

Supporting Information

Promotion of the selective catalytic reduction of NO_x with NH₃ over microporous Cu-SSZ-13 by H₂O and OH group at low temperatures: a density functional theory study

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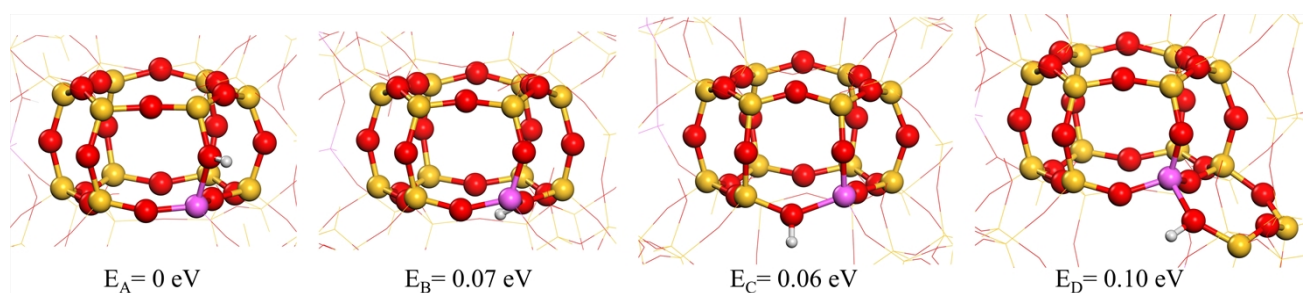


Figure S1. Four possible H atom positions on the Al-O sites in CHA zeolite. The relative energies (E) of each structure are presented below. Atom color codes: Si (yellow), Al (pink), O (red), H (white).

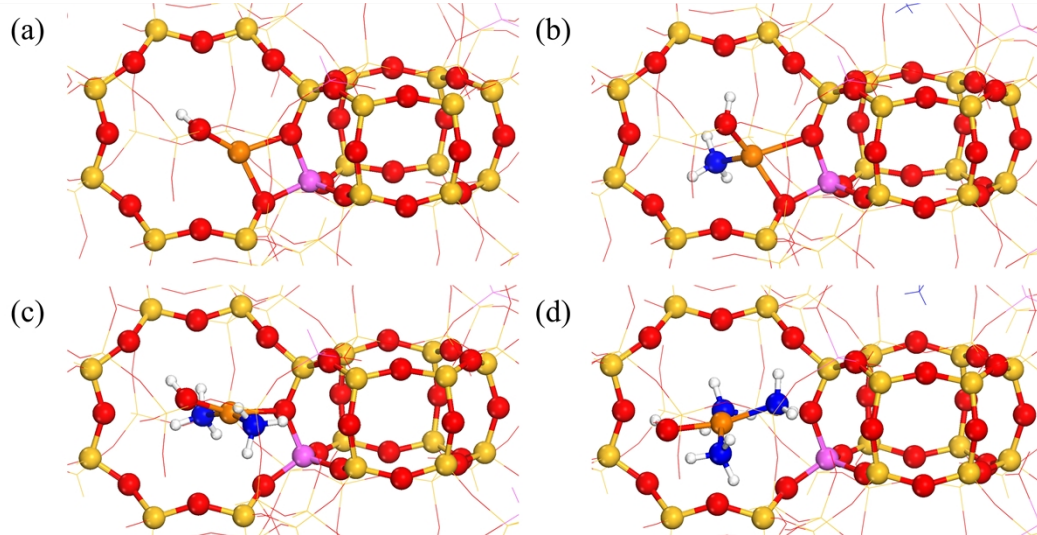


Figure S2. Structures of NH_3 adsorbed on the Cu-OH site in the 8-MR of Cu-SSZ-13. (a) $\text{Cu}(\text{OH})^+$ species anchored on the framework without any adsorption; (b), (c), and (d) corresponding to the adsorption of one, two, three NH_3 ligands respectively. Atom color codes: Cu (gold), Si (yellow), Al (pink), O (red), N (blue), H (white).

