

**Supplementary Information for**  
**Band engineering of  $\text{AgSb}_{1-x}\text{Bi}_x\text{O}_3$  for photocatalytic water**  
**oxidation under visible light**

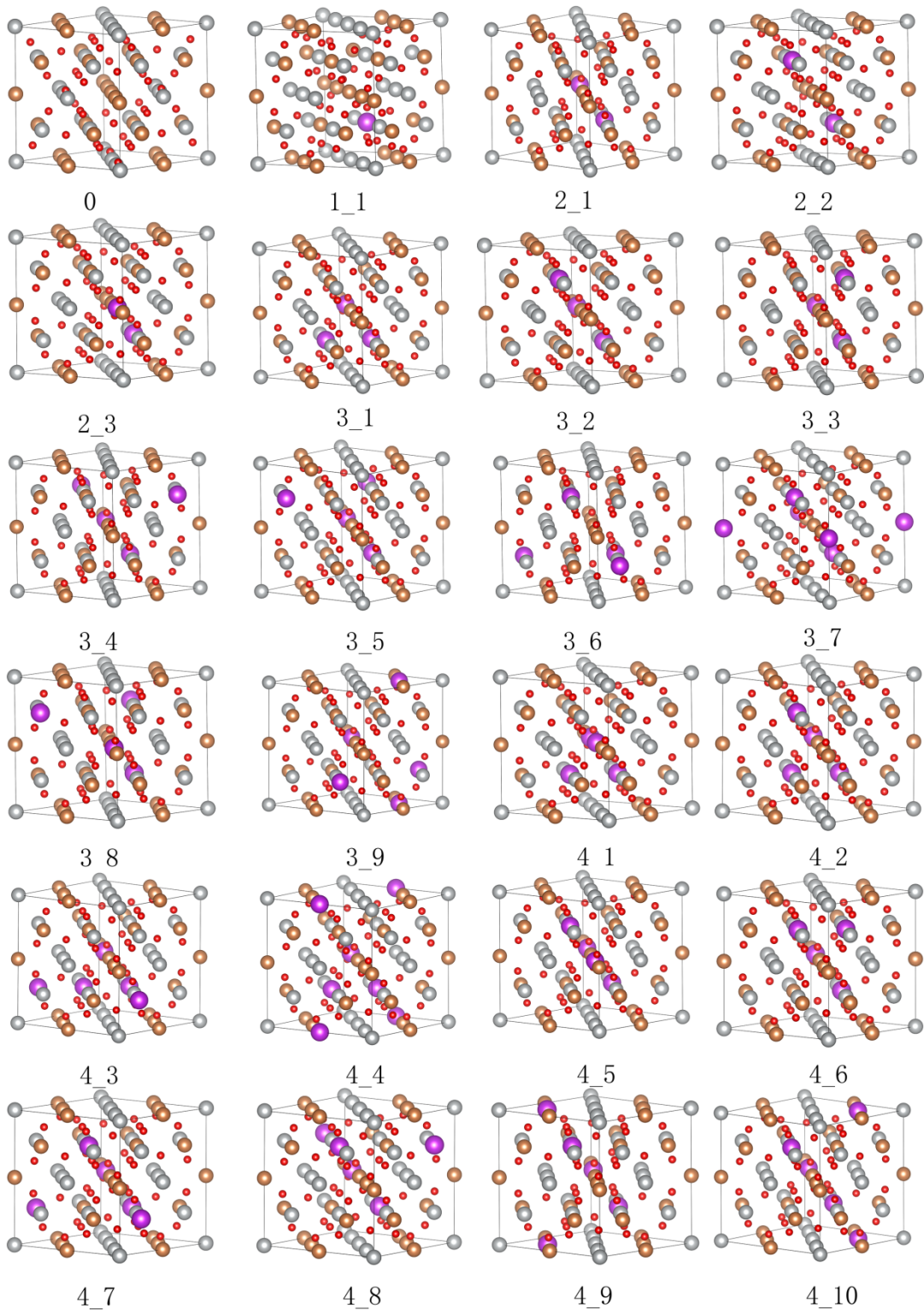
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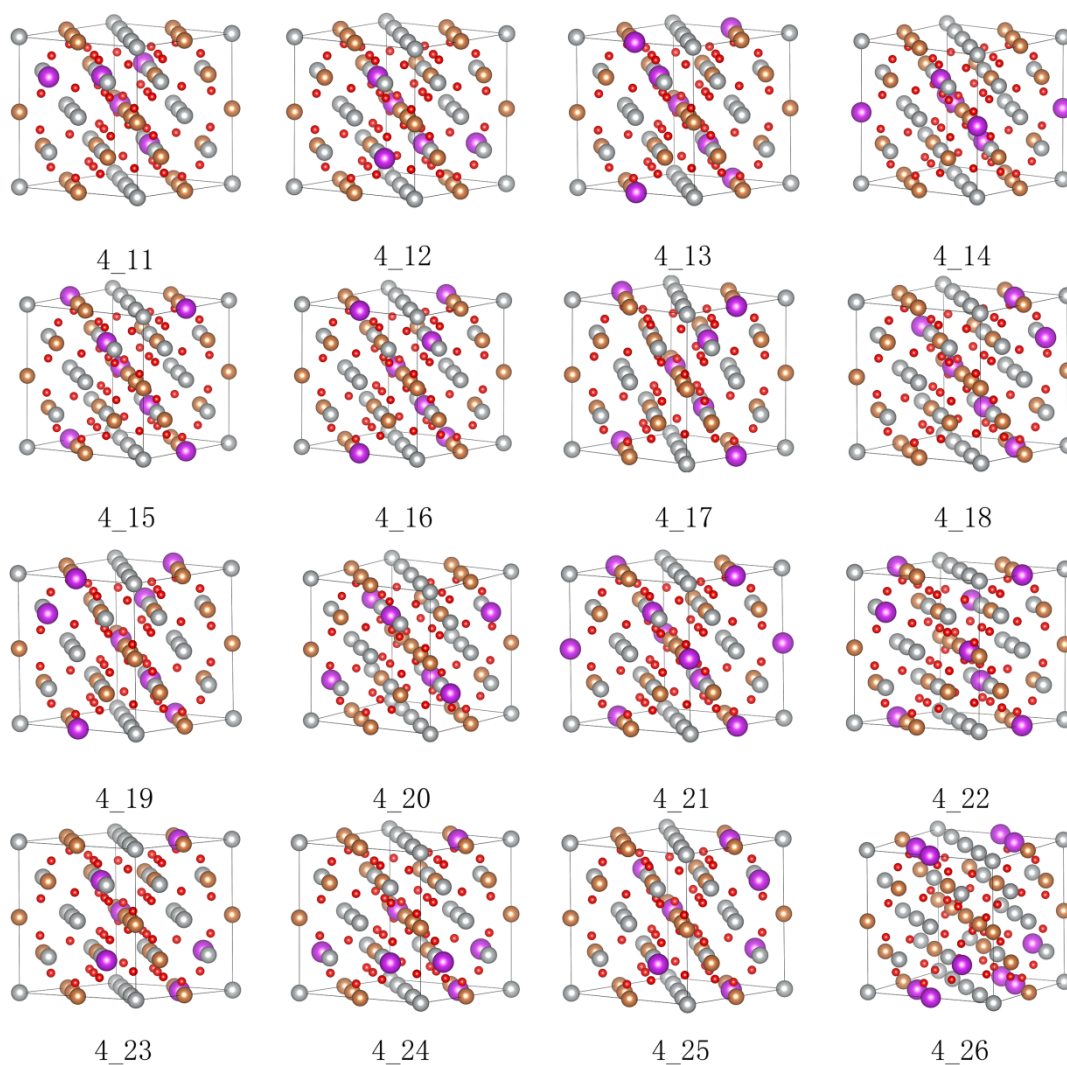
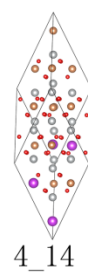
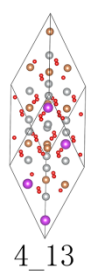
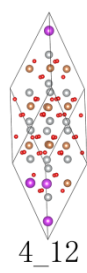
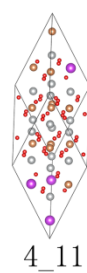
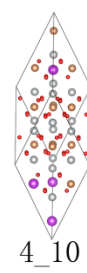
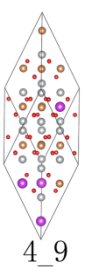
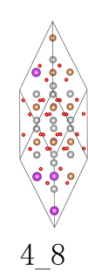
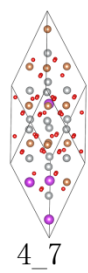
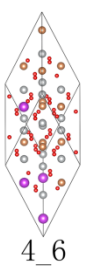
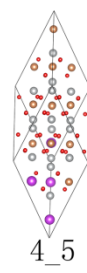
