

High Reactivity of Dimethyl Ether Activated by Zeolite Ferrierite within a Fer Cage: A Prediction Study

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Figure S1. The pore sizes of (a) 8- and (b) 10-member channels of zeolite ferrierite, and (c) the molecule size of dimethyl ether (DME).

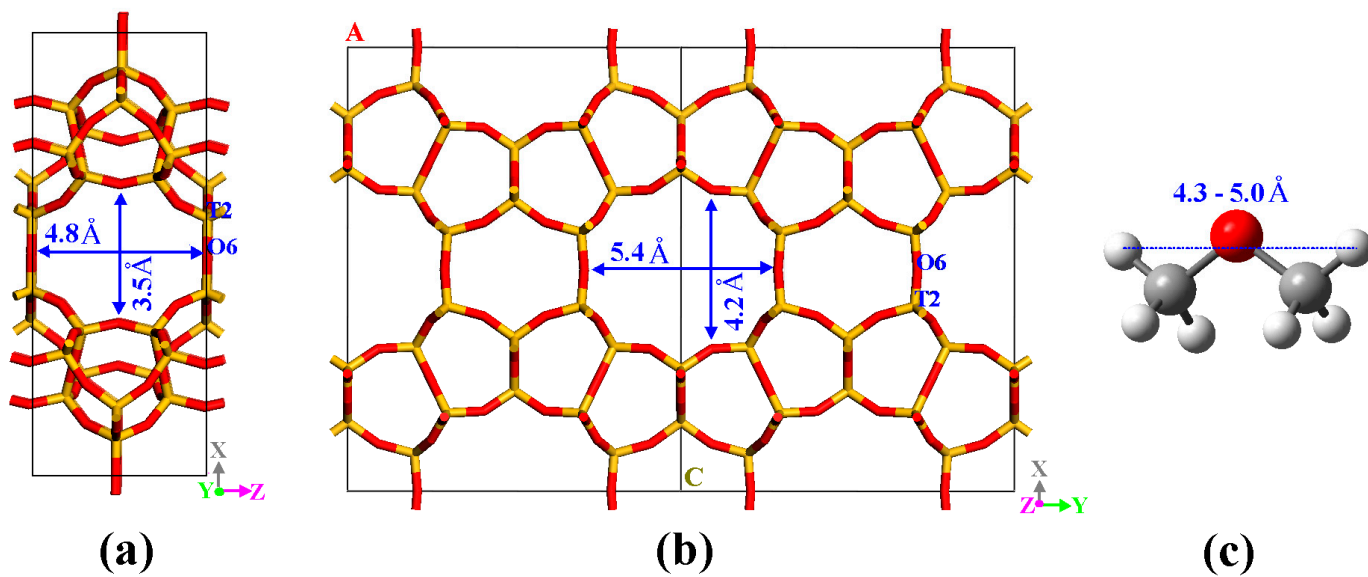


Figure S2. Total energy of zeolite ferrierite dependant on the energy cutoff

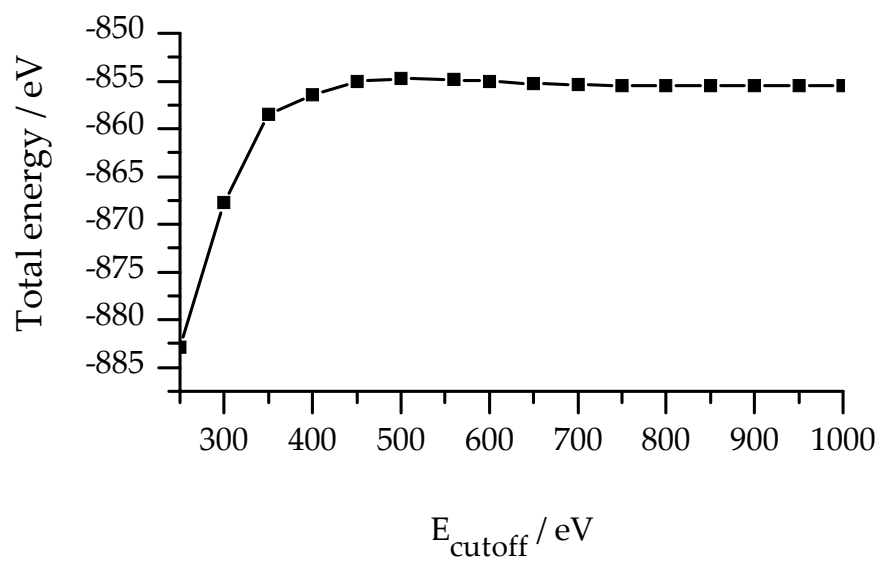


Figure S3. Total energy of zeolite ferrierite dependant on the unit cell volume.

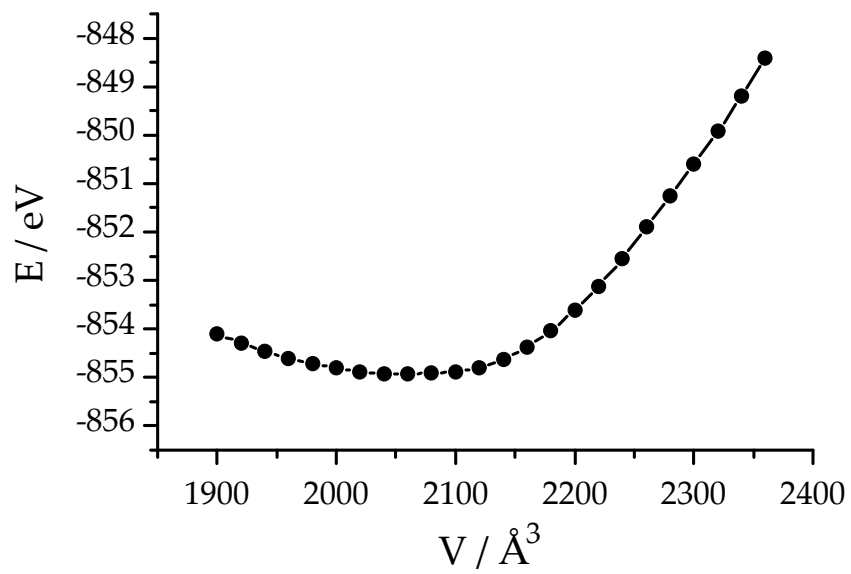
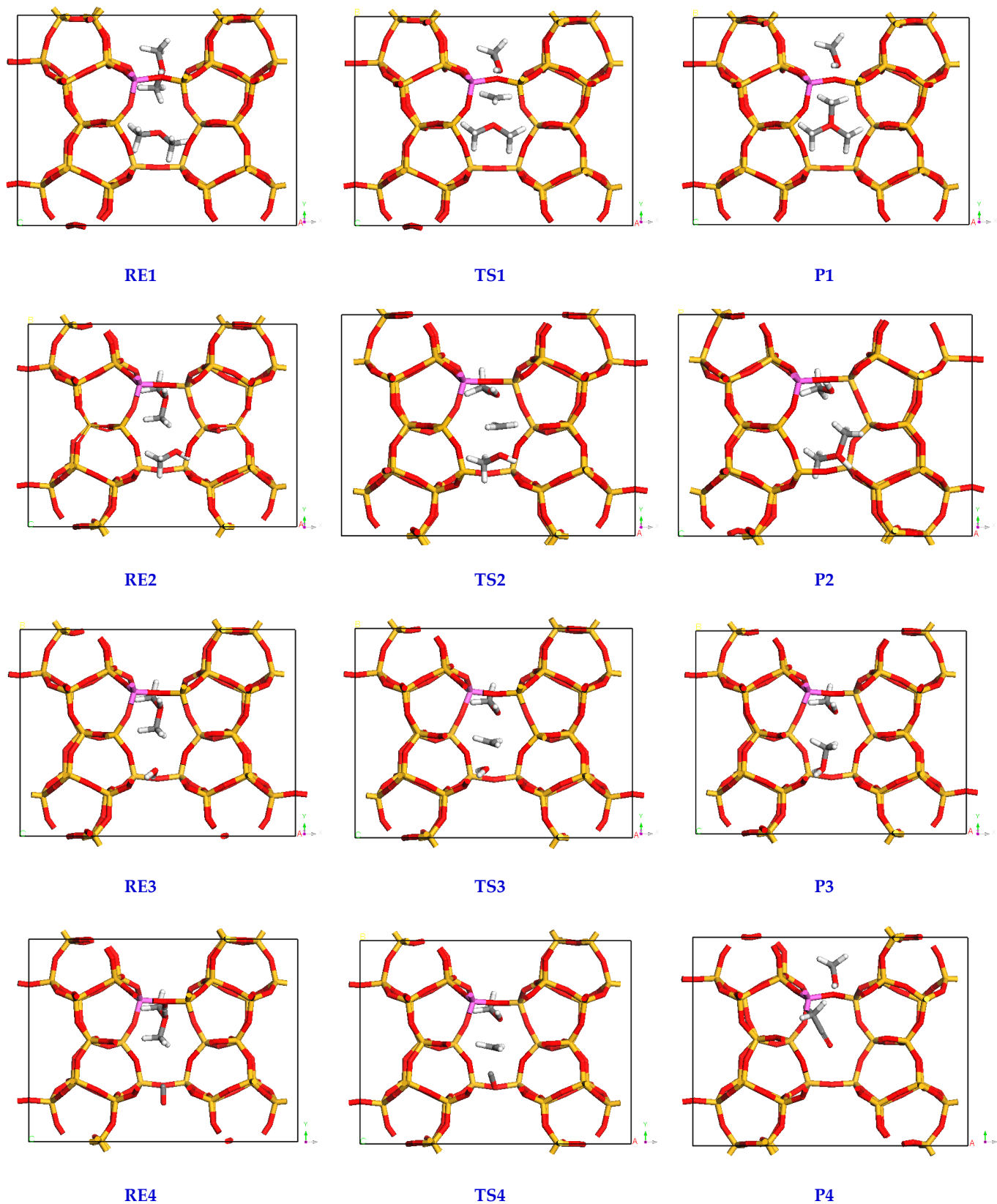
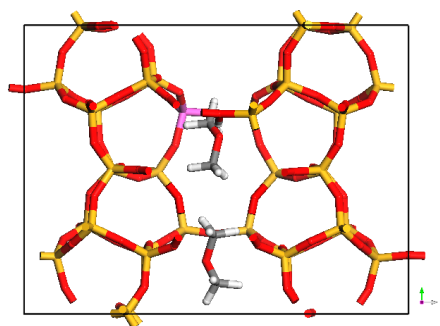


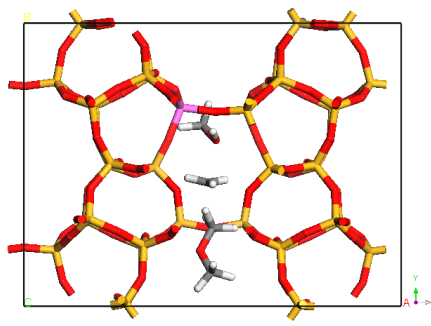
Figure S4. Schematic structures of reactants (Rex), transition states (TSx), and products (Px) from Eq.x ($x = 1-6$). For Eq.x, please refer to the section 1.