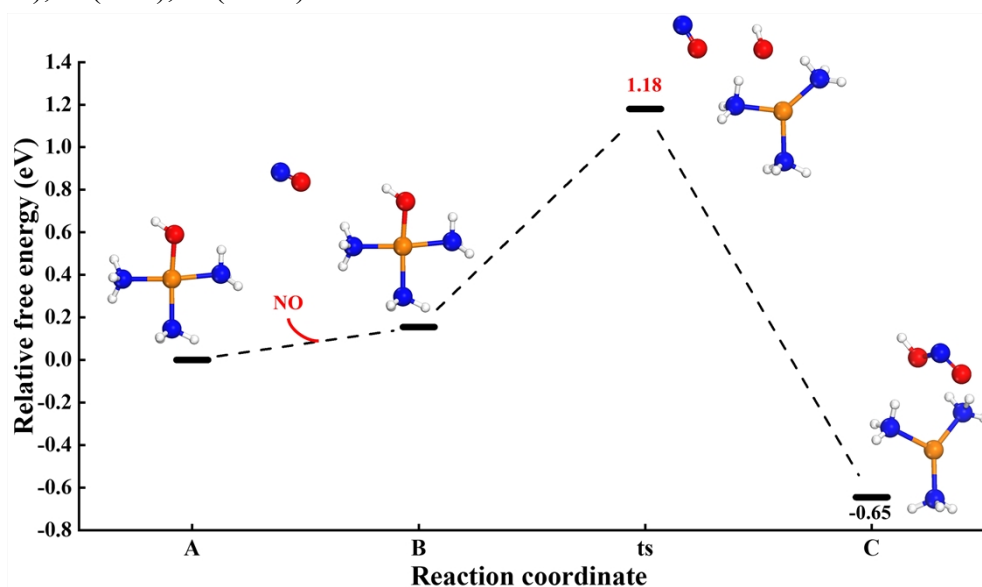


Figure S3. Gibbs free energy profile for the reaction of NO molecule with the OH group of $\text{Cu}^{\text{II}}(\text{OH})(\text{NH}_3)_3^+$. The structures of A, B, ts, and C are presented as insets. The zeolite framework is not shown for clarity. All legends are the same as those in Figure S2.

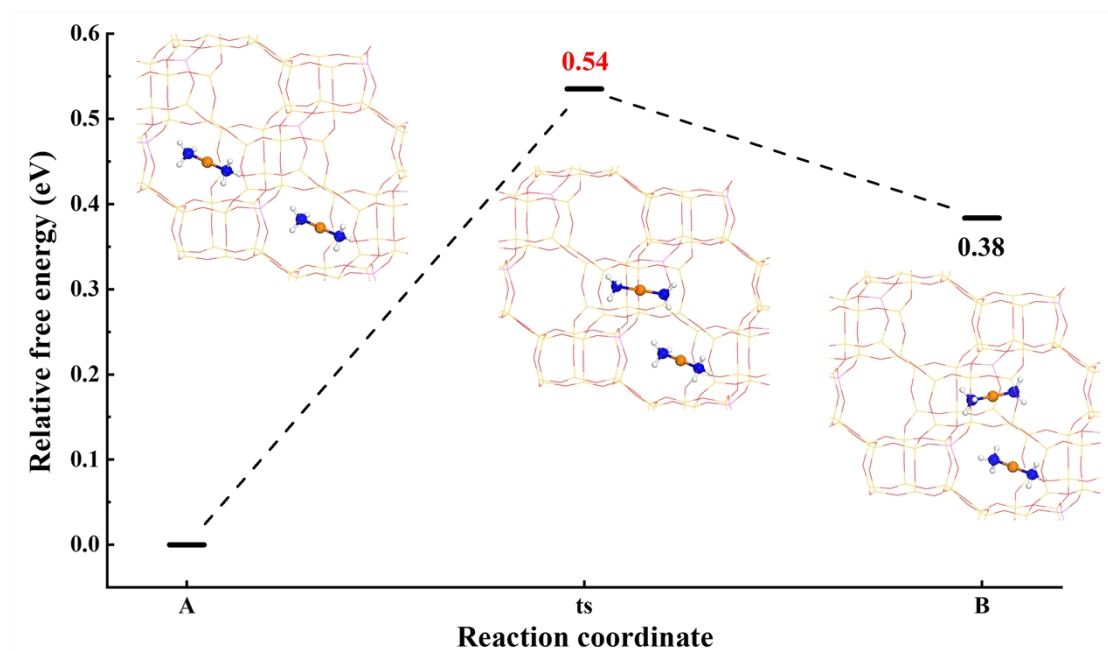


Figure S4. Gibbs free energy profile for the diffusion of $\text{Cu}^{\text{I}}(\text{NH}_3)_2^+$ through an 8-MR window into an adjacent cage. The structures of A, ts, and B are presented as insets. The zeolite structure is displayed by thin lines. All legends are the same as those in Figure S2.