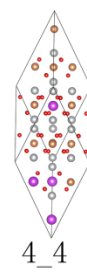
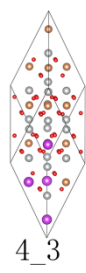
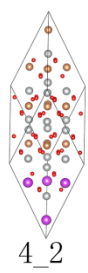
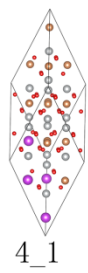
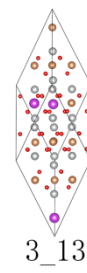
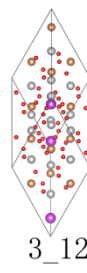
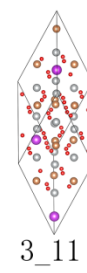
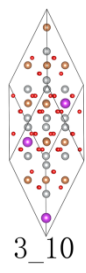
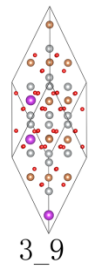
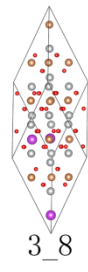
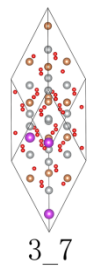
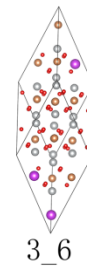
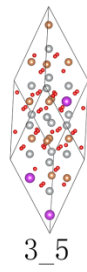
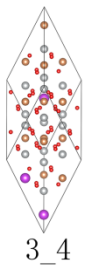
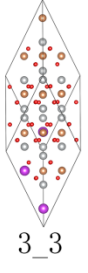
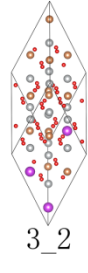
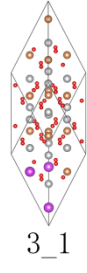
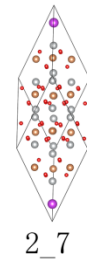
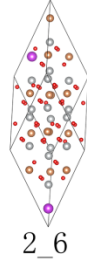
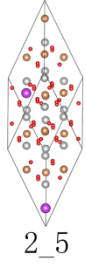
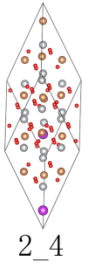
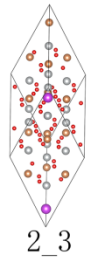
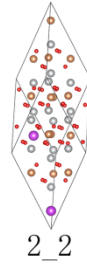
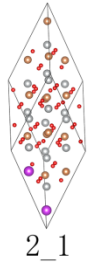
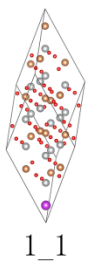
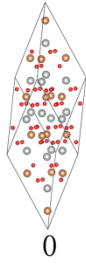


Figure S1. The optimized 80-atom supercell of  $\text{AgSb}_{1-x}\text{Bi}_x\text{O}_3$  solid-solution with the defective pyrochlore structure. The value of “a” in “a\_b” represents the number of Bi atom in the supercell. “b” represents the sequence number of all inequivalent configurations with same Bi concentration. Ag, Sb, Bi, and O atoms are colored by silver, brown, purple and red, respectively.