Noting that (1) O in red, Si in yellow, Al in pink, C in grey, and H in white; (2) the detailed coordinates are provided in following S3 in this Supplementary Materials.

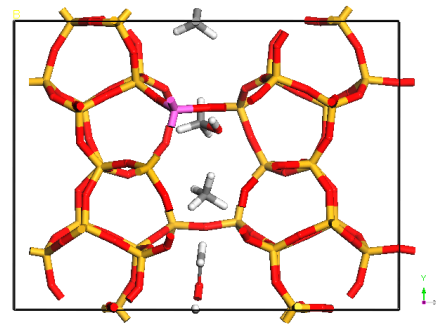




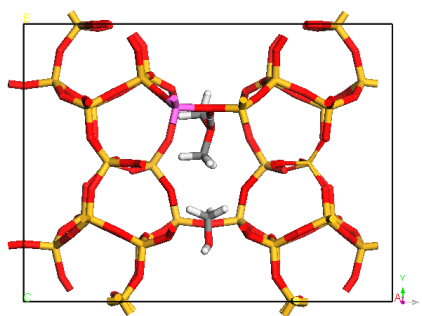
RE5



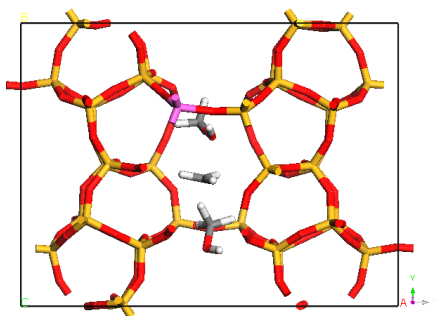
TS5



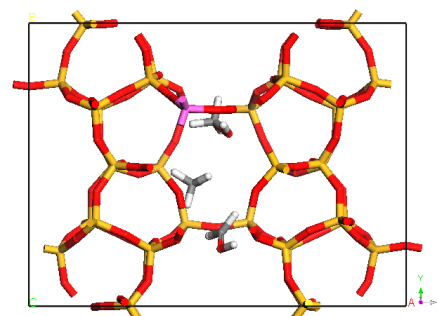
P5



RE6



TS6



P6

Table S1. The energy difference (in kcal/mol) between two types of K-meshes (i.e., 1×1×1 and 2×2×2) of H-FER.

item	in kcal/mol					
	$\Delta E^\ddagger(1^*1^*1)$	$\Delta E^\ddagger(2^*2^*2)$	$\Delta E^\ddagger(2^*2^*2) - \Delta E^\ddagger(1^*1^*1)$	$E_r(1^*1^*1)$	$E_r(2^*2^*2)$	$E_r(2^*2^*2) - E_r(1^*1^*1)$
Eq.1	18.47	17.70	-0.77	9.39	7.61	-1.78
Eq.2	22.13	22.97	0.84	14.78	15.79	1.01
Eq.3	23.49	22.97	-0.52	17.67	16.75	-0.92
Eq.4	30.06	29.47	-0.59	-8.37	-7.85	0.52
Eq.5	34.00	34.21	0.21	26.41	26.27	-0.14
Eq.6	36.63	36.65	0.02	18.43	16.75	-1.68

Noting that 1) $\Delta E^\ddagger(1^*1^*1)$ or $\Delta E^\ddagger(2^*2^*2)$ represents the activation internal barrier when K-mesh is 1×1×1 or 2×2×2; 2) $E_r(1^*1^*1)$ or $E_r(2^*2^*2)$ represents the reaction heat when K-mesh is 1×1×1 or 2×2×2.

Table S2. The fractional coordinates for Rex, TSx, and Px from Eq.x (x = 1-6).

Re1(H13C4O74Al1Si35):

0.5138429324990170	0.7288688809139430	0.7558005565670385
0.5093438279171778	0.8321353742116884	0.3968493583751567
0.5361824539989186	0.8822565488952208	0.6060155747878468
0.4457364644550381	0.8482580277826841	0.5709184239321203
0.5177085226575642	0.6647771467005725	0.3731287739090305
0.4371397386944409	0.6599489872256967	0.4997984813923182
0.5148787259904992	0.5984665060213246	0.5742139802721340
0.5734255452100996	0.3417491334143037	0.5140207032454072
0.5673661835847383	0.4452507383875570	0.6460685600310825
0.6152851208281973	0.4473675685340766	0.4411676811772125
0.4008906723518137	0.4376908110712776	0.4164635869848325
0.4454032934098251	0.3362893910553524	0.5010115932988342
0.4416732452327494	0.4408302767629237	0.6315530748167149
0.5008108431826059	0.8324805616095645	0.5403797784315856
0.4947205665952339	0.65999273062217361	0.5054141462851973
0.5690518863600218	0.4185756335664621	0.5083034235325457
0.4458908050678545	0.4133023572402834	0.4949809991749134
0.3307456882333426	0.0648518279204922	0.7683680602016452
0.4037436349709722	0.2185575452770649	0.8195945858041398
0.8295195595104872	0.5724492240946546	0.2509557086213832
0.8790652600725863	0.7404984646701612	0.3292598594202119
0.6953601188261160	0.8879667897153496	0.7156106849075314
0.6452219736634461	0.7261922205622611	0.8284286991951006
0.1851938302203635	0.3943075509853671	0.2278634708495346
0.1185230823992427	0.2397512736873253	0.3241106994712126
0.6905219499373203	0.0692811771367801	0.2296633101231791
0.6252663323435517	0.2602813279829081	0.1704272303372321
0.1737437196824345	0.5647935328956564	0.7287025188174425
0.1042350172331368	0.7216307741021240	0.6650238371197474
0.3239158749105613	0.8915417649700359	0.2549154505735771
0.4016045920326405	0.7424114592152975	0.1781093084127079
0.8269834742426099	0.3870399185307605	0.7639544441446873
0.8847472518149715	0.2252334487884085	0.6740015588578174
0.6871223076416797	0.8863291872809285	0.2542564805866405
0.6131619316337691	0.7335880790393006	0.1743415492369706
0.1871557701288040	0.3833403251437346	0.7592770025678703
0.1293591548307162	0.2205158542662460	0.6778903605389104
0.3173673595460968	0.0735552046837142	0.2243540671075337
0.3907542216104929	0.2274856150297424	0.1743882370016152
0.8385473705655500	0.5695527706429502	0.7361490409898721
0.9136925468081714	0.7229187946983373	0.6723550945430574
0.3124696484383236	0.8861250379680357	0.7078898524231079
0.3805117825797737	0.7317989676642753	0.7978163563675764
0.8261682489634268	0.3897253606976179	0.2318428387145985
0.8964864741899774	0.2369049935379692	0.3195092817096992
0.6843226018315249	0.0689015271476094	0.7701818572947587
0.6115379340553773	0.2242431344620286	0.8176071376290395
0.1891618494760792	0.5768596093314855	0.2587612644848321
0.1356246197643713	0.7438000710977377	0.3198892205396078
0.3577495980727861	0.1774548549610699	0.4986632504126973
0.1013402235554111	0.0728794764487191	0.4741399371764459
0.8632397240373422	0.6909858803372089	0.9938839021659334
0.6080812398952560	0.5713598650638332	0.9972430679483750
0.6762482347057528	0.7491455027237492	0.4876714265062532
0.9037077170045578	0.8906399670292018	0.5216841090307014
0.1734668579648826	0.2514834984772207	0.0038017036951530
0.3900083408085493	0.3816016705710297	0.9790378166296492
0.6549100459699702	0.1787106405203289	0.4972506041756048
0.9089749259061009	0.0732066839889853	0.4812759690757105
0.1470235357985672	0.6832123077936672	0.9905267051228392
0.4097508205082576	0.5645312724276081	0.9953525362303282
0.3276904824262843	0.7489081435901994	0.4768655336201988
0.1106104716567771	0.8910590885800076	0.5216898897269644
0.8395257245842487	0.2511473570629192	0.0006647507312252
0.6204639716288227	0.3871135792964751	0.9824217869254710
0.2668013611817628	0.2311214418006458	0.7466366370991651
0.7778203434406947	0.7378106967042797	0.7269316140707573