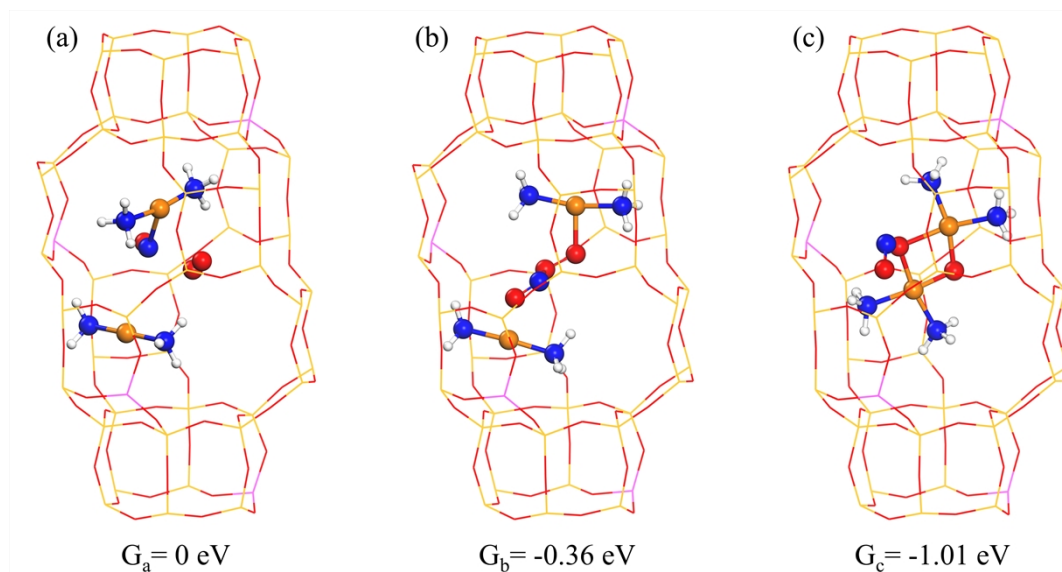


Figure S5. Optimized structures and relative free energies of NO and O_2 co-adsorption on a pair of $\text{Cu}^{\text{I}}(\text{NH}_3)_2^+$ complexes. The zeolite structure is displayed by thin lines. All legends are the same as those in Figure S2.

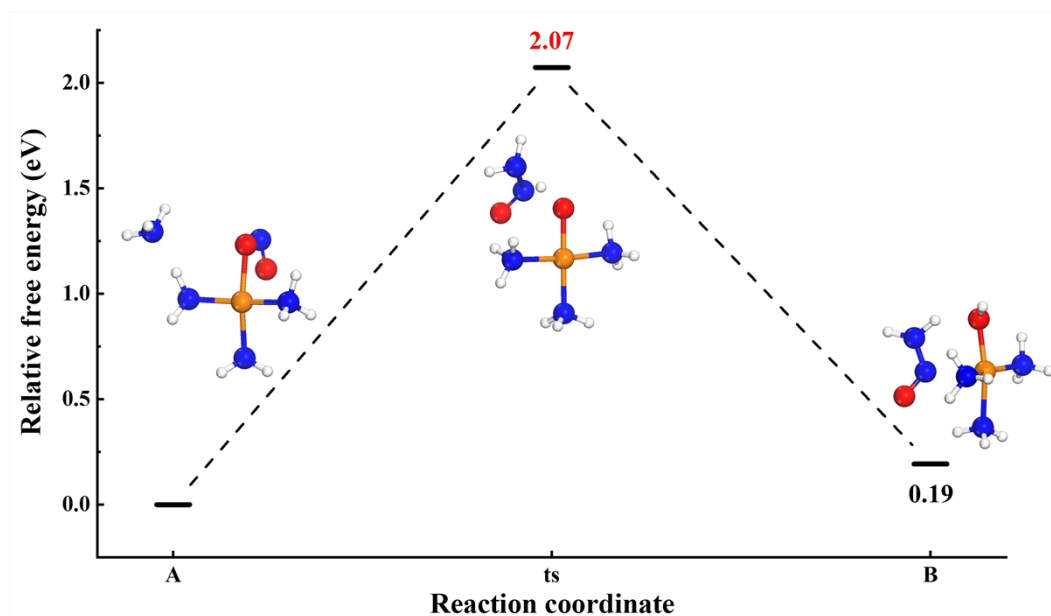


Figure S6. Gibbs free energy profile for the reaction of NO₂ ligand with NH₃ molecule from the gas phase. The structures of A, ts, and B are presented as insets. The zeolite framework is not shown for clarity. All legends are the same as those in Figure S2.

