918011623
H	1.3742045864	1.7068754299	0.0976944446
H	2.2021063939	0.3311410667	0.1084176623
H	2.2213092690	7.2088197814	3.7025348781
H	3.0491915258	5.8330747028	3.6918011379
H	3.0500183616	5.8070796942	7.0485051516
H	2.2396315611	6.2605546839	5.7355262258
H	1.3733823249	1.7328720090	3.4543795252
H	2.1837813889	1.2794079774	2.1414064772
H	4.3954335055	2.4905648527	5.7355262406
H	3.5850467895	2.0370898524	7.0485051992
H	0.0279222775	5.0494328741	2.1414177517
H	0.8383194489	5.5028911015	3.4543921386
24			
N=5, SG 29 (Pca21), Cell	params	4.424 7.543 7.180	90.000 90.000 90.000
O	-0.0013234025	5.0468696260	0.4487682398
O	-0.0013231054	2.4963557154	4.0388488084
O	2.2133213908	1.2752252357	0.4487724364
O	2.2133216950	6.2680001059	4.0388530050
O	2.2093663566	6.2680317688	6.7314246608
O	2.2093660647	1.2751936541	3.1413440946
O	4.4265921688	2.4964191645	6.7314246556
O	4.4265918607	5.0468062585	3.1413440893
H	0.8385671774	5.4792114917	0.1035656218
H	0.0093255297	4.1028236892	0.1076357189
H	0.8385674821	2.0640138683	3.6936461935
H	0.0093258147	3.4404016597	3.6977162970
H	1.3734287227	1.7075676237	0.1035756316
H	2.2026760084	0.3311785296	0.1076331865
H	1.3734290190	5.8356577371	3.6936562034
H	2.2026763246	7.2120468196	3.6977137645
H	3.0508599578	5.8080969876	7.0322985948
H	2.2228195818	6.2623259528	5.7274678474
H	2.2228192885	1.2808994595	2.1373872812
H	3.0508596627	1.7351284452	3.4422180236
H	4.4131388027	2.4907133712	5.7274678419
H	3.5850985873	2.0364843797	7.0322986416
H	4.4131384961	5.0525120412	2.1373872757
H	3.5850982830	5.5067410541	3.4422180702
24			
N=6, SG 19 (P2121), Cell	params	4.415 7.619 7.145	90.000 90.000 90.000
O	-0.0019472808	5.0999518788	0.4519599911
O	4.4166080846	2.5185544146	4.0242189535
O	2.2413892528	1.2579787971	0.4225149359
O	2.1732991743	6.3605180121	3.9947668062
O	2.2054108545	6.3277977151	6.6924920804
O	2.2093019291	1.2906808809	3.1202470165
O	4.4487193754	2.5512748458	6.7219442922