0.7580781952270286	0.2299517693962372	0.2844921670455420
0.2614679312011603	0.7302758479111020	0.1689245438397080
0.7514526912126129	0.7234546824360706	0.1910009231855980
0.2574675153787922	0.2387263099342505	0.2864315303735054
0.2402937437497101	0.7290372463967003	0.7437785943376412
0.7474532159411069	0.2353724148949681	0.7387639640455816
0.0069315004929180	0.2047918814216771	0.5192954602457505
0.5142707163733746	0.7056259464226002	0.9233250332107374
0.0078043157777614	0.7756944666314070	0.4352898737776059
0.5067881570172617	0.2821475689331550	0.0186996833001061
0.2051280303230030	0.0044582668107580	0.6655127094733473
0.7073991183039468	0.4865202208791288	0.1825595160941162
0.8080109793280812	0.9983542724494896	0.6737658918027662
0.3078148419366116	0.4837236094358559	0.1827942018614550
0.8078188068234695	0.9760768013028169	0.3213503199893424
0.2975224976742865	0.4940264768964013	0.8258053753699151
0.2014784563929766	0.9782951963332849	0.3118120481854589
0.7151206186728842	0.4955218086277995	0.8271778115971458
0.2510978796036341	0.9666160050414092	0.9882319636684755
0.7620197055951223	0.4759503441954251	0.5005421491584769
0.7593031050422141	0.96555710507536521	0.9444551251563425
0.2536246164650464	0.4716251041172939	0.5002176797625779
0.5198861952195273	0.7405407497975247	0.6069443970116168
0.5083051291706724	0.4465628675052145	0.4114772801707289
0.4218519960806049	0.6840806671321786	0.9821131882839325
0.3387802401374245	0.1732296216580878	0.7082072181798083
0.8314490266373795	0.6816498809612739	0.1922374077520672
0.6987190855943624	0.7749992220734825	0.6907277622893560
0.1837755092266420	0.2811532083448043	0.2100698359087687
0.6823328850318404	0.1773282940189560	0.2937765306269142
0.1672146963687595	0.6746644865174645	0.7818630742406043
0.3298668159294493	0.7776115760307292	0.2681074191810850
0.8249278192400666	0.2744909530111315	0.7932658275756310
0.6829157693255326	0.7735492628839822	0.2778837772640657
0.1894068916579599	0.2717840281421289	0.7959636657780180
0.3303696676773527	0.1792708229265969	0.2945207903932356
0.8482506547273871	0.6797575953122674	0.7830424742845992
0.3158671670214659	0.7724011086292748	0.6863085607297208
0.8299843035444141	0.2768839861629431	0.2086271307839098
0.6751714767627917	0.1769347740136098	0.7064612927788474
0.1837966458425200	0.6833824506871480	0.1855030575354277
0.0903528677714860	0.1846766469917753	0.4985126659624655
0.5957399603924571	0.6833925685933337	0.9836079962808810
0.9262321125850335	0.7824061031351235	0.4905602283070465
0.4219610457533705	0.2780922523584195	0.9985603915136352
0.9239631415959551	0.1847688126958360	0.4986936730928377
0.0907425838936717	0.7823989450456672	0.4861636647723600
0.5907874922433720	0.2810061665705987	0.9978573339006616
0.2746580514818078	0.9792351655023452	0.7829872777419595
0.7815209392756586	0.4810526025340920	0.2913691496973030
0.7371625193023377	0.9801292766183778	0.7881993439464310
0.2342258469894531	0.4819937801385237	0.2912283448115858
0.7366505786485646	0.9750147224499344	0.2011996576382060
0.2287032125226034	0.4785212805186561	0.7057525024143203
0.2734448459355860	0.9772865507041573	0.1955400568238161
0.7855908421954325	0.4816668845304193	0.7076722412174874
0.1555125237495574	0.9858072308738315	0.4926373528969705
0.6630706195653104	0.4842745780611324	0.9972247478812619
0.8570083652668217	0.9841945801134457	0.4986862992345209
0.3523492279807456	0.4832000495197377	0.9968658845677396

Re2 (H11C3O74Al1Si35)

0.5053514223413984	0.6683385203704901	0.7757797671973847
0.5065697723019653	0.6429520320117916	0.3687736370235086
0.5032944838356741	0.7503909605375370	0.4922974829453395
0.4268673618820316	0.6764087781447330	0.4827661262672223
0.4291324918598463	0.5311936640027426	0.6333696636755946
0.5000014624374316	0.5096482054869469	0.7868294301851151

0.1032914287735736	0.7344879583558708	0.6667594482468289	0.3143264251312488	0.2058654181537136	0.3040381613360736
0.3186789286891809	0.9160457963923818	0.2108539760090338	0.8313845751939226	0.6968456682850857	0.7847540108772293
0.4000353826057221	0.7656325458901918	0.1834242020243693	0.3183567894281580	0.8015207257846626	0.6955622657390848
0.8190577190762625	0.4011457093866397	0.7423974405562959	0.8324512063192415	0.2973322297169645	0.2201227446979743
0.8752695381048383	0.2351578868513755	0.6819094695126182	0.6733138339622187	0.1956432252415539	0.7240470054585657
0.6732515563776786	0.9085629880090735	0.2494760940171048	0.1832609063263604	0.7062312369907886	0.1911988511559954
0.5999730234231819	0.7544502423071506	0.1759790174997420	0.0830107616323374	0.1959395755853990	0.5031410687597386
0.1802495589469260	0.4044246627071431	0.7376990751640733	0.5885318825557562	0.6928800736732796	0.9962170604048666
0.1272035453773555	0.2368621039530439	0.6702768584048542	0.9172289354156291	0.7903504878798628	0.4942550345394849
0.3041149724894581	0.0942729508172704	0.2822256291211502	0.4151937798545831	0.2912652272642973	0.0075043746074570
0.3758048965046115	0.2422617306732917	0.1737638291760462	0.9172440718040065	0.1933886999694181	0.5123614472493969
0.8253638125408429	0.5839706569922356	0.7646955920134104	0.0828492112031185	0.7927113152050751	0.4884985063399725
0.8996016932442927	0.7351098682626613	0.6784221862305699	0.5825334398602635	0.2923746775976426	0.0116048512086024
0.3106567192930925	0.9066739382433866	0.7782518247977848	0.2681046223708137	0.0038919562274131	0.7922238548993334
0.3752360599610967	0.7424231614365340	0.8037443446569057	0.7756140513563921	0.4940799749640874	0.2966481795019362
0.8300532405186232	0.4072594445258417	0.2759755980388121	0.7301745213824091	0.9954399119901112	0.8008093500788718
0.8946521173737239	0.2462620919596361	0.3300596709809724	0.2205250350931180	0.4981511059879580	0.2859684367563844
0.6798982362108461	0.0831765036389882	0.7489514863611717	0.7259037806562390	0.9965728410890335	0.51265140314109948
0.6068426134252931	0.2334857010418574	0.8375678851006754	0.2270566815236563	0.4978039323681926	0.7009693904516539
0.1817705848030613	0.5943458500182430	0.2284248182929431	0.2646420465119590	0.0028679184325853	0.2003739220459337
0.1252897621364539	0.7564037911306372	0.3160495018002365	0.7750539153654969	0.4967178586197107	0.7099170367369751
0.3399638233607973	0.2282034968740092	0.5066613023830868	0.1479540728487478	0.9935287585003110	0.4937974120967681
0.0986639051804445	0.0855372111098092	0.4783229544120928	0.6561625231021679	0.4894624291171869	0.0059795043443032
0.8379737350909409	0.7230810465613970	0.9935105643694939	0.8489781002555574	0.9924124343189078	0.5090882349921912
0.6117562044761513	0.5852448661321006	0.0323438700217977	0.3437738506557722	0.4916217944274095	0.0005360746564946
0.6505287906493606	0.7819665012477941	0.4984890405011555			
0.8978353140703632	0.9002173018746120	0.5159718820917831	Re4(H7C3O74Al1Si:		
0.1501345024231995	0.2885779264522554	0.0015177827723747	0.5043977903800752	0.6544902803295187	0.7971678829665763
0.3952315799992405	0.4004030302117059	0.9938270409946099	0.5080602062028703	0.6289196835024455	0.3737668731567183
0.6619914698435423	0.2186956966902542	0.5152150691291695	0.5000513891014506	0.7328863940801398	0.5059350828882145
0.8995221620137102	0.0828690821179023	0.492652233253303	0.4260185219573529	0.6559300027283470	0.4820817021508574
0.1618572716219191	0.7259655213133840	0.9857514415933935	0.4295996901107912	0.5074908717880717	0.6293971738324871
0.3904340037336667	0.5827899450309886	0.0279878587316773	0.5140671820597333	0.4767039358331999	0.5382573541921261
0.3426964640261048	0.8109316245945521	0.4903765632779340	0.5028217902913283	0.4837832027835773	0.7745154504263283
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0.4139317927360295	0.7018360533612267	0.0017128095807166	0.3112405809743137	0.0987052475404937	0.2817824845992760
0.3199792158197994	0.2069748748089140	0.7214613583493161	0.3777223990486505	0.2527453515308409	0.1845640172705103
0.8178038767125955	0.7017220215047928	0.1954412144942594	0.8234917532296180	0.5883805262947490	0.7599719729866479
0.6844744034020849	0.7955164698876374	0.6957628883167928	0.9001444170390371	0.7379988829833408	0.6764952088138259
0.1629405487560760	0.3080262873410575	0.2147527250628229	0.3106599630462483	0.9094494824807740	0.7798927345173325
0.6855444039494714	0.26384161669915127	0.3022914278901449	0.3745409797672394	0.74481403048080093	0.8108461089427550
0.1738612973968898	0.7064748705157058	0.7822490221288305	0.8311901322494819	0.4090053045028981	0.2737499542744928
0.3366360690422496	0.8140381124619083	0.2840432121479353	0.8985179402327574	0.2495550687191113	0.3253628517110414
0.8246868713917550	0.2960755742955925	0.8041914844671467	0.6815969316251511	0.0886000992852871	0.7422803172249104
0.6678967195226306	0.7985290443185349	0.2869538679499897	0.6083470325090730	0.2394896249188960	0.8284306542727862
0.1748450692945056	0.3036601498226972	0.8075278559100099	0.1897398818815219	0.5958162842154806	0.2252257430767912
0.3134768450393324	0.2134628755299204	0.3089207107115897	0.1274199253384722	0.7528082261059978	0.3223629957260954
0.8317945650877405	0.6995172705903414	0.7830580558757063	0.3310065133630076	0.2356251397738589	0.5142575544123389
0.3204099751118576	0.8069937817103110	0.7014157091676836	0.1024513479614768	0.0888730037068015	0.4774251792182227
0.8365346675972702	0.2987053428881055	0.2136429154178998	0.8389709284740263	0.7253421110023766	0.9920666251559851
0.6768336471152665	0.2007822820476335	0.7214811090992512	0.6131002814981201	0.5883912445623736	0.0295690263607824
0.1886519422230108	0.7095031743029310	0.1950594987754641	0.6517928668974946	0.7865693299088719	0.4966283353726197
0.0839951629607540	0.1998533821349540	0.5068241712164863	0.8999501339072182	0.9032091577313892	0.5138323670320233
0.5917343924536524	0.6933655641080065	0.9947234582266518	0.1455220175211451	0.2967273434882722	0.0039750675009387
0.9195272036964113	0.7905942952897504	0.4930650234082492	0.3973048461447419	0.4016189990365646	0.9805234506771967
0.4144680025031064	0.2946039673491256	0.0097970916976422	0.6701756397105001	0.2278002049874388	0.5112058025253319
0.9180018900921709	0.193268957668752	0.5083117783837565	0.8994388930338246	0.0859746102431842	0.4888100241631435
0.0849296798983659	0.7961860450055696	0.4885581132600691	0.1621570366774066	0.7273885969351639	0.9890175245055346
0.5830118278776553	0.2919484977109761	0.0093444542337338	0.3937836696235948	0.5831737562257331	0.0300513767629127
0.2650610161971017	0.2067454817641490	0.8021727936342842	0.3437525803537724	0.8112206430283209	0.4951996244569372
0.7778386556837305	0.4945702094356292	0.2923305762437565	0.0969372700292368	0.9062956009285372	0.5052832111502710
0.7308927127939100	0.9984040944932033	0.7975659870535878	0.8548282650482548	0.2934206057828206	0.0052992612956970
0.2272606322297506	0.5004258844236986	0.2934612133287615	0.6010580292014680	0.4060950347431671	0.9861246166767685
0.7279262345748236	0.9965646949567954	0.2139194547086163	0.2569907864353453	0.2569778588932508	0.8107896074650611
0.2262948371505047	0.5036186955733868	0.7067461613722159	0.7629154479041347	0.7532339492249136	0.6978178905454797
0.2725787365523686	0.0082828189461779	0.2122720596437588	0.7613972861962424	0.2475287243849955	0.2522544230653949
0.7749781295948992	0.4975132042778228	0.7051769789314122	0.2628367308496991	0.753813630887004	0.2271898427125407
0.1505468243646462	0.9965229654773680	0.5011998872036330	0.7379510411486905	0.7440779005268183	0.2282652051808753
0.6573379449124417	0.4883704361276813	0.0022209989397410	0.2401718634460579	0.2569293120050133	0.2533355631753267
0.8501860476789673	0.9912653871657184	0.5054701080590291	0.2405904414014657	0.7543503837014143	0.6988628382295161
0.3462189420748274	0.4937705129561962	0.0056991282423624	0.7457271491993183	0.2513888406677083	0.8048404143136949
			0.0014632492388031	0.2093028392138976	0.5480088654391935
			0.5069394681771371	0.6958512383253677	0.9318940145205090
			0.0002257666684287	0.7785158745762288	0.4472916791418058
			0.5005309853111228	0.2809338347798089	0.0315841439126601
			0.1930021340751509	0.0003416257567679	0.6854973867172021
			0.7066366239351893	0.4748210476088559	0.1741262944273885
			0.8038832514768899	0.0011437849866809	0.6867950680148383
			0.2954034846086415	0.47418638868875290	0.1748638868875290
			0.7980814666956846	0.9870094360495614	0.3329236275567169
			0.2982261056985749	0.5001501211046033	0.8229010411161539
			0.2017715544297403	0.9846713661845712	0.3304812753835122
			0.7021888248699781	0.4991023397716248	0.8203212297068063