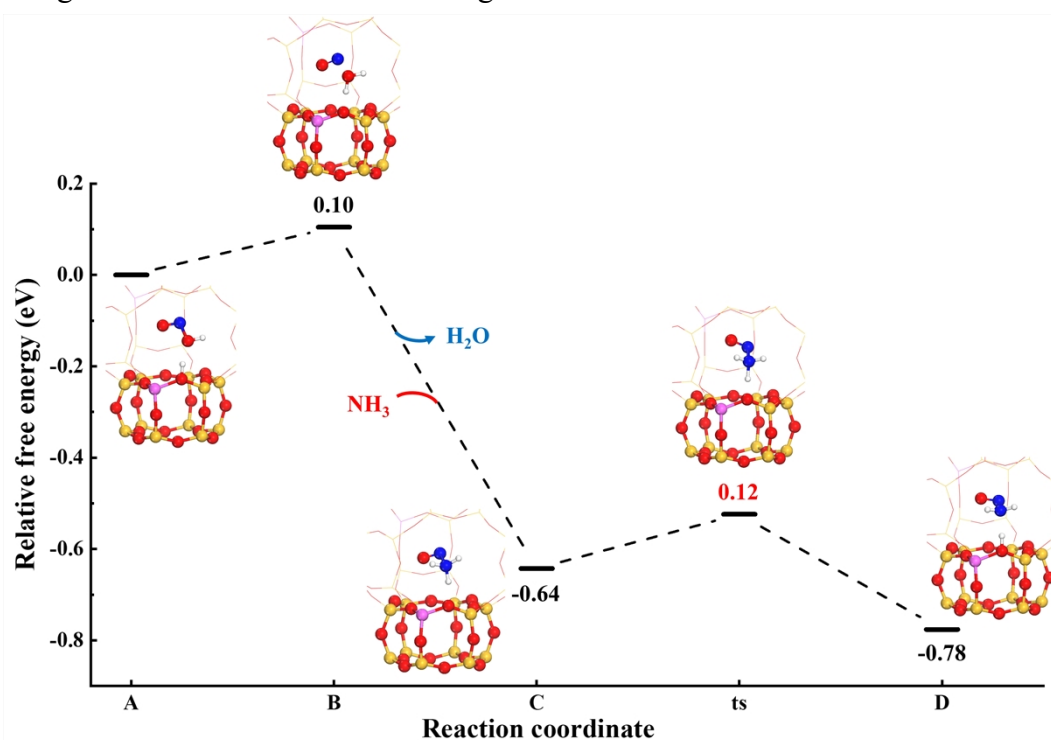


Figure S7. Gibbs free energy profile of the reaction of HONO with NH₃ over Brønsted acid sites. The structures of all elementary steps are presented as insets. Reactants are marked in red, and products are marked in blue. All legends are the same as those in Figure S2.

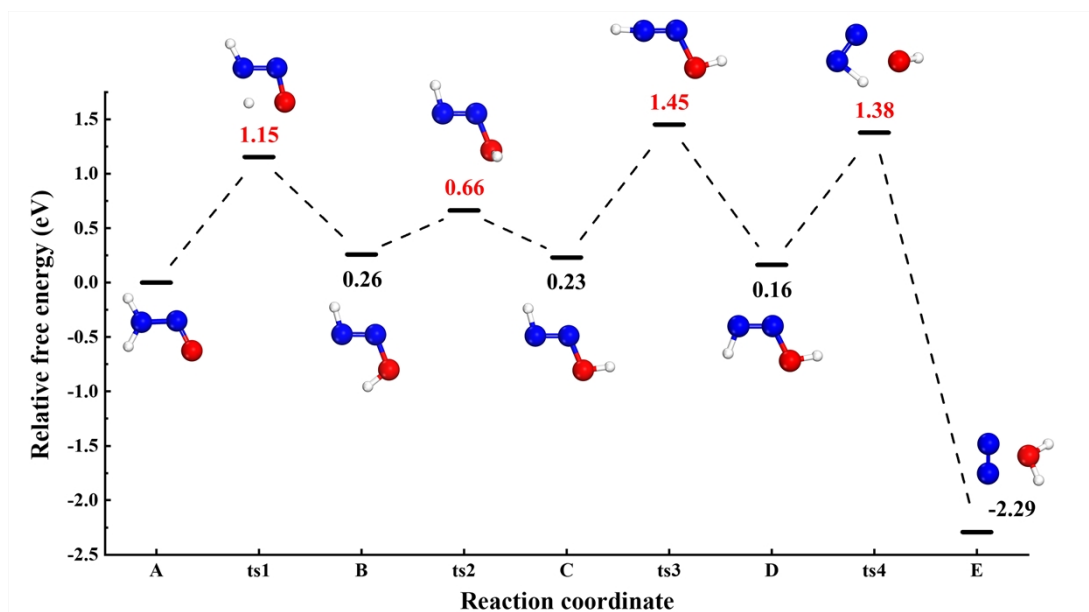


Figure S8. Gibbs free energy profile for the self-decomposition of NH_2NO in the CHA cage. The structures of all elementary steps are presented as insets. The zeolite framework is not shown for clarity. All legends are the same as those in Figure S2.