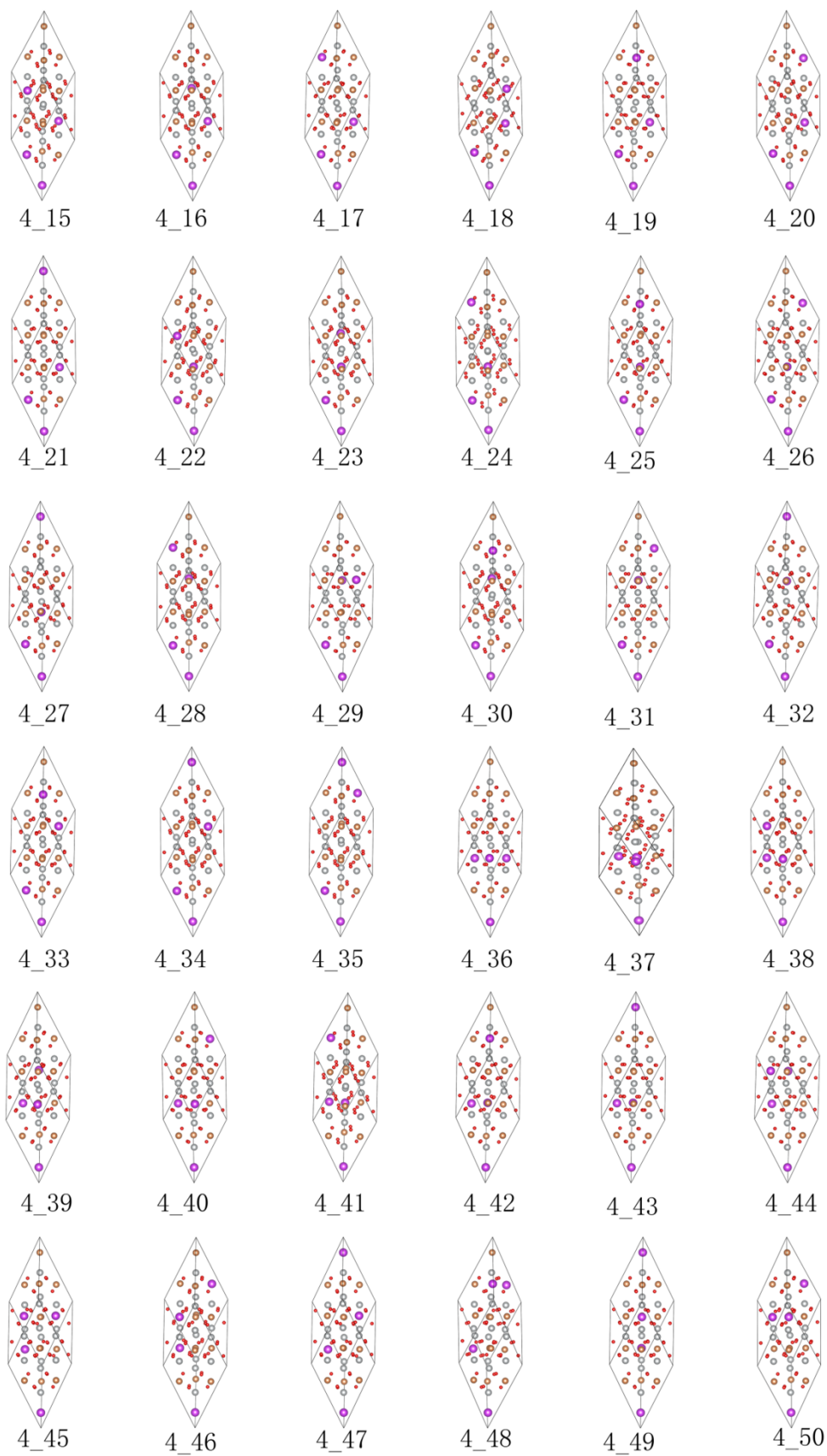


Figure S2. The optimized 80-atom supercell of  $\text{AgSb}_{1-x}\text{Bi}_x\text{O}_3$  solid-solution with the ilmenite structure.