Re6(H11C3O74Al1Si35):

0.5049294567026834	0.6629328623945199	0.7938142220789786
0.5094041040658013	0.6415885467328550	0.3695760625308679
0.5011419224790288	0.7444848613465140	0.5043720590303948
0.4271910294169246	0.6676184944375620	0.4780908408553017
0.5034109219893566	0.4931927752097138	0.7652107092584970
0.5123931843274363	0.4891677919346833	0.5279153095983702
0.4290726416691939	0.5201817247223488	0.6256784980263745
0.4893174297901908	0.1829378208308512	0.6292419294360414
0.4502618393090003	0.3296107432212665	0.5495215004634488
0.5070916903875897	0.3202435040949752	0.3632528398070676

0.2448079382841470	0.0229842949147994	0.0058097446997962	0.1034869340585800	0.7175266363495325	0.6690452031689702
0.7524635736582326	0.5075185169357752	0.4976358259238793	0.3226737109014621	0.8860767340538160	0.2551083860354311
0.7500221014777964	0.0045238668586407	0.0066171112197893	0.3982416411728877	0.7335210387527908	0.1865217636668248
0.2498552476968072	0.5081309771537832	0.4977985723188212	0.8232258858977701	0.3819152548649427	0.7698006442338325
0.5091896187237808	0.6208061555669602	0.6414731152063169	0.8788443230943273	0.2194568845330522	0.6759481813125134
0.5008533045040835	0.2008947632642943	0.5083425822349383	0.6850063315848587	0.8807317525473763	0.2638435578028009
0.4130773697397672	0.7000042336673715	0.9997953767328767	0.6134576291089289	0.7260210743656614	0.1838349108105177
0.3233104662414448	0.2034454436153439	0.7195641834239979	0.1834611102213728	0.3783460922367752	0.7595402424511306
0.8167343163535179	0.7026380633516638	0.1951185134619990	0.1291267833476297	0.2138616572661221	0.6760496153731452
0.6840610016033324	0.7967146165257191	0.6959089783126728	0.3180945619408959	0.0686448529672674	0.2365238915099326
0.1647684884019895	0.3062686599216704	0.2132502935212131	0.3833157933294444	0.2283521212385651	0.1777275092721737
0.6846052564324125	0.2056632820267339	0.3032235838353969	0.8331243586955850	0.5648868641362839	0.7362697595001890
0.1715948995716303	0.7034609074013503	0.7801300364207648	0.9114603526236138	0.7161111504401774	0.6797639258896808
0.3341926306974727	0.8118885685047132	0.2815186989913343	0.3090304169329343	0.8820885487179595	0.7123230537738223
0.8241851145219528	0.2971716091318868	0.8046886086208360	0.3799797292942984	0.7299562588791346	0.8027251951734868
0.6675103799269166	0.8005055674881589	0.2866564988996956	0.8251937848806961	0.3820328532923867	0.2438409922317675
0.1775986307287596	0.3004068074923012	0.8051772413422782	0.8957900203807441	0.2277121684185914	0.3233343359137493
0.3153120323200937	0.2108620757643394	0.3070357766429268	0.6792220663536668	0.0634208775497527	0.7694238663305626
0.8315856528120307	0.7008356714219630	0.7827564906467401	0.6057806728753334	0.2179854639524947	0.8218144308221653
0.3183544225576469	0.8037557683206131	0.6997633665736629	0.1872380290225308	0.5711309067510157	0.2616137281211834
0.8359146735520753	0.2995605211446986	0.2144373785894302	0.1309239070370865	0.7366914656915853	0.3216771276876642
0.6763740998401815	0.2013167549416153	0.7195484502030851	0.3527110367426900	0.1822108955231201	0.5033759128359421
0.1861455059136503	0.7079712405505063	0.1927220576352227	0.0989283032325261	0.0672598414443399	0.4733806423260916
0.0846164650743901	0.198467314280731	0.5058628509119174	0.8628260210867253	0.6800974717969339	0.0006237764590864
0.5906047812039290	0.6961333446483735	0.9951927125876949	0.6054866748409324	0.5650538268371577	0.0092775757461112
0.9181697363960666	0.7929261368792666	0.4921134636425819	0.6787089926967127	0.7409579066839527	0.4947843891650763
0.4158528343620134	0.2923410148217158	0.0082046512003515	0.8975554157563863	0.8825992402264475	0.5258630537745717
0.9186364873306445	0.1960334001969670	0.5089085632162025	0.1655043162729299	0.2480507967065293	0.0056845676499506
0.0833799185415671	0.7946531809255077	0.4875765180508509	0.3910697350344350	0.3792362718446896	0.9763763361375339
0.5842265557601820	0.2945925507996350	0.0079374464255153	0.6522011138597890	0.17919388602238047	0.5025463851431624
0.2657505622005729	0.0046875957818457	0.7998092419205776	0.9061461305096259	0.0653762540995686	0.4925306544321373
0.7768117776461381	0.4958470357493709	0.2925969243216429	0.1448217590138015	0.6761456209465351	0.9933732891995959
0.7306118051742629	0.0001213887727474	0.7970873366522682	0.4054453726864864	0.5610676584373167	0.9963421812500286
0.2260682687334068	0.4994943229506532	0.2911325311471487	0.3244908953677097	0.7444868286188751	0.4823538352118106
0.7272838414097151	0.9996855694743729	0.2136236937107441	0.1103350089981561	0.8857955193599025	0.5229898274956994
0.2266146237753262	0.5018486130036663	0.7047226137456590	0.8386384314880004	0.2465111415453620	0.0061422522005827
0.2705735777484080	0.0063254583969795	0.2093254583234222	0.6139983902234789	0.3822296518231454	0.9813680256732056
0.7746945232049356	0.4996881802524911	0.7053122519965243	0.2649241789424082	0.2276838730040893	0.7647639209345414
0.1495614187198271	0.9952214818904892	0.4995974474224028	0.7763560923287756	0.7362650768596737	0.7426947812988303
0.6566674478182719	0.4917669418664019	0.0019844092295287	0.7573638093824542	0.2216028717952412	0.2895799970340676
0.8499899691233992	0.9945098358117477	0.5052501927781989	0.2577954135408547	0.7264342627240126	0.1751889987313007
0.3460695049087548	0.4926152671943029	0.0035634102358415	0.7516288309281904	0.7205835792033142	0.1945365040773908

TS1 (H13C4O74AlSi35):