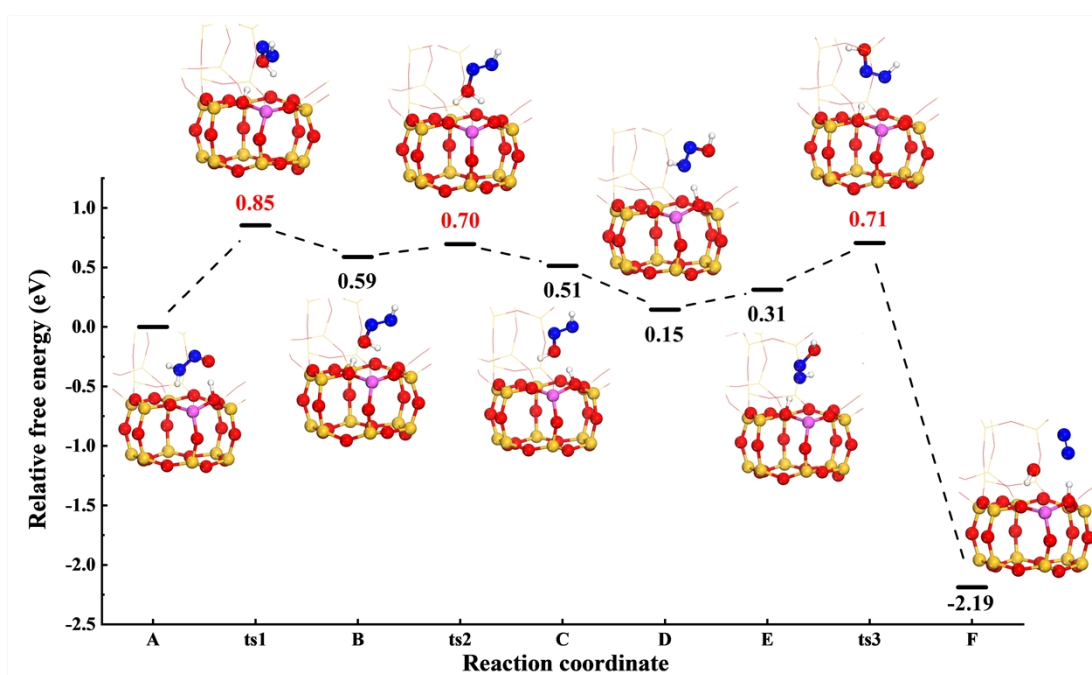


Figure S9. Gibbs free energy profile of NH_2NO decomposition with the assistance of Brønsted acid sites. The structures of all elementary steps are presented as insets. All legends are the same as those in Figure S2.

Table S1. Ground-state spin multiplicity of gas molecules

Molecules	Spin multiplicity
NO	2
NH ₃	1
O ₂	3
H ₂ O	1

Table S2. Comparison of adsorption free energies for different reactants on Cu-OH site^a

Adsorption order	Reactant	Adsorption energy/eV ^b
1	NH ₃	-0.58
	NO	-0.04
	O ₂	0.41
	H ₂ O	0.14
2	NH ₃	-0.64
	NO	-0.10
	O ₂	0.29
	H ₂ O	-0.10
3	NH ₃	-0.25
	NO	0.26
	O ₂	0.65
	H ₂ O	-0.05

^a When adsorbing the second or third ligands, the adsorption is on the basis of the structure with the lowest adsorption energy in the last adsorption.

^b The adsorption free energy (E_{ad}) was calculated according to

$$E_{ad} = E_{zeolite + adsorbate} - E_{zeolite} - E_{adsorbate}$$

where $E_{zeolite+adsorbate}$, $E_{zeolite}$, and $E_{adsorbate}$ are the Gibbs free energies of the adsorption complex, the zeolite, and the adsorbate in the gas phase, respectively.

Table S3. Electronic energies (E) and Gibbs free energies (G) for cycle I, II, III and gas-phase species. The Gibbs free energies are evaluated at 150°C.

	Reactant species				Step	Cycle I			
	E/eV	$\Delta E/eV$	G/eV	$\Delta G/eV$		E/eV	$\Delta E/eV$	G/eV	$\Delta G/eV$
NO	-12.34	-	-12.78	-	A	-648.89	0.00	-641.26	0.00
O ₂	-9.88	-	-10.55	-	B	-661.30	-0.14	-653.83	0.21
NH ₃	-19.63	-	-19.24	-	ts1	-660.89	0.41	-653.32	0.71
H ₂ O	-14.29	-	-14.23	-	C	-662.50	-2.53	-654.81	-1.54
					D	-649.83	-7.16	-642.98	-7.02
					E	-1247.06	-7.39	-1234.19	-6.62
					ts2	-1246.73	-7.05	-1233.65	-6.08