Table S1. The relaxed lattice constants, degeneracy, total energy and band gap ( $E_g$ ) for  $\text{AgSb}_{1-x}\text{Bi}_x\text{O}_3$  solid-solution with the defective pyrochlore structure.

py- $\text{AgSb}_{1-x}\text{Bi}_x\text{O}_3$	Degeneracy	Volume( $\text{\AA}^3$ )	a( $\text{\AA}$ )	b( $\text{\AA}$ )	c( $\text{\AA}$ )	Energy(eV)	$E_g$ (eV)
0	1	1105.94	10.3410	10.3410	10.3410	-453.342	2.50
1_1	16	1116.76	10.3750	10.3750	10.3750	-450.691	2.34
2_1	48	1126.61	10.4065	10.4065	10.4032	-448.006	2.20
2_2	24	1126.91	10.4101	10.4045	10.4045	-448.115	2.14
2_3	48	1126.71	10.4076	10.4076	10.4021	-448.010	2.19
3_1	32	1134.20	10.4287	10.4287	10.4287	-445.298	2.10
3_2	191	1134.55	10.4352	10.4303	10.4240	-445.414	2.03
3_3	96	1135.33	10.4313	10.4313	10.4339	-445.321	2.07
3_4	48	1134.68	10.4298	10.4298	10.4310	-445.404	2.05
3_5	96	1137.62	10.4411	10.4354	10.4411	-445.333	2.07
3_6	16	1135.01	10.4313	10.4313	10.4313	-445.627	1.92
3_7	48	1134.80	10.4268	10.4324	10.4324	-445.411	2.02
3_8	32	1135.58	10.4329	10.4329	10.4329	-445.314	2.07
3_9	1	1134.68	10.4245	10.4307	10.4355	-445.415	2.03
4_1	8	1142.65	10.4545	10.4545	10.4545	-442.585	2.02
4_2	96	1143.31	10.4635	10.4531	10.4531	-442.720	1.95
4_3	191	1142.69	10.4552	10.4579	10.4509	-442.704	1.96
4_4	96	1144.94	10.4614	10.4616	10.4616	-442.625	1.99
4_5	48	1142.68	10.4595	10.4595	10.4451	-442.817	1.90
4_6	96	1143.41	10.4608	10.4549	10.4549	-442.728	1.94
4_7	96	1143.45	10.4601	10.4601	10.4511	-442.934	1.83
4_8	96	1143.27	10.4585	10.4585	10.4526	-442.929	1.84
4_9	48	1143.13	10.4644	10.4563	10.4474	-442.817	1.90
4_10	96	1142.90	10.4604	10.4558	10.4499	-442.808	1.90
4_11	96	1143.24	10.4631	10.4530	10.4530	-442.725	1.94
4_12	96	1143.56	10.4626	10.4548	10.4548	-442.719	1.94
4_13	191	1143.09	10.4599	10.4551	10.4527	-442.715	1.95
4_14	191	1143.42	10.4571	10.4599	10.4537	-442.722	1.93
4_15	191	1143.78	10.4581	10.4589	10.4571	-442.717	1.93
4_16	96	1143.07	10.4552	10.4571	10.4552	-442.611	1.99
4_17	24	1143.95	10.4570	10.4570	10.4614	-442.636	1.98
4_18	12	1142.73	10.4522	10.4522	10.4601	-442.789	1.93
4_19	24	1142.23	10.4529	10.4540	10.4529	-442.611	2.00
4_20	4	1144.81	10.4560	10.4638	10.4638	-442.810	1.87
4_21	12	1143.08	10.4559	10.4559	10.4559	-443.256	1.67
4_22	8	1142.06	10.4527	10.4527	10.4527	-442.574	1.98
4_23	1	1143.51	10.4564	10.4578	10.4575	-442.714	1.93
4_24	1	1142.90	10.4520	10.4578	10.4562	-442.716	1.94
4_25	1	1143.24	10.4528	10.4553	10.4611	-442.716	1.95
4_26	1	1142.35	10.4491	10.4575	10.4542	-442.699	1.96

Table S2. The relaxed lattice constants, degeneracy, total energy and band gap ( $E_g$ ) for  $\text{AgSb}_{1-x}\text{Bi}_x\text{O}_3$  solid-solution with the ilmenite structure.