O	-0.0340155958	5.0672154964	3.1497079131
H	0.8359090934	5.5427757069	0.1164281178
H	0.0198329777	4.1556324458	0.1100924418
H	4.3948188327	3.4628730052	3.6823500662
H	3.5787595267	2.0757174404	3.6886809301
H	2.2058644735	1.2735201681	1.4264953017
H	1.4110138052	1.7305284227	0.1114926500
H	2.2088299645	6.3449721293	4.9987474356
H	3.0036714591	5.8879633356	3.6837401053
H	3.0432593293	5.8849608107	7.0280300317
H	2.2271997796	7.2721162176	7.0343610143
H	1.3714432049	1.7335068147	3.4557721470
H	2.1875130500	0.3463625577	3.4621224661
H	4.4131886526	2.5357289275	5.7179637817
H	3.6183471439	2.0787203336	7.0329710542
H	0.0015076785	5.0827729511	2.1457298397
H	0.7963510080	5.5397752610	3.4607406907
24			
N=7, SG 19 (P2121), Cell params			
O	-0.0009922759	5.0947053345	0.4521289694
O	4.4212886138	2.5166067519	4.0189001689
O	2.1767881658	1.2545942365	0.4208353696
O	2.2435369848	6.3566794742	3.9875712745
O	2.2091859053	6.3222505525	6.6813207438
O	2.2111655866	1.2890263999	3.1145771121
O	-0.0333425842	2.5510462244	6.7126368058
O	4.4536847537	5.0602382537	3.1459051597
H	0.8355699401	5.5356065234	0.1124199762
H	0.0151851792	4.1502516344	0.1089531972
H	4.4051214608	3.4610593584	3.6757180450
H	3.5847367805	2.0756972853	3.6791754735
H	2.1927939262	1.2711228579	1.4256355921
H	3.0067234604	1.7342171338	0.1214761848
H	1.4136001698	5.8770598609	3.6882140777
H	2.2275381927	6.3401482733	4.9923721798
H	3.0457377012	5.8813406145	7.0210454708
H	2.2253540441	7.2667031508	7.0245030241
H	1.3746000714	1.7299240153	3.4542848012
H	2.1949969505	0.3445730199	3.4577577372
H	0.7965866275	2.0714172482	7.0120037166
H	-0.0173440522	2.5344986976	5.7078389231
H	4.4376788254	5.0767668150	2.1411048330
H	3.6237493623	5.5398613160	3.4452645437
24			
N=08, SG 9 (C1c1), Cell params			
O	-0.0004856590	5.0480885315	0.4482494130
O	0.0000525994	2.4994281685	4.0397720179
O	2.2107009146	1.2743043772	0.4482529371
O	2.2112392227	6.2732123234	4.0397755420
O	2.2106320434	6.2724023508	6.7347586640
O	2.2100937544	1.2751142632	3.1432360493
O	-0.0005512942	2.4986263923	6.7347640068
O	-0.0010895336	5.0488902215	3.1432413919
H	0.8344929552	5.4860615823	0.0982369661
H	0.0225274700	4.1034302247	0.1084803917
H	0.8350312306	2.0614551630	3.6897595726
H	0.0230657437	3.4440865077	3.7000030511
H	2.2337184515	0.3296468428	0.1084760930
H	3.0456702215	1.7122904033	0.0982362945
H	2.2342567747	7.2178698901	3.6999987522
H	3.0462085468	5.8352263430	3.6897589011
H	3.0479225033	5.8086329582	7.0419639822
H	2.2370198177	6.2680399280	5.7309899526

H	2.2364815128	1.2794767577	2.1394673374
H	3.0473841979	1.7388836882	3.4504413711
H	0.8367450595	2.0348680910	7.0419671078
H	0.0258334574	2.4942578970	5.7309967476
H	0.0252952021	5.0532587880	2.1394741323
H	0.8362068038	5.5126485550	3.4504444966

24			
N=9, SG 7 (P1c1), Cell params	4.395	7.567	7.185 90.590 90.000 90.000
O	-0.0016998416	5.0699385371	0.4487918301
O	-0.0007917935	2.5331139267	4.0407566946
O	2.1994180357	1.2765872357	0.4487970377
O	2.1985076084	6.3264254045	4.0407590389
O	2.1947926324	6.2383293559	6.7356274623
O	2.1976777007	1.2642502609	3.1438786474
O	4.3983251631	2.4450144687	6.7356274535
O	0.0000488212	5.0575543809	3.1438776027
H	0.8348818074	5.5065870349	0.1003441452
H	0.0085690516	4.1272049975	0.1036721788
H	0.8032908894	2.0389577060	3.6952866192
H	-0.8027970942	2.0405921447	3.6877165100
H	1.3628356644	1.7132365449	0.1003527414
H	2.1891528659	0.3338521016	0.1036719561
H	1.3944225757	5.8322711084	3.6952916920
H	3.0005114375	5.8338992100	3.6877146354
H	3.0315105973	5.7704679175	7.0391780522
H	2.2183628639	6.2465098709	5.7319854954
H	2.1880949254	1.2424208950	2.1401431016
H	2.1966027127	0.3066965530	3.4508611139
H	4.3747549074	2.4531950195	5.7319854867
H	3.5616072078	1.9771530274	7.0391780445
H	0.0096303334	5.0357391592	2.1401430462
H	0.0011207717	4.0999995819	3.4508535555