F	-1247.25	-7.57	-1234.21	-6.64					
G1	-1261.04	-9.03	-1247.81	-7.46					
H1	-1275.05	-10.70	-1261.77	-8.65					
ts3	-1274.75	-10.40	-1261.67	-8.55					
I1	-1275.21	-10.86	-1262.10	-8.98					
J1	-658.14	-13.12	-650.57	-10.52					
ts4	-656.26	-11.24	-648.69	-8.64					
K1	-657.63	-12.11	-650.02	-9.42					
L1	-660.05	-16.94	-652.83	-15.03					
A	-648.83	-18.70	-641.24	-15.73					
Cycle II					Cycle III				
Step	E/eV	$\Delta E/eV$	G/eV	$\Delta G/eV$	Step	E/eV	$\Delta E/eV$	G/eV	$\Delta G/eV$
A	-648.89	0.00	-641.26	0.00	A	-648.89	0.00	-641.26	0.00
B	-661.30	-0.14	-653.83	0.21	B	-661.30	-0.14	-653.83	0.21
ts1	-660.89	0.41	-653.32	0.71	ts1	-660.89	0.41	-653.32	0.71
C	-662.50	-2.53	-654.81	-1.54	C	-662.50	-2.53	-654.81	-1.54
D	-649.83	-7.16	-642.98	-7.02	D	-649.83	-7.16	-642.98	-7.02
E	-1247.06	-7.39	-1234.19	-6.62	E	-1247.06	-7.39	-1234.19	-6.62
ts2	-1246.73	-7.05	-1233.65	-6.08	ts2	-1246.73	-7.05	-1233.65	-6.08
F	-1247.25	-7.57	-1234.21	-6.64	F	-1247.25	-7.57	-1234.21	-6.64
G1	-1261.04	-9.03	-1247.87	-7.52	G3	-1260.18	-8.17	-1247.20	-6.85
H2	-1281.30	-9.66	-1267.28	-7.69	H3	-1280.35	-8.71	-1266.31	-6.72
ts3	-1280.14	-8.50	-1266.03	-6.44	ts3	-1279.85	-8.21	-1265.93	-6.34
I2	-1281.77	-10.14	-1267.68	-8.09	I3	-1281.62	-9.99	-1267.54	-7.95
J2	-1284.19	-12.55	-1270.13	-10.54	J3	-1284.25	-12.61	-1270.13	-10.54
K2	-1266.64	-14.51	-1253.18	-11.90	K3	-1265.04	-12.96	-1251.58	-10.39
L2	-1286.68	-14.92	-1272.45	-11.93	L3	-1265.60	-13.53	-1252.11	-10.93
ts4	-1285.62	-13.86	-1271.46	-10.94	M3	-1287.98	-16.28	-1274.04	-13.61
M2	-1287.57	-15.82	-1273.23	-12.71	N3	-1256.86	-17.05	-1243.23	-14.19
N2	-1289.38	-17.62	-1275.34	-14.82	ts4	-1256.44	-16.63	-1243.06	-14.02
O2	-1278.39	-18.28	-1264.06	-15.35	O3	-1258.06	-18.26	-1244.59	-15.55
P2	-1298.66	-18.92	-1283.36	-15.42	P3	-1278.39	-18.91	-1264.06	-16.08
ts5	-1298.08	-18.35	-1282.70	-14.75	Q3	-1298.66	-19.56	-1283.36	-16.14
A	-1298.36	-18.62	-1282.92	-14.97	ts5	-1298.08	-18.98	-1282.70	-15.48
					A	-1298.36	-19.25	-1282.92	-15.70

Table S4. Electronic energies (E) and Gibbs free energies (G) for the transformation pathways of NH_2NO and HONO intermediates. The Gibbs free energies are evaluated at 150°C.

Self-decomposition of NH_2NO					NH_2NO decomposition with B acid				
Step	E/eV	$\Delta E/eV$	G/eV	$\Delta G/eV$	Step	E/eV	$\Delta E/eV$	G/eV	$\Delta G/eV$
A	-647.85	0.00	-640.81	0.00	A	-648.33	0.00	-641.20	0.00
ts1	-646.44	1.41	-639.65	1.15	ts1	-647.52	0.81	-640.34	0.85
B	-647.61	0.25	-640.55	0.26	B	-647.94	0.39	-640.61	0.59

ts2	-647.42	0.73	-640.31	0.66	ts2	-647.52	0.81	-640.50	0.70
C	-647.95	0.20	-640.74	0.23	C	-647.84	0.48	-640.68	0.51
ts3	-646.55	1.60	-639.52	1.45	D	-648.15	0.18	-641.05	0.15
D	-647.93	0.22	-640.81	0.16	E	-648.08	0.24	-640.88	0.31
ts4	-646.57	1.66	-639.70	1.38	ts4	-647.64	0.69	-640.49	0.71
E	-650.24	-2.01	-643.37	-2.29	F	-650.31	-1.98	-643.39	-2.19
NH ₂ NO decomposition with B acid and Cu-OH					HONO transformation with B acid				
Step	E/eV	ΔE/eV	G/eV	ΔG/eV	Step	E/eV	ΔE/eV	G/eV	ΔG/eV
A	-616.25	0.00	-610.57	0.00	A	-642.27	0.00	-635.41	0.00
ts1	-615.90	0.36	-610.38	0.19	B	-642.06	0.21	-635.31	0.10
B	-615.90	0.35	-610.39	0.18	C	-647.85	-0.95	-640.77	-0.64
C	-615.70	0.55	-610.32	0.24	ts	-647.73	-0.83	-640.65	-0.52
ts2	-615.63	0.63	-610.24	0.32	D	-647.91	-1.00	-640.91	-0.78
D	-618.70	-2.44	-613.24	-2.67					

Table S5. Cartesian coordinates of the reactant complex (RC), transition state (TS), intermediate (IM), and product complex (PC) for cycle I.