il- $\text{AgSb}_{1-x}\text{Bi}_x\text{O}_3$	Degeneracy	Volume( $\text{\AA}^3$ )	a( $\text{\AA}$ )	b( $\text{\AA}$ )	c( $\text{\AA}$ )	Energy(eV)	$E_g$ (eV)
0	1	1113.99	12.6517	12.6517	12.6517	-452.160	2.44
1_1	16	1117.41	12.5738	12.5738	12.5738	-449.881	2.18
2_1	24	1117.14	12.4911	12.5055	12.5109	-447.663	1.95
2_2	24	1117.11	12.5137	12.4962	12.5087	-447.546	1.99
2_3	8	1115.30	12.4847	12.4847	12.4847	-447.635	1.95
2_4	8	1117.30	12.4968	12.4968	12.4968	-447.645	1.93
2_5	24	1117.14	12.5027	12.5000	12.5042	-447.664	1.95
2_6	24	1117.54	12.5421	12.5113	12.5163	-447.562	2.03
2_7	8	1116.75	12.5065	12.5065	12.5065	-447.642	1.96
3_1	48	1119.22	12.4610	12.4369	12.4599	-445.425	1.76
3_2	48	1119.30	12.4559	12.4571	12.4570	-445.405	1.77
3_3	48	1118.78	12.4445	12.4399	12.4387	-445.519	1.70
3_4	48	1119.77	12.4821	12.4384	12.4552	-445.430	1.80
3_5	48	1119.25	12.4694	12.4707	12.4439	-445.427	1.80
3_6	48	1119.10	12.4562	12.4499	12.4715	-445.416	1.80
3_7	16	1120.51	12.4724	12.4724	12.4724	-445.176	1.85
3_8	48	1118.90	12.4895	12.4348	12.4517	-445.281	1.81
3_9	48	1120.07	12.4585	12.4509	12.4736	-445.419	1.77
3_10	48	1119.33	12.4628	12.4495	12.4568	-445.403	1.77
3_11	48	1119.01	12.4671	12.4708	12.4841	-445.203	1.89
3_12	16	1118.67	12.4404	12.4404	12.4404	-445.487	1.72
3_13	48	1119.24	12.4510	12.4506	12.4818	-445.409	1.80
4_1	12	1122.15	12.4232	12.4023	12.4172	-443.256	1.59
4_2	16	1121.79	12.4169	12.4169	12.4169	-443.123	1.64
4_3	48	1120.96	12.4067	12.3978	12.3926	-443.241	1.59
4_4	48	1121.47	12.4108	12.3971	12.4064	-443.120	1.63
4_5	48	1120.82	12.3952	12.3852	12.4041	-443.358	1.53
4_6	48	1120.74	12.4281	12.3834	12.4039	-443.230	1.61
4_7	48	1121.44	12.4415	12.3979	12.4062	-443.230	1.61
4_8	48	1121.63	12.4359	12.4001	12.4220	-443.241	1.64
4_9	48	1121.99	12.4204	12.4305	12.4338	-443.143	1.69
4_10	48	1120.97	12.4069	12.4183	12.4008	-443.234	1.63
4_11	48	1121.16	12.4059	12.4063	12.4252	-443.230	1.64
4_12	48	1121.01	12.4069	12.4104	12.4240	-443.132	1.68
4_13	12	1121.31	12.4058	12.4026	12.4060	-443.216	1.60
4_14	48	1120.27	12.3893	12.3911	12.4209	-443.211	1.60