24			
N=10, SG 7 (P1c1), Cell params	4.372	7.641	7.180 90.000 90.000 90.014
O	-0.0029081770	5.1239028506	0.4503343240
O	-0.0007150512	2.5934083311	4.0367172900
O	2.1861585340	1.3072899536	0.4469266644
O	2.1856909688	6.4151371872	4.0393947372
O	2.1845785234	6.4136547721	6.7332990738
O	2.1842135104	1.3036614535	3.1396633733
O	0.0004040026	2.5948932786	6.7306233754
O	-0.0009755407	5.1275210659	3.1430733315
H	0.8252628469	5.5731754028	0.1020788384
H	0.0180750939	4.1787498903	0.1097906327
H	0.8253409978	2.1082035613	3.7332077856
H	0.0166378110	2.5775019789	5.0409163658
H	2.1941328008	1.2766234559	1.4508806065
H	2.1969582181	0.3544627850	0.1286404407
H	1.3812942383	5.9206362198	3.6948585849
H	2.9846220456	5.9160607005	3.6890815624
H	3.0106329163	5.9284468388	7.0368090775
H	2.2019301910	6.3977498268	5.7290994759
H	3.0123846755	1.7529309709	3.4879257317
H	2.2051936791	0.3585070222	3.4802034611
H	0.7993376839	2.0958212816	7.0809330414
H	-0.8039913752	2.1003911317	7.0751613085
H	0.0070012819	5.0968554000	2.1391208747
H	0.0098246830	4.1746953922	3.4613613309

24			
N=11, SG 4 (P1211), Cell params	4.430	7.544	7.174 90.000 89.971 90.000
O	-0.0002809852	5.0474552168	0.4484564163
O	0.0020419054	2.4948421656	4.0338097479
O	2.2150499331	1.2769693204	0.4469674006

O	2.2163570004	6.2680880523	4.0352982593
O	2.2167370557	6.2673778716	6.7276957365
O	2.2166537121	1.2703227404	3.1339657532
O	0.0036570005	2.5014774594	6.7208252949
O	0.0001005449	5.0481655589	3.1408616037
H	0.8367198066	5.4799991546	0.0963656419
H	0.0171549018	4.0987681596	0.1199695210
H	0.0090261730	3.4507169698	3.7273064338
H	0.0010279754	2.5116363982	5.0389266581
H	2.2140356309	1.2601670512	1.4520846477
H	2.2220376110	0.3210942425	0.1404543088
H	2.2337953200	7.2167709328	3.7067950446
H	3.0533496318	5.8355309738	3.6832041320
H	3.0561049586	5.8062020747	7.0325039530
H	2.2435253439	6.2656730715	5.7236175732
H	1.4088701438	1.7517642265	3.4873383829
H	3.0215821137	1.7565201617	3.4866562484
H	0.8085909682	2.0152904325	7.0735091482
H	-0.8041242918	2.0200312341	7.0741985507
H	0.0268874290	5.0498718938	2.1367852480
H	0.8394743798	5.5093286245	3.4456681616
24			
N=12, SG 4 (P1211), Cell params			
O	-0.0020745838	5.0987398003	0.4514209331
O	-0.0013534358	2.5218570563	4.0220991568
O	2.2437835674	1.2570000027	0.4220607145
O	2.1770319814	6.3630420567	3.9914788180
O	2.2064948317	6.3313200813	6.6878838519
O	2.2072176326	1.2920634152	3.1171974660
O	4.4523275398	2.5569567984	6.7172623580
O	-0.0314951544	5.0670011755	3.1478480950
H	0.8361805313	5.5409635664	0.1160960933
H	0.0195858701	4.1541647113	0.1099239333
H	0.8348519475	2.0802677931	3.6823270349
H	0.0151550401	3.4659070925	3.6783772920
H	2.2241015945	1.2735025177	1.4265430209
H	1.4118132368	1.7319413045	0.1199562392
H	2.2089196140	6.3473093612	4.9957831386
H	3.0053921667	5.8857838803	3.6831391028
H	3.0447420554	5.8890834582	7.0232152149
H	2.2281642759	7.2758939923	7.0293831649
H	3.0434120981	1.7336619384	3.4569851457
H	2.2237154920	0.3480162601	3.4609306835
H	4.4326385764	2.5404585159	5.7127803103
H	3.6203584675	2.0820106741	7.0193680429
H	0.0003854907	5.0827449279	2.1435459412
H	0.7968594908	5.5442655071	3.4561936262
24			
N=13, SG 4 (P1211), Cell params			
O	-0.0003075230	5.0978963819	0.4523002444
O	4.4197587550	2.5171479429	4.0205826365
O	2.2422688837	1.2572638446	0.4215653069
O	2.2416803922	6.3591078871	3.9903391154
O	2.2082490629	6.3232193185	6.6856356358
O	2.2112618008	1.2886160529	3.1173727014
O	4.4507910441	2.5485206843	6.7163813096
O	4.4502038772	5.0619745902	3.1476170021
H	0.8371256072	5.5397452176	0.1150125381
H	0.0186914982	4.1534962247	0.1099021397
H	4.4006768474	3.4615515829	3.6779609836
H	3.5827487793	2.0751905523	3.6826671938
H	2.2073666020	1.2724607151	1.4257459880
H	1.4115726448	1.7296844876	0.1112437440