Structure A			Structure B			ts1					
Si	-0.028297722	2.758152962	8.151423454	Si	-0.029726028	2.756790876	8.149905205	Si	-0.035175025	2.754082203	8.143242836
Si	7.703778744	1.007079482	3.117919445	Si	7.703464985	1.007366896	3.118304968	Si	7.705681324	1.007878661	3.118867397
Si	2.240016699	8.486470222	0.895689309	Si	2.239417076	8.486422539	0.895544589	Si	2.237642050	8.483605385	0.890744448
Si	5.333650589	8.668211937	1.249793768	Si	5.332723618	8.668834686	1.251062036	Si	5.330864906	8.657846451	1.246812344
Si	7.722766399	0.954755902	6.256845951	Si	7.722712994	0.953097522	6.257001400	Si	7.706669807	0.947243333	6.250041485
Si	-0.073300302	5.934364796	8.352061272	Si	-0.074040890	5.933443069	8.354169846	Si	-0.075961471	5.931731701	8.348664284
Si	-0.017412663	8.237659454	6.252862453	Si	-0.017677903	8.235490799	6.253303528	Si	-0.018914312	8.231376648	6.245858192
Si	5.447589874	0.716152489	8.395402908	Si	5.446925163	0.714873970	8.395470619	Si	5.439025879	0.718799174	8.392709732
Si	2.312567711	0.663371742	8.179399490	Si	2.311973333	0.662996829	8.178683281	Si	2.307134628	0.656591535	8.168780327
Si	-0.034654617	8.265520096	3.132427692	Si	-0.034803003	8.262008667	3.132460117	Si	-0.036265045	8.254689217	3.123343945
Si	7.836153984	3.294283628	0.986540854	Si	7.831700802	3.296249866	0.987968385	Si	7.842007637	3.281250000	0.968411922
Si	9.382879257	2.802717209	8.182695389	Si	9.380640984	2.801840782	8.184583664	Si	9.371917725	2.790520906	8.174399376
Si	17.072635651	0.959131062	3.081121683	Si	17.072164536	0.957785606	3.080664158	Si	17.070426941	0.949506700	3.070237398
Si	11.610020638	8.525442123	0.895436883	Si	11.606787682	8.526420593	0.898474097	Si	11.602599144	8.525306702	0.887670875
Si	14.700273514	8.624283791	1.165774584	Si	14.696202278	8.622453690	1.168063760	Si	14.697489738	8.617797852	1.157442927
Si	17.158870697	0.944022834	6.232077599	Si	17.158798218	0.942618251	6.231687546	Si	17.156425476	0.938720942	6.224454403
Si	9.240896225	5.940318108	8.313284874	Si	9.239109993	5.940173149	8.315531731	Si	9.232294083	5.944304943	8.304066658
Si	9.383009911	8.245381355	6.194309711	Si	9.379977226	8.241434097	6.194568157	Si	9.375052452	8.242195129	6.181064129
Si	14.819309235	0.737580776	8.356811523	Si	14.816211700	0.730631530	8.356814384	Si	14.816907883	0.727166235	8.352415085
Si	11.718410492	0.679169416	8.115897179	Si	11.715466499	0.677481234	8.115482330	Si	11.711750031	0.677067935	8.102153778
Si	9.377953529	8.236913681	3.069099903	Si	9.377391815	8.237329483	3.070527792	Si	9.375853539	8.242964745	3.058042288
Si	17.235275269	3.230849504	0.937731564	Si	17.230686188	3.226961851	0.936152458	Si	17.227006912	3.222273111	0.932296276
Al	7.680119514	6.443420887	1.157969952	Al	7.679252148	6.445194244	1.161682963	Al	7.682808876	6.461930752	1.125080824
Al	17.046363831	6.410267353	1.059174299	Al	17.043031693	6.408944607	1.059118390	Al	17.043113708	6.402755260	1.051837206
O	1.421663523	2.026816845	8.229351044	O	1.421237111	2.026721716	8.229400635	O	1.413040161	2.017933607	8.221134186