0.5083114200024141	0.7496223302064351	0.7174439336403680	0.2397522670217924	0.7231602452613188	0.7523951790522219
0.4951275212955863	0.8227132909042467	0.3628536386711048	0.7424862261337566	0.2306916585162142	0.7544166696592640
0.5331896864751542	0.8938746308566650	0.5346300523616847	0.0035428138802445	0.1968398941046843	0.5344051037389761
0.4436745437384246	0.8543635344617044	0.5521964328644984	0.5121331102749735	0.6999644256776278	0.9415614769330176
0.5558564638544752	0.6286069884712049	0.4390227529439841	0.0053153588914086	0.7730412844785164	0.4453199632762477
0.4578734802703650	0.6429490092592616	0.4328692372665444	0.50350271268423704	0.274353840588444	0.0347128259469400
0.5025342684005167	0.6033987088646811	0.6430169762513884	0.2023150362480663	0.0013517370689513	0.6703387395535358
0.5542395415473180	0.3703683729510914	0.4496058661939202	0.7043107369573960	0.4731459427876672	0.1859699673814958
0.5597219566176506	0.4435252833453589	0.6432248743662541	0.8027033872699363	0.9915466928483312	0.6779473207343827
0.6051740125393152	0.4759244022092943	0.4429062559382047	0.3043560823442348	0.4748283251504546	0.1817323987671031
0.3893500309761961	0.4962532918837681	0.4456083712288006	0.8048858460255772	0.9733453786903965	0.3241656853981496
0.4282653886802734	0.3822873695324489	0.4524946208620833	0.2951918720124809	0.4866503557261197	0.8286192336283804
0.4323164566542204	0.4563959445450152	0.6455707101262718	0.2011282492722941	0.9744541416287475	0.3162450149561380
0.4966031800213315	0.8362001575447735	0.5057552163430401	0.7106244542887694	0.4890448067943893	0.8308743639217866
0.5053411859583221	0.6227999228700725	0.5042393386835613	0.2508683789454267	0.9674229544290469	0.9924904764673244
0.5580760061588634	0.4427158517832126	0.4973417707497845	0.7565450344645512	0.4679194677415950	0.5054333005251053
0.4325365276231707	0.4546396031239865	0.4998452842696892	0.7535960405725817	0.9631729280277597	0.9998983156279166
0.3291997964432340	0.0611613260432975	0.7628889837513810	0.2516934871557339	0.4647511449305881	0.5006310534081422
0.4024379043726825	0.2139369785909295	0.8239008720990668	0.5225874397468360	0.7528800441781485	0.5910763427601738
0.8242678619710659	0.5648349655679539	0.2568134691546931	0.4975803563199577	0.4941635047589656	0.4332655269129688
0.8790289260880257	0.7296629965157138	0.3356992059903803	0.4215511621722925	0.6807215526567916	0.9861609403543596
0.6900003971038871	0.8815336694340132	0.7242014159803034	0.3361526729066924	0.1709168284566260	0.7131988342764046
0.6436234158733143	0.7165050570825500	0.8354580314869793	0.8297891735530385	0.6738558386119848	0.198021449895041
0.1808096291352115	0.3884193093817316	0.23203669401065259	0.6960901747659776	0.7684988891233431	0.7003333254128208
0.1107673739209076	0.2357671772196284	0.3257935432289898	0.1768566519076984	0.2754263466489490	0.2124772743059680
0.6855014079725308	0.0637443774068700	0.2409315610493152	0.6803038089732354	0.1727392488219692	0.2999642559740323
0.6249684533436408	0.2275688138447052	0.1741111775874771	0.1661004707081872	0.6695955275842707	0.7852647600681522
0.1720872230794157	0.5600544799168503	0.7279651149860058	0.3271300292976207	0.7720555655454575	0.2734484340505716
			0.8210642209793519	0.2693799406641446	0.8001156143960202

0.6825146392755386	0.7676103062605932	0.2854181859966261	0.6130534249526960	0.2336405605337291	0.8474938419056741
0.1858838591323817	0.2671132798736977	0.8001416415679117	0.1897478990686992	0.5813487897040091	0.2129776508945369
0.3252070714143969	0.1764651535855322	0.2995280713219728	0.1201268971227165	0.7315782416137111	0.3157181804546951
0.8454963829245798	0.6739676371332877	0.7901891820167748	0.3367532045508526	0.2220831961723277	0.5017963197586468
0.3146058502578057	0.7683792069543927	0.6919779120383964	0.0977606665543433	0.0775734716751870	0.4759721598786655
0.8291773127299109	0.2695086706329235	0.2151047088166322	0.8370956254381241	0.7243053077929531	0.0058182925046992
0.6708556207365177	0.1723448443673092	0.7122984736031981	0.6158598443297691	0.5875267204146652	0.0467796186612759
0.180828889560572	0.6778259657598653	0.1890625550345675	0.6513761777362248	0.7909639599814469	0.5117635923741517
0.0866182158717734	0.1785042356889193	0.5017937141473965	0.8981402405967955	0.9004969470100832	0.5088479312419523
0.5923833264692249	0.6778862571279518	0.9923163124171026	0.1489765052933905	0.2825721072343654	0.9933803892831037
0.9234028764412869	0.775502804427377	0.49775151726171997	0.3934380136773896	0.3917880385468280	0.9539291363355460
0.4189454376367223	0.2740412219404504	0.0028893053885284	0.6595227043719447	0.2301808588452232	0.5215194508549175
0.9207515061847502	0.1770475465932790	0.5065385675587564	0.8987626528653010	0.0838634970044083	0.5104329220250250
0.0886663974867616	0.7776113218239971	0.4902908956022074	0.1607334827484408	0.7147134719781008	0.9837914904180565
0.5872291752683267	0.2750468858513244	0.0028503178721166	0.3959975941208214	0.5724138774035481	0.0141325320665970
0.2726720777253036	0.9763115605468116	0.7853158883840763	0.3416599067108450	0.8042741458209406	0.4890281886021057
0.7780654331568044	0.4722341353672732	0.2972492246183194	0.1013889515430435	0.8951262030596823	0.4782031464261678
0.7317058656973003	0.9743509601993807	0.7926782119212987	0.8499313899495391	0.2897741829163820	0.0195096800723533
0.2310158244091696	0.4753561085508480	0.2921270856692075	0.6009481229332678	0.4047788774220606	0.9904752841107509
0.7326488525399100	0.9704224485113073	0.2079587433081400	0.2598556784252679	0.2510791193046629	0.7922493794150967
0.2258819670295793	0.4727596471005242	0.7056923405825088	0.7632699487338428	0.7547160165354541	0.7072172890371888
0.2731790635078752	0.9734591261673984	0.2004185299064503	0.7559760118983476	0.2491963304178668	0.2683623319516570
0.7812139781928877	0.4758640540583912	0.7116897942856468	0.2560061683476889	0.7447030234204703	0.2351748595109697
0.1540980619958603	0.9813820391217831	0.4953061716747058	0.7380162143066400	0.7464415195329082	0.2464530841107759
0.6592271869930428	0.4775663083078854	0.0017570776744975	0.2412305882956360	0.2403071977610267	0.2475411732393411
0.8525888149528384	0.9776169526628422	0.5045065532566042	0.2414733760144756	0.7424303583760619	0.6977665088674954
0.3495648732616772	0.4784365899049945	0.9967701228470602	0.7489027005961120	0.2523390754504078	0.7907142159641580

TS2 (H11C3O74Al1Si35):

0.5159724309764826	0.6545544384007798	0.7220592285647243	0.5084058807769978	0.6925570817135807	0.9444307575812942
0.5009201768207348	0.6424970099233605	0.3411678740203143	0.9984197798362473	0.7748095813844174	0.4530922812011937
0.4801148873250298	0.7418354549610200	0.4733363350204769	0.4994980303937311	0.2789857026236220	0.0244834829050760
0.4280117893580595	0.6383426371193437	0.4925036159267364	0.1906398316266475	0.9896983862767073	0.6799288093576834
0.4963948822521473	0.4873110639263416	0.6978458630571609	0.7031124717618980	0.4666852525268226	0.1943876874673123
0.5911831320532102	0.4975534719924255	0.6320895416712702	0.8064650341302055	0.9926228041005487	0.7062574351363509
0.5208482023362748	0.4971649788697832	0.4576041768501042	0.2988781611841986	0.4642243406489381	0.1703329528894528
0.5846937793805580	0.3356608554274487	0.5437120984408566	0.7942114511968867	0.9933010000440774	0.3512131504485723
0.4853195954351222	0.2481778317739938	0.4787102663882123	0.2930775763598064	0.4961907709505056	0.8205219349943604
0.4876285798131974	0.3502019197265085	0.3398022554439493	0.2041479261476979	0.9890305405791153	0.3258178745013041
0.4336075746720525	0.3481260572435545	0.5352741604384903	0.7054058126012634	0.4956850289032104	0.8399821758107322
0.4814023740949835	0.6654552457517013	0.4706769220514175	0.2443758455589418	0.0164779621846591	0.9969293084600821
0.5362791527613595	0.4888962645573969	0.5953671933708193	0.7516122947825608	0.5040186674043383	0.5140117055468778
0.4828849117979033	0.3244773127305862	0.4759538079162695	0.7480435033056239	0.0111873319888147	0.0210488931281034
0.3119772573843704	0.0807262931698176	0.7158758102302656	0.2493754285837966	0.4966945415626469	0.4906116989657860
0.3953765320427749	0.2195001891092545	0.8221558995321914	0.5303191845774364	0.6314940784794345	0.6021242318392979
0.8093824156144009	0.5870336371714444	0.2306264844377850	0.5395176201124698	0.3611673160115458	0.5860410924748010
0.8714871248387439	0.7405782808079024	0.3448878702229266	0.41666356754759875	0.6904065292943216	0.9896387845498253
0.6851570478993807	0.9050527367997176	0.7759384103044269	0.3249046131080675	0.1921882620137509	0.7077239169867156
0.6375090085311186	0.7361119156715930	0.8487810155474378	0.8142166687214285	0.7000152523798988	0.2078725797425207
0.1717742748077100	0.4015331530736646	0.2587847703228050	0.6834628966061373	0.7962447964787529	0.7116205322855294
0.1039926809875382	0.2422977183661246	0.3132548870516985	0.1669799770971991	0.2920914210674042	0.2031099135605245
0.6792168279254938	0.0946092003786276	0.2820628731655788	0.6792845491988615	0.2065810090238571	0.3140870031430083
0.6177797317540126	0.2571649039583162	0.1993619390356756	0.1707078400680402	0.6943928799905450	0.7738572837534221
0.1724179632489538	0.5819665006097452	0.7379981374244338	0.3299959537659021	0.7997909003616144	0.2760800415753479
0.1030398422230121	0.9038184656341490	0.6697586372097248	0.8271172502652391	0.2976016619185984	0.8132782994374637
0.3215250136200751	0.7073370003644412	0.2060220812675837	0.6662117488770889	0.8010781590912401	0.3006173863277724
0.3954730141877931	0.7510415762214961	0.1818601927064805	0.1793120102757442	0.2908325890404626	0.7933661185456344
0.8243969446847430	0.4067102106941149	0.7543329757410362	0.3183565974171998	0.1991500277783231	0.2948784369607154
0.8824699253410202	0.2411316038139475	0.6928407520229243	0.8311846591265990	0.7024623439755615	0.7950925229243708
0.6736884019449292	0.9116994967667793	0.2526925725927072	0.3186520997933542	0.7938535408705576	0.6948265725321789
0.6011736546968578	0.7560853839835460	0.1888156280745861	0.8321481094190020	0.2975802080025218	0.2285938903236513
0.1780491161923266	0.3989948709718831	0.7300725528679521	0.6781715466065847	0.1992808034831626	0.7260762792386828
0.1314912033468900	0.2282673252676162	0.6613174208965447	0.1825925774441330	0.6938191975314609	0.1882192893933166
0.3200754581123206	0.0875730388937939	0.2612707430300389	0.0849949339828555	0.1888091483096233	0.4970484976521732
0.3789846323150385	0.2481932850040494	0.1755852472361710	0.5887235767682739	0.6946253650250966	0.0078145828671978
0.8242308156380318	0.5898416602296095	0.7683262723217794	0.9170905150562376	0.7897872792566432	0.5013149344323509
0.9003913629993363	0.7411204093787518	0.6929274642504453	0.4147939320854093	0.2848440355982049	0.9932692642831071
0.3089298128281683	0.8995636871713160	0.7754135006949738	0.9191750026485366	0.1936947134762690	0.5204515393151112
0.3763906309196798	0.7367067100996181	0.8025152745163595	0.0827238490867472	0.7847176873286941	0.4798378709114672
0.8298760228961655	0.4070223519741276	0.2877651848072205	0.5831111601093966	0.2940815956650482	0.0136958408312609
0.8930190128262012	0.2444491615183679	0.3388376562638342	0.2641642531477117	0.9946962844389660	0.7914864596956122
0.6866430078606811	0.0870816831499184	0.7370939092485500	0.7740459924515122	0.4925789269627074	0.3071508514481707
			0.7319248735154744	0.9980402852589592	0.8107222773009752