4_15	48	1120.67	12.3880	12.3914	12.4058	-443.326	1.54
4_16	48	1121.05	12.4228	12.4059	12.4001	-443.228	1.63

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4_17	48	1122.27	12.4373	12.4322	12.4258	-443.126	1.70
4_18	48	1121.53	12.4046	12.4403	12.3936	-443.234	1.63
4_19	48	1120.96	12.4234	12.4215	12.3964	-443.127	1.68
4_20	48	1120.22	12.3910	12.3928	12.4187	-443.190	1.62
4_21	48	1119.49	12.3913	12.3867	12.4154	-443.207	1.63
4_22	12	1121.14	12.3903	12.3936	12.3862	-443.462	1.48
4_23	48	1121.17	12.4294	12.3954	12.4018	-443.351	1.58
4_24	48	1121.17	12.4228	12.3964	12.4083	-443.221	1.62
4_25	48	1121.71	12.4133	12.4311	12.3994	-443.226	1.61
4_26	48	1121.39	12.3977	12.3949	12.4260	-443.219	1.61
4_27	48	1120.57	12.3994	12.3906	12.4223	-443.320	1.57
4_28	12	1121.66	12.4638	12.3970	12.4117	-443.244	1.68
4_29	48	1121.76	12.4389	12.4371	12.4040	-443.139	1.69
4_30	48	1121.18	12.4313	12.4177	12.3988	-443.228	1.67
4_31	48	1121.00	12.4210	12.4040	12.4190	-443.233	1.67
4_32	48	1121.24	12.4346	12.4006	12.4214	-443.131	1.69
4_33	12	1121.21	12.4125	12.4521	12.3859	-443.247	1.67
4_34	48	1121.31	12.4187	12.4265	12.4152	-443.127	1.69
4_35	12	1120.30	12.4046	12.4041	12.4319	-443.215	1.67
4_36	4	1122.23	12.4411	12.4411	12.4411	-442.743	1.76
4_37	48	1121.92	12.4464	12.4359	12.4217	-442.875	1.74
4_38	16	1122.74	12.4288	12.4288	12.4288	-443.112	1.65
4_39	48	1121.85	12.4106	12.4043	12.4165	-443.110	1.65
4_40	16	1122.75	12.4612	12.4612	12.4612	-442.806	1.81
4_41	12	1121.58	12.4662	12.4135	12.4080	-442.954	1.72
4_42	48	1121.23	12.4393	12.4296	12.4220	-442.889	1.76
4_43	48	1120.76	12.4339	12.3955	12.3997	-443.186	1.62
4_44	12	1122.03	12.4177	12.4120	12.4233	-443.233	1.60
4_45	48	1121.78	12.4206	12.4003	12.4058	-443.233	1.60
4_46	48	1121.60	12.4063	12.4261	12.4368	-443.120	1.69
4_47	12	1121.64	12.4121	12.4207	12.4119	-443.206	1.61
4_48	12	1121.79	12.4231	12.4651	12.4629	-442.816	1.83
4_49	4	1120.51	12.3955	12.3955	12.3955	-443.380	1.52
4_50	12	1120.42	12.3991	12.3951	12.4469	-443.203	1.67

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