H	1.4119676945	5.8790443559	3.6908816726
H	2.2262423383	6.3419054412	4.9949828346
H	3.0456724462	5.8813584701	7.0229361082
H	2.2272543227	7.2676190937	7.0280329077
H	1.3742392873	1.7305590565	3.4552751469
H	2.1921799652	0.3442105790	3.4599895077
H	4.4158827135	2.5333191583	5.7121999814
H	3.6200974916	2.0760959249	7.0267074023
H	4.4347593503	5.0791751163	2.1429735455
H	3.6204931729	5.5420413790	3.4470773196
24			
N=14, SG 4 (P1211), Cell	params	4.430 7.544 7.169	90.000 90.000 90.116
O	-0.0117028073	5.0471807052	0.4484313904
O	-0.0049680967	2.4951389427	4.0309215621
O	2.2122567260	1.2769077892	0.4466108012
O	2.2037040960	6.2690769848	4.0327425748
O	2.2005760848	6.2681381260	6.7226009345
O	2.2111772079	1.2708728648	3.1322759238
O	-0.0039041662	2.5011684814	6.7165994483
O	4.4212152484	5.0480945884	3.1382966165
H	0.8270613619	5.4810769148	0.1024762442
H	0.0081174563	4.0985468237	0.1198868813
H	-0.0137687588	3.4510776870	3.7246773549
H	-0.0039064892	2.5116351530	5.0362011529
H	2.2111922062	1.2604067611	1.4518904283
H	2.2210613384	0.3209681061	0.1403595275
H	1.3649398164	5.8351775049	3.6867921254
H	2.1838850907	7.2177093218	3.7041840883
H	3.0415564500	5.8051312911	7.0189300882
H	2.2112738524	6.2653870547	5.7180705215
H	1.4059288315	1.7568179113	3.4846793256
H	3.0190714516	1.7527634521	3.4853554156
H	0.8013413685	2.0152183568	7.0690018915
H	-0.8118029021	2.0192893634	7.0696753912
H	4.4105176008	5.0508457735	2.1337662047
H	3.5802348582	5.5111013944	3.4346257425
24			
N=15, SG 4 (P1211), Cell	params	4.372 7.641 7.181	90.000 90.022 90.000
O	-0.0013899992	5.1243722159	0.4504328487
O	4.3706585038	2.5936220000	4.0374188099
O	2.1863860946	1.3072487513	0.4470632025
O	2.1844522983	6.4157955392	4.0400067398
O	2.1833168706	6.4141751076	6.7341161967
O	2.1860618465	1.3038309500	3.1400708315
O	-0.0025872118	2.5952431007	6.7315328997
O	-0.0017017042	5.1277843940	3.1434429654
H	0.8266523257	5.5736901199	0.1019545364
H	0.0196965729	4.1792614532	0.1098231948
H	3.5447053274	2.1084978711	3.7334896615
H	4.3522498524	2.5779557343	5.0415818792
H	2.1748908134	1.2764736559	1.4509496710
H	2.1949227498	0.3543970427	0.1288243042
H	1.3838107969	5.9151145701	3.6963468515
H	2.9869918023	5.9228327472	3.6887602174
H	3.0092700295	5.9290509183	7.0380453427
H	2.2017254442	6.3985086199	5.7299531527
H	1.3580154078	1.7531429962	3.4885475484
H	2.1649753434	0.3587182556	3.4806780928
H	0.7980547769	2.0945624812	7.0751925491
H	-0.8051267408	2.1022823633	7.0827770125
H	0.0097945404	5.0970071348	2.1395572397
H	-0.0102394404	4.1749349987	3.4616856548
24			