0.2278866141922293 0.4871267843697993 0.2826077849401472
0.7243546495649866 0.0017867762140895 0.2273386752273936
0.2235727436963231 0.4938931606412638 0.6960243707835048
0.2723246359374301 0.9986016148870362 0.1982963177163626
0.7767943798131469 0.4993400470308345 0.7205846076888420
0.1496141198611411 0.9876669793669777 0.4903246612734904
0.6567517943586694 0.4902895990540159 0.0176237239164294
0.8490543470304317 0.9922888838141830 0.5185345938364563
0.3454176981305395 0.4851073337432936 0.9916002340833288

TS3 (H9C2O74Al1Si35):

0.5049760847699289 0.6242036959011799 0.7390613217506257
0.5017634879312425 0.6237384424170074 0.3564964996533675
0.5000252255937028 0.7238782569794182 0.4976803007808712
0.4253850346843819 0.64773121115976659 0.4889359901280059
0.4340617128798101 0.4757598701792531 0.5925742858807368
0.5193463227127708 0.4637103938856981 0.4684151839420423
0.5174268546542820 0.4436347949914463 0.7122352988937095
0.4434386227878804 0.3207236409812495 0.4456117305468368
0.4501030887182225 0.2998890867844040 0.6480279276961696
0.4831179230895941 0.6510709217228268 0.4838146286491281
0.4892724588112785 0.4561470885435526 0.5892147772803327
0.4752085420358938 0.3297105286417903 0.5469562444301701
0.5150486641728236 0.5950620828937829 0.6213026376328230
0.3225157041951690 0.0937742900564231 0.7407775507737000
0.3965451626361656 0.2471263753972224 0.8179552290618304
0.8160904757295455 0.5875454032520651 0.2251776639028193
0.8767333068121772 0.7459142662323828 0.3257170188500851
0.6840643003531923 0.9058356650203265 0.7545290702051872
0.6321390706983578 0.7385152059992990 0.8303805814223253
0.1633914945502184 0.4118372314982395 0.2700437313519259
0.1020906105633230 0.2477325325361832 0.3205491583174762
0.6851124400770985 0.0915638540524029 0.2674901592133452
0.6252076570668663 0.2522069540478569 0.1785115060963989
0.1870758036892539 0.59033048465537794 0.7605195963085620
0.1054434775115496 0.7335397482220998 0.6726436641287989
0.3188249489737842 0.9155792147872504 0.2140605696109006
0.4011267750481551 0.7663187721928750 0.1864986478260207
0.8220878193505499 0.4040041523030808 0.7426071411632691
0.8727564692621357 0.2359710531228814 0.6713248919737325
0.6768930161524978 0.9092334839093894 0.2411583714705117
0.6033161110776817 0.7551179305199724 0.1744996544096722
0.1797438820289372 0.4077702902855620 0.7394726044886681
0.1290022552070980 0.2388920644886738 0.6685651773791150
0.3080330616080076 0.0944722585364062 0.2842353846524759
0.3770152001980946 0.2456833130158245 0.1784426232215495
0.8202607137708497 0.5869535932022885 0.7587689879204902
0.8985930285323960 0.7344699933747023 0.6768111537966206
0.3152564744764277 0.9116612124495660 0.7798679130864841
0.3760187549547283 0.7444220334570275 0.8100430335006052
0.8343263218530907 0.4063163754073429 0.2689971130803741
0.8987361114305918 0.2446694624883179 0.3222900592486369
0.6794136450677613 0.0888322659098506 0.7455962953589506
0.6051869800850795 0.2406706805337180 0.8248904558904684
0.1838466357374671 0.5928854016900473 0.2310137865629116
0.1258654426499248 0.7537354331743344 0.3212268011167552
0.3363581101795958 0.2326116095364625 0.5079181376828501
0.0985439988313459 0.0848223424954426 0.4871297795384919
0.8383858513192450 0.7225916620351853 0.9926841529189758
0.6188638607438506 0.5881770459349269 0.0309313988752180
0.6514580883313101 0.7874572294367539 0.4968319806178627
0.8972917670864504 0.8997833360241074 0.5160136885338815
0.1473199002331995 0.2918221096294644 0.0016049549715476
0.4000804684083974 0.4044391205700535 0.0040909892395078
0.6634704544959789 0.2237792037811275 0.5084523901920477
0.9017973151830532 0.0822760969526684 0.4913066303537619
0.1645126607116154 0.7256134592532391 0.9914851013920156
0.3855592465916828 0.586088205798887 0.0346814333191503
0.3451046019877779 0.8133439640776672 0.4949739225475511
0.1020646777810796 0.9024282941791242 0.5239019899973414
0.8516467764973754 0.2860788416418316 0.0038528027610667
0.5994540871171381 0.4060484583603667 0.9888706448031499

0.2577278066395436 0.2568438222487046 0.8007743384494788
0.7614930012230872 0.7537290970294066 0.7012344202795475
0.7611244814957274 0.2473988446557485 0.2632466392591368
0.2625709081743892 0.7461313203950297 0.2403888720386007
0.7408995756888501 0.7436786304849718 0.2382357922169618
0.2399116892731499 0.2564869338966247 0.2576164866512087
0.2416678745970415 0.7599449439244736 0.7020522794595152
0.7427943767989760 0.2534795131454857 0.7960398003772795
0.0005669525843288 0.2103718951208791 0.5503654024458413
0.5066109829989003 0.6868809879494364 0.9454824189362370
0.0012800059646025 0.7802101930258090 0.4593329846182499
0.5005404766814365 0.2794454804025293 0.0399563222217338
0.2018046041538213 0.0078894955883371 0.6689967096380656
0.7094605521151607 0.4683006559037821 0.1679113764298847
0.8013372499291478 0.0026490327953184 0.6808020515603914
0.2873324546284479 0.4700116259948075 0.1605550920569598
0.8001153368075222 0.9879480939098002 0.3271006040667999
0.3042025281094922 0.4876824644164017 0.8091502725459492
0.1946578824935372 0.9860758885521435 0.3158722425541214
0.7011549652988975 0.4912946284634430 0.8142626017806904
0.2447827445643895 0.0247663924120047 0.9989199810839793
0.7535783803777676 0.5008820988920917 0.4941567018415398
0.7506993378097491 0.0047668452057508 0.0034827005381857
0.2494415121317957 0.5017568329146404 0.4915962835206997
0.4163636979692100 0.6991724676386113 0.9980667082120007
0.3257405757421949 0.2054422710845003 0.7164467961638366
0.8180378085736066 0.7002144658659191 0.1970760141951260
0.6819223215431620 0.7960806140488330 0.6976480489499224
0.1631247111213412 0.3023118435177565 0.2123171411557578
0.6842242508909493 0.20340562601683704 0.3032967686476837
0.1757342445747341 0.7026127746133923 0.7828158518205797
0.3333880507711129 0.8085602290534055 0.2821550377978284
0.8226650578783605 0.2949383763087638 0.8022310617976487
0.6685573619534253 0.7987135638723188 0.2872237339118300
0.1776570956762740 0.2994322314300391 0.8016501941395546
0.3137389178716106 0.2062825892111633 0.3037140310404141
0.8294207952709201 0.6991940234509215 0.7834189117988259
0.3212409559395297 0.8050441941399953 0.7003191356289591
0.8359866235620359 0.2961918149535165 0.2141155021716870
0.6733690382906303 0.2009442048517940 0.7175964814172531
0.1851104752667894 0.7054345662300463 0.1972718848374342
0.0830487662711334 0.1955405185880608 0.5061909727383096
0.5884669025197979 0.6935541638819700 0.9951292261613389
0.9181006633762223 0.7902850288979195 0.4948222244806857
0.4168622212445854 0.2944834842694988 0.0122458254483817
0.9180821271098978 0.1931957188801121 0.5085555810792641
0.0848980624920870 0.7921088237612324 0.4946315999439932
0.5842758363711056 0.2943826199192188 0.0081568379650108
0.2708110553780827 0.0067657280652324 0.7963866225681429
0.7784601452376592 0.4918570806981251 0.2891203834473828
0.7291016481650630 0.9998064094939849 0.7953489903742366
0.2212746254375944 0.4959752823352304 0.2876598762527820
0.7283969755048503 0.9981225658862698 0.2104804821497055
0.2301090670788852 0.4979940527190081 0.7013347504749987
0.2664471854187269 0.0034621562091317 0.7027636951224471
0.7743611444929996 0.4960096727126171 0.2029988305676298
0.1500005433460885 0.9946021338467332 0.4989729043293423
0.6578407527836063 0.4898135241118098 0.0000594826657121
0.8496345502142404 0.9929274755905979 0.5037591396182890
0.3440199675211275 0.4921468868876602 0.0031555370409606