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N=16, SG 1 (P1), Cell params 4.424 7.544 7.181 89.974 90.000 89.973
O      0.0020358840      5.0479365265      0.4485135287
O      -0.0003643889      2.5001743461      4.0391274747
O      2.2135366689      1.2754369639      0.4490859471
O      2.2143505773      6.2715352496      4.0387566459
O      2.2124144963      6.2718308908      6.7328882805
O      2.2101927460      1.2753155195      3.1421874906
O      4.4270477507      2.5001019482      6.7323171732
O      0.0010850152      5.0481768970      3.1425828903
H      0.8401421690      5.4794786315      0.0972843720
H      0.0118081128      4.1036453825      0.1080725451
H      0.8364948956      2.0615915023      3.6951761406
H      0.0234876236      3.4445516049      3.6985859179
H      1.3737678463      1.7077662609      0.1034902443
H      2.2027529869      0.3313926189      0.1079433816
H      2.2375296194      7.2161479923      3.6988136133
H      3.0493360920      5.8335066158      3.6888760405
H      3.0524240717      5.8138850801      7.0418395019
H      2.2413804053      6.2673425518      5.7291977076
H      2.2210404827      1.2807233461      2.1381596977
H      3.0489825216      1.7408776038      3.4412990489
H      4.4129332008      2.4948955787      5.7283687392
H      3.5855584033      2.0402912473      7.0333083364
H      0.0282032828      5.0526237486      2.1388038691
H      0.8384203167      5.5115728123      3.4502178291

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VASP PBE, Hard PP - XIc

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24
Ice XIc (I41md), Cell params 8.796 4.398 6.277 90.000 90.000 90.000
O      8.796003254      0.000024075      -0.053272751
O      2.198991295      2.198904307      3.085055664
O      8.795998570      2.198889590      1.515472458
O      2.198971122      4.397771890      4.654844998
O      4.398000949      0.000022270      -0.053247817
O      6.596991552      2.198905909      3.085036668
O      4.398023230      2.198889706      1.515485936
O      6.597027547      4.397771803      4.654831437
H      8.796000908      -0.800647867      0.549696567
H      8.796000918      0.800623207      0.549676241
H      7.397594623      4.397768735      5.257844547
H      1.398365909      4.397768777      5.257869964
H      9.596583984      2.198886422      2.118417596
H      3.597396366      2.198886489      2.118443947
H      2.198988250      1.398339395      3.688062767
H      2.198988231      2.999400502      3.688042660
H      4.397999790      -0.800640301      0.549703455
H      4.397999806      0.800615902      0.549683329
H      2.999611234      4.397768624      5.257871893
H      5.796351103      4.397768600      5.257868433
H      5.198575346      2.198886577      2.118426475
H      7.995408652      2.198886541      2.118422444
H      6.596991122      1.398335739      3.688052385
H      6.596991128      2.999403936      3.688032041