TS4 (H7C3O74Al1Si35):

0.5060489401466484 0.6381007100257676 0.7419819384452353
0.4998500192709727 0.6314293122467021 0.3570475535596032
0.4959736415901830 0.7334665798570299 0.4931993085823194
0.4237207944687640 0.6533781378038626 0.4924915371196548
0.4359927868163069 0.4870577341612261 0.6030162637212371
0.5247963049921083 0.4759101902504597 0.4922503598659844
0.5165149532910078 0.4622695138715400 0.7397885688601136
0.4811681385400490 0.6597182155086614 0.4835481620180317
0.4921787949299556 0.4725095246699524 0.6105066635455429
0.4831140051750893 0.3421150399158392 0.5635409446415593

0.0981761494250421	0.2775002979539849	0.4844320632805363	0.7505500084527128	0.0053784521016240	0.0061028553721343
0.5160249503275836	0.6081005447958603	0.6232199683630668	0.2505688132720252	0.5043289046464210	0.4916868444801921
0.3219018741176995	0.0932015997135167	0.7366341963766274	0.4165386372431925	0.7007129429995516	0.9974066235626040
0.3968417498310117	0.2431997939263866	0.8244889762004206	0.3268762172714474	0.2055183364784128	0.7186108813469119
0.8164168580132412	0.5889711908179862	0.2291173724178890	0.8180640421226357	0.7015926630067923	0.1996420910914409
0.8754196137078196	0.7483935045883996	0.3301412014155147	0.6831595545027422	0.7977510494516906	0.7002489730770094
0.6840822253608252	0.9077769584768589	0.7550240140081002	0.1640423997877463	0.3055141304911544	0.2134362705655164
0.6345526437166527	0.7398041404499480	0.8352570603996128	0.6847288611919282	0.2046407545124325	0.3048937781559928
0.1644203752908169	0.4155674932226106	0.2682714057232545	0.1750978932259528	0.7031808063069391	0.7805840559116675
0.1025523054277642	0.2522081963142710	0.3229590849833599	0.3338023035046547	0.8114095829497998	0.2808572142393402
0.6851669466842338	0.0928197810950095	0.2694613711214942	0.8234841692183679	0.2967314802967636	0.8045410650492855
0.6264310706571905	0.2542971120661619	0.1791026922412300	0.6687095025791722	0.7998096495312765	0.2901418782446825
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0.8433724593273766	0.0097135422927909	0.5206795760535243	0.7418914323323378	0.2536675082759743	0.7961604388552100
0.3382150272928115	0.4872190388098616	0.9945935395389114	0.0006345552933382	0.2150566100457780	0.5519241002752366
			0.5068645793348026	0.6928692274683002	0.9502821842704989
			0.0008282786411664	0.7857077898424265	0.4628998374499034
			0.4999281057936500	0.2826282561679037	0.0436523704821710
			0.2053217099259872	0.0137173208440728	0.6575540460740115
			0.7105658436166209	0.4715097684095255	0.1694453534541296
			0.7986007115417451	0.0085260482087861	0.6794850939803183
			0.2835981652579633	0.4751780065055797	0.1536302781273449
			0.8028902053756539	0.9928587353948473	0.3262745264970874
			0.3051630432203751	0.4885412291900550	0.8041871437506956
			0.1894392834672445	0.9885693847841921	0.3074798848842661
			0.6997607422862870	0.4942188626375810	0.712047386110677
			0.2427427423758459	0.0267965742289746	0.9935045292410720
			0.7534282166837087	0.5008490320673360	0.4977241175245055
			0.7509113889461929	0.0060448204440817	0.0051852736767728
			0.2479466581222667	0.5019551407144363	0.4885223754350747
			0.4164711357540583	0.7011831667644515	0.9957738138597350
			0.3270208506606167	0.2060741783530275	0.7139507944154815
			0.8190838827641613	0.7014708212318820	0.2011208212318820
			0.6827271992694364	0.7970319634297454	0.7017576471868949
			0.1631559729934793	0.3036193664145230	0.2126269986934659
			0.6832847215595947	0.2043943932067123	0.3075156033876425
			0.1753895127429672	0.7037276764772642	0.7825574059592029
			0.3311080375395150	0.8092494356754045	0.2801320424415010
			0.8214870830818626	0.2960305497808378	0.8062874482250422
			0.6698651045842468	0.7999593255613391	0.2910500230382524
			0.1787359223835665	0.3007331608771224	0.8002578402021143
			0.3129115454700226	0.2056919848568128	0.3013796768910382
			0.8302069409821513	0.7002046404175104	0.7874841578351663

P3(H9C2O74Al1Si35):

0.5076763531600292	0.6291027856933908	0.7250622816482348
0.5009918505586697	0.6105627583980393	0.3478550916332992
0.5044443193418715	0.7174898968913439	0.4684129660345420
0.4272108295174348	0.6465290877672700	0.4779520043423702
0.4365285982632869	0.4466461270421505	0.5868293104375510
0.5125117437595037	0.4318729693313088	0.4434834955618925
0.5223555756276355	0.4199483768606243	0.6794577480944994
0.4402944276055791	0.2928791111646447	0.4561105450538037
0.4485963149940139	0.2832095931497065	0.6652747503376872
0.4851347817863569	0.6451915925846308	0.4715764109834808
0.4869252136047564	0.4114419814492152	0.5666170857049693
0.4741914467343378	0.3074698550191215	0.5519584562530895
0.5153154082834988	0.5932779343132424	0.6153648213088232
0.3253044525470585	0.0952732606822835	0.7454401616387045
0.3988219589314355	0.2502326100162051	0.8130799003989253
0.8179699377409477	0.5890814832315456	0.2332742414389415
0.8769004079795266	0.7493739926934708	0.3294457122151044
0.6837033056210444	0.9072391723938011	0.7569465508329500
0.6337735291106910	0.7390571547615536	0.8349676254115934
0.1613084007902259	0.4133534565383599	0.2670840178763925
0.1025305977337680	0.2475237860381228	0.3193937326708607
0.6858698565860735	0.0929782578970775	0.2698059424504393
0.6238796928659909	0.2522855338476901	0.1820630897649309
0.1880069424434367	0.5916658562710495	0.7606743681343886
0.1051055610622882	0.7328352881088520	0.6704950542105692
0.3140411184616170	0.9158083038527067	0.2113132688036288

0.3208595002338868	0.8062364226941199	0.6986776565879396	0.6038835238907510	0.5985485157169066	0.0157436464970644
0.8348981703641130	0.2974461228310474	0.2188349926210265	0.6712722751768112	0.7763770520268949	0.4999747395736236
0.6716444119420686	0.2019456578258101	0.7213590066412578	0.8976534130262621	0.9164308222829050	0.5333775570062329
0.1827443167774661	0.7071356690617847	0.1975918632562141	0.1659822746204540	0.2844216810542832	0.0147815702290544
0.0826758579227800	0.1973497208206680	0.5068210369786854	0.3936086122855471	0.4140856381334430	0.9846204297207350
0.5883804702397839	0.6964935301542283	0.9994465147515541	0.6506978466348556	0.2086834410071887	0.5103202391765080
0.9176177412684225	0.7928399393229668	0.5000909438969003	0.9043122373718617	0.0992452918239835	0.4959619069594723
0.4164994328564404	0.29656442357602363	0.0132874773029528	0.1445934519258003	0.7119730216911009	0.0005927496245590
0.9180600472818057	0.1954028452293670	0.5133166011785661	0.4032633187678769	0.5951267565537393	0.0400297823565978
0.0846107509434404	0.7946061390485397	0.4965594488983456	0.3254294693908761	0.7786627565149260	0.4906935103156655
0.5841105665860766	0.2971743514425000	0.01266820369785937	0.1077235230879978	0.9179601148011258	0.5307287671465701
0.2715656103088762	0.0084873801419789	0.7933226543626972	0.8363092026757712	0.2779272347044710	0.0157624945094241
0.7790502585692352	0.4935758766393903	0.2930828568931005	0.6120176256542891	0.4152864725653629	0.9909499311015111
0.7275979045165997	0.0018369130076579	0.7981286480730319	0.2633496990278488	0.2578965577354850	0.7699642079644562
0.2185697741120407	0.4984789736846480	0.2854346218919730	0.7724286048423679	0.7642172335713866	0.7407158735413475
0.7300143357222311	0.0000208839234475	0.2131500682220704	0.7568311896220123	0.2543037328769273	0.3030322014751832
0.2304833073605650	0.4993960692400066	0.6992654721809259	0.2578582470540951	0.7582991229678626	0.1849940054760566
0.2624265066006615	0.0039786246673188	0.1991952909009553	0.7467219953105442	0.7513660830656903	0.2038163489645726
0.7732544081946386	0.4976065514833365	0.7071262524624089	0.2482704610427575	0.2669967706609313	0.3004101464613385
0.1492240233716728	0.9970572775289241	0.4973022484156431	0.2352552148319873	0.7667958142166356	0.7540655653687054
0.6574059197538134	0.4932537837699797	0.0045519775402880	0.7413424139215579	0.2620332741573321	0.7606618790107547
0.8495499819824559	0.9961364209195338	0.5079906605190203	0.0022190260426171	0.2298665016491483	0.5447660347123389
0.3427653332866569	0.4951852850205185	0.0008864388689531	0.5089228491586084	0.7295303478386970	0.9379216186572137
			0.0031070397379764	0.8036418256676328	0.4499850695151864
			0.5027784647412830	0.3043503500895852	0.0448355116288042
			0.2077368611943484	0.0256902602463498	0.6668069557291716
			0.7023249216798462	0.5076087532851687	0.1938368927896761
			0.8020838085549826	0.0247486152507861	0.6849101114935152
			0.2969097179217499	0.4981926492451905	0.1773688810606302
			0.8033722464033417	0.0036103905512377	0.3319210646970703
			0.3030044026558372	0.5264814918954457	0.8266192452975289
			0.1933482628906233	0.0106361198821716	0.3133447836763850
			0.7094051468642988	0.5223407396244113	0.8395829241707915
			0.2496050518308692	0.9986713896936052	0.9961695319968698
			0.7561654898661914	0.5008068089640574	0.5134966816794773
			0.7535038638908205	0.9940732531627461	0.0064675390334159
			0.2527607652415895	0.5007383566390153	0.5059166936239450
			0.4179336067954651	0.7132880818988880	0.0007187740022232
			0.3359026758864587	0.2038274011082493	0.7195860067132713
			0.8260624015650606	0.7074952123263003	0.2049276652708656
			0.6933488653724780	0.8013328305597724	0.7036628763921371
			0.1743167418857610	0.3086529521144996	0.2240049891206439
			0.6796146010231610	0.2053474534594173	0.3084369102921301
			0.1651738848853199	0.7057741788164620	0.792124600083357
			0.3252855469259543	0.8088594147244947	0.2828113681849231
			0.8194049951844633	0.3010556376405589	0.8092620102231791
			0.6778733802820369	0.8011043371326139	0.2902738998881276
			0.1868100134755224	0.3037855769074298	0.8095484971888283
			0.3228284320677588	0.2112523680315448	0.3064837623276020
			0.8427934904897967	0.7056576432704134	0.7953843864245584
			0.3140449293257461	0.8009465135072986	0.7005995904657070
			0.8276213461419957	0.3029718769682717	0.2243301385420224
			0.6693484844516817	0.2042749668856629	0.7201222787593053
			0.1800668926141782	0.7111370118684022	0.1969088638098171
			0.0855200554545874	0.2124541132276150	0.5152520815049328
			0.59033646462043544	0.7103235679139958	0.9969109531875517
			0.9210963163329637	0.8084848095691299	0.5031864070587773
			0.4186263928543923	0.3072454654944821	0.0100132510425226
			0.9193862655187885	0.2107580593644229	0.5149527988326525
			0.0863294885843544	0.8095835892251131	0.4972714599086316
			0.5863923416397370	0.3075704727637927	0.0112591975767700
			0.2760492059913560	0.0071137147383453	0.7922087362795978
			0.7759986200354874	0.5057302281661435	0.3046618287663492
			0.7312279156541166	0.0071137364043494	0.7999112991592057
			0.2273470036992862	0.5067009344908584	0.2999487909891556
			0.7316094737765297	0.0027415456474387	0.2138178831284350
			0.2308731126314569	0.5097256082923280	0.7133531312449790
			0.2676997238577101	0.0087552867480341	0.2059759735916700
			0.7797626573944072	0.5077129166632588	0.7202157135697149
			0.1526591106919639	0.0128539921216628	0.5031979196455936
			0.6575189228142406	0.5101913808349110	0.0093143502624571
			0.8516514857139441	0.0106900941339774	0.5108939592861930

P4(H7C3O74Al1Si35):

0.5072156504714798	0.7450265366120092	0.7489970382533997
0.5443719548935562	0.8840653297929393	0.5593663240956701
0.4515411885341010	0.8745605895357542	0.6041031631583564
0.4860172750482477	0.8350575292151277	0.3944411810176476
0.3970377756853622	0.5823908504340264	0.5732902499729278
0.4809322567260352	0.6955540348272322	0.5521553608558847
0.4345860395184005	0.5944371029843651	0.3444338826660527
0.4965667909803315	0.8429818762187224	0.5363499122357993
0.4432779716048216	0.5857350315532344	0.4872150169779417
0.4948171506404719	0.5279166873783581	0.5348061914943116
0.5101097180316785	0.7496739813990061	0.6072845765052293
0.5426139515103543	0.4823514619331419	0.5795651284218124
0.3304418930533330	0.0942991565680202	0.7735669398217695
0.4014211602613145	0.2493016923915121	0.8288385531914315
0.8225221448275875	0.5984694623001729	0.2637766195219768
0.8750937201996294	0.7651012869388794	0.3411229930854489
0.6898373164080880	0.9142109738001167	0.7296855162151701
0.6390237708704021	0.7520954667379414	0.8386585569211036
0.1732522308834916	0.4212436005391993	0.2552731821822576
0.1090541068034412	0.2616312335002107	0.3300383265556803
0.6855948743537041	0.0968622013501275	0.2452183360054576
0.6253488198752777	0.2604893711719072	0.1810742925611066
0.1769491357604949	0.5967360881399628	0.7385573076300886
0.1004140364114292	0.7482888112399451	0.6754694831136092
0.3160871181067506	0.9222828140998729	0.2723244557791205
0.3976889253435019	0.7775898747084895	0.1902023485121092
0.8212844076852548	0.4135426282265229	0.7791670374362738
0.8778549676928264	0.2514061814683402	0.6863696336012666
0.6823749831659711	0.9139559215048578	0.2675698437423577
0.6081980222473575	0.7617717887276072	0.1862117530271590
0.1902136618860624	0.4157485302106565	0.7768473908824305
0.1274452283796066	0.2574073668496411	0.6827474486535081
0.3119671955670000	0.1042352916635636	0.2410028730999088
0.3804206890753790	0.2613168076120331	0.1810757619984997
0.8328600019947245	0.5957359488879845	0.7466487423213692
0.9083729541335188	0.7490508171545542	0.6850301942610955
0.3180833659356779	0.9140990552716630	0.7312332043144920
0.3748685951151103	0.7499950493550074	0.8101783479594928
0.8229223294838306	0.4156910196129004	0.2484712248347378
0.8950026558101314	0.2634257076589464	0.3332745228704113
0.6781231834062851	0.0954391367910858	0.7794260795111470
0.6048583345345335	0.2503508504292640	0.8303419806232029
0.1857020800141456	0.6039869273577949	0.2665358289455639
0.1303652073825248	0.7698392827954024	0.3302074109564899
0.3517867226459757	0.2130109685946664	0.5091876004748883
0.0987836377917333	0.1006140860748630	0.5047186580789429
0.8579388106950248	0.7159012127729767	0.0063798829766029

0.3495400010319187 0.5106442025854108 0.0083294602972472

P5(H13C4O74Al1Si35):

0.5118302822446594 0.6540605794698706 0.7069120989418565
0.5048735201026773 0.6059785710761574 0.3390071080834431
0.4873877935749604 0.7195393261382748 0.4261718881847258
0.4295466663487062 0.6250000282734476 0.4758931586492849
0.5126148233734469 0.4647834095331120 0.5769856718418040
0.5434177780611975 0.3483978548374154 0.5442624719777811
0.5015223653204828 0.4100859046098719 0.3660130592334596
0.4502090315803713 0.3720689750738586 0.5510558095866145
0.4888424301112479 0.2228902751402657 0.3964979372717607
0.4811031104431507 0.1617789787098189 0.6214750021668607
0.4279906280083381 0.9622165904077278 0.4280374144189096
0.5225453683025592 0.9525095197468616 0.4481106480493722
0.4718140058314404 0.0051485082336882 0.6271145919640873
0.4851050315778380 0.6442622070778725 0.4548193601148185
0.5018429513856475 0.3983962519102988 0.5095974402904844
0.4830964750577493 0.1597400750187035 0.4761602427502822
0.4759663363724371 0.9933345366914708 0.4839480194138019
0.3248337230098883 0.0816008516983118 0.749956553716039
0.3991545666217391 0.2301028213375886 0.8298626489433900
0.8150478524114604 0.5977513740526632 0.2272638381765688
0.8727145612191194 0.7579168148750952 0.3278831555142858
0.6827052952304200 0.9147836699757050 0.7496733792447330
0.6358344110453515 0.7474404104156847 0.8384055602913065
0.1696032153461715 0.4135165269642727 0.2483889291931263
0.1071614983652012 0.2532299581357336 0.3326758533646981
0.6838541228738180 0.10078273734259479 0.2607198893129095
0.6236573310349911 0.2609982397456250 0.1761330810826180
0.1695704878502653 0.5837186324031904 0.7242077478718727
0.0974627731014408 0.7396202487127965 0.6718731142835566
0.3196213154703074 0.9181805366701141 0.2645863503344827
0.3924466617436835 0.7688039214463913 0.1701914694557374
0.8202638945034550 0.4145416858745108 0.7498963011068724
0.8742759210218836 0.2485062277564225 0.6745341315412503
0.6751706979267382 0.9191254379109708 0.2498407076400895
0.6012201980181118 0.7668552862822011 0.1769080108503616
0.1811827579348702 0.4021496396534090 0.7665001921111667
0.1257708840450888 0.2373062552948468 0.6862881751411010
0.3103700225111368 0.0986336381317443 0.2396463794535038
0.3778373999515239 0.2555301319890901 0.1790954740843773
0.8218803271158421 0.5973105100417868 0.7551854134431863
0.8999076250614024 0.745575633373174 0.6771252301159834
0.3133416486817993 0.9011450935366909 0.7300188715879159
0.3735256019781872 0.7368807002300954 0.7963523604595579
0.8322084546520259 0.4165936418953251 0.2657336659401395
0.8969158319682577 0.2556243671018592 0.3236472399330310
0.6774774428664827 0.0967206055584171 0.7509630530998663
0.6034849568809477 0.2481970921553511 0.8248069031939878
0.1946954149010693 0.5953775044533387 0.2543428685776732
0.1236624608610342 0.7493287740682320 0.3230149170425136
0.3535574715554688 0.2062686696561471 0.5054578765269113
0.0953584296790666 0.0878815160238418 0.4918602549433047
0.8389935723309847 0.7316215009932066 0.9925423993674869
0.6142868800336956 0.5982826495592661 0.0350340057801333
0.6514760434328011 0.7941887859123682 0.4987152438733347
0.8967223874845445 0.9109653938425168 0.5173910453437855
0.1660379414390434 0.2723276137141042 0.0158103838811670
0.3904239997420973 0.4012079545032066 0.9611764272336671
0.6559851549132745 0.2259560889181529 0.5067388308415914
0.8999487694502122 0.0936118433268192 0.4932115685008540
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