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VASP PBE, Hard PP - XIh

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24
Ice XIh (Cmc21), Cell params 4.407 7.678 7.190 90.000 90.000 90.000
O      4.407411678      5.089270352      0.435562724
O      4.407412137      2.588266856      4.030660246
O      2.203703010      1.250514353      0.435553027
O      2.203703296      6.427030382      4.030695875

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O	2.203706750	6.377481034	6.734793687
O	2.203706498	1.300096753	3.139654478
O	4.407412911	2.538714456	6.734779204
O	4.407412551	5.138865532	3.139676385
H	4.407411764	4.129694572	0.147129955
H	4.407411815	5.087901210	1.437231533
H	4.407412212	3.547869020	3.742234807
H	4.407412371	2.589662411	5.032351685
H	2.203703669	1.249132177	1.437217449
H	2.203703572	0.290917832	0.147113401
H	2.203703905	6.428428180	5.032362132
H	2.203703738	7.386633655	3.742252004
H	1.402875740	5.878030029	7.071144072
H	3.004535168	5.878030463	7.071143850
H	1.402871801	1.799559619	3.476011850
H	3.004538671	1.799559075	3.476011674
H	5.208242400	2.039260028	7.071132316
H	3.606580920	2.039260993	7.071131552
H	5.208243555	5.638328586	3.476026340
H	3.606578905	5.638327648	3.476025573

VASP optPBE-vdW, Hard PP - XIc

24			
Ice XIc (I41md), Cell params			
O	0.000005547	4.469004799	-0.047779459
O	2.232248988	2.234499950	3.113224276
O	-0.000002230	2.234499897	1.531382587
O	2.232251878	4.468995640	4.692384187
O	4.464495879	0.000008570	-0.047779789
O	6.696749544	2.234505994	3.113216273
O	4.464502664	2.234503275	1.531382727
O	6.696751708	0.000000997	4.692385358
H	0.000003681	3.672225890	0.551518469
H	0.000003647	5.265769019	0.551514138
H	7.493293431	0.000000928	5.292096497
H	1.435707983	4.468997565	5.292097444
H	0.796546857	2.234498644	2.131098681
H	3.667950045	2.234500829	2.131098669
H	2.232249673	1.437720395	3.712517615
H	2.232249695	3.031264179	3.712516074
H	4.464496950	-0.796770141	0.551519093
H	4.464496999	0.796772848	0.551513556
H	3.028792188	4.468998790	5.292096044
H	5.900207945	0.000002124	5.292097136
H	5.261034720	2.234502759	2.131090355
H	-0.796537820	2.234500554	2.131090265
H	6.696750019	1.437727363	3.712517840
H	6.696750009	3.031269133	3.712514223

VASP optPBE-vdW, Hard PP - XIh

24			
Ice XIh (Cmc21), Cell params			
O	4.471997806	5.151378279	0.439573088
O	4.471997829	2.632623533	4.068575070
O	2.235996822	1.259380240	0.439574337
O	2.235996987	6.524623979	4.068576396
O	2.235997705	6.454624342	6.804991746
O	2.235997924	1.329379418	3.175990779
O	4.471996982	2.562623868	6.804989656
O	4.471997009	5.221379991	3.175990405
H	4.471997598	4.195172058	0.158939593

H	4.471997570	5.154750429	1.436250701
H	4.471997550	3.588829112	3.787941587
H	4.471997504	2.629251775	5.065253322
H	2.235997150	1.262752504	1.436252329
H	2.235997080	0.303174165	0.158941522
H	2.235997231	6.521252199	5.065254411
H	2.235997353	7.480829756	3.787942809
H	1.439182580	5.955907439	7.136466733
H	3.032813122	5.955907771	7.136466536
H	1.439182835	1.828095362	3.507467279
H	3.032813276	1.828095177	3.507467043
H	5.268812197	2.063907845	7.136465808
H	3.675181550	2.063908150	7.136465570
H	5.268812012	5.720095916	3.507467195
H	3.675181718	5.720095612	3.507467035