O	18.393110275	0.009952769	2.900413752	O	18.391235352	0.005803809	2.901173830	O	18.385282516	0.006986216	2.886759281
O	8.031728745	2.396239758	2.343765259	O	8.029395103	2.398169518	2.344977617	O	7.986664772	2.400135279	2.337935686
O	2.709106684	0.536208928	0.165559947	O	2.709568739	0.536147594	0.165095970	O	2.703093290	0.528634608	0.153277382
O	1.238818288	8.466297150	2.195789337	O	1.238760710	8.466366768	2.196044683	O	1.239334226	8.465112686	2.192356348
O	-0.184289724	3.129253626	0.131464064	O	-0.191280454	3.126071692	0.125479177	O	-0.196599424	3.122029066	0.118839562
O	6.225518227	7.358359814	1.308751106	O	6.223078728	7.358628750	1.317366123	O	6.204253674	7.334271908	1.288806915
O	8.644580841	0.391506732	6.361008167	O	8.642842293	0.393604457	6.361337662	O	8.638611794	0.394723713	6.351188660
O	6.303020477	0.655949056	7.004187107	O	6.302284718	0.655115545	7.004567146	O	6.293451309	0.639834046	7.003153324
O	7.805616856	6.004161835	8.996222496	O	7.803557396	6.006106853	8.998807907	O	7.787387371	6.048413754	8.961050034
O	-0.091867030	6.768632412	6.934632301	O	-0.092379570	6.766379833	6.935735226	O	-0.097092390	6.763628960	6.929662704
O	5.517845154	0.710864305	9.167399406	O	5.517076969	0.712674439	9.167206764	O	5.512294769	0.702401400	9.174270630
O	1.162952900	6.513711929	9.262027740	O	1.164280057	6.513066292	9.261600494	O	1.162624359	6.510019302	9.257102013
O	17.975839615	2.216856480	6.845140457	O	17.978181839	2.216004133	6.841602802	O	17.971176147	2.215082169	6.834159851
O	6.377321243	0.317837358	2.473839045	O	6.376366138	0.318951428	2.473620653	O	6.398391247	0.281180263	2.478596449
O	6.041357517	1.885207891	9.350538254	O	6.038777351	1.883813858	9.351661682	O	6.027444839	1.909284949	9.325904846
O	18.031360626	6.819167137	2.645239592	O	18.037195206	6.813067436	2.641967535	O	18.046457291	6.802798271	2.628103256
O	1.840780020	0.232429475	6.889398575	O	1.840700626	0.233932436	6.889379501	O	1.846362829	0.242834389	6.876411915
O	0.353634834	8.005980492	4.670880795	O	0.353895396	8.002192497	4.671162128	O	0.347901881	7.996301174	4.663043022
O	3.880999565	1.044545174	8.033178329	O	3.880537271	1.044359922	8.033326149	O	3.873367071	1.044819593	8.027157784
O	7.388134480	4.755484104	1.412033319	O	7.378810883	4.756982803	1.413182855	O	7.456199169	4.763882637	1.386128426
O	7.439861298	1.327987671	4.697875977	O	7.440929890	1.329912782	4.698017120	O	7.413079739	1.311375499	4.694895744
O	3.742074251	8.308362007	1.434511900	O	3.741570950	8.308055878	1.434725285	O	3.737864971	8.309566498	1.434395790
O	0.200490177	4.358762741	8.003448486	O	0.200260162	4.357779503	8.005804062	O	0.200103402	4.355557919	8.002902031
O	10.826325417	2.027904987	8.268493652	O	10.824960709	2.027392387	8.269462585	O	10.831989288	2.037556648	8.214969635
O	8.992518425	0.037125856	2.931237221	O	8.991059303	0.036988825	2.931042194	O	9.013111115	0.062869757	2.934937000
O	17.371429443	2.348337412	2.308375597	O	17.372587204	2.348015785	2.309297323	O	17.370908737	2.343850136	2.305901527
O	12.246270180	0.580765009	0.145274043	O	12.246311188	0.580495656	0.145817846	O	12.228462219	0.577730179	0.126058608
O	10.751324654	8.697121620	2.272518635	O	10.748757362	8.705576897	2.274878740	O	10.762123108	8.681215286	2.274903774
O	9.322198868	3.300861835	0.248590574	O	9.317598343	3.302698851	0.250197172	O	9.324139595	3.226590872	0.230838120
O	15.604740143	7.311442852	1.195831895	O	15.602705002	7.311000824	1.203552008	O	15.605561256	7.308444023	1.198513389
O	18.064098358	0.411576450	6.345840454	O	18.064628601	0.412912220	6.345626831	O	18.065292358	0.413739890	6.345601559
O	15.756542206	0.702464700	7.022362232	O	15.757191658	0.702471197	7.023921967	O	15.754814148	0.702973902	7.018169403
O	17.375257492	6.134076118	9.126413345	O	17.375745773	6.135022640	9.129495621	O	17.372671127	6.133711338	9.121708870
O	9.311693192	6.769769669	6.891219616	O	9.311903000	6.767284393	6.893330097	O	9.323027611	6.768810749	6.879198074
O	14.876616478	0.704938233	9.113392830	O	14.873529434	0.713557899	9.111235619	O	14.876395226	0.717072904	9.103639603
O	10.402011871	6.583588123	9.303068161	O	10.400543213	6.583484173	9.305901527	O	10.395262718	6.581923485	9.295671463
O	8.449985504	2.229073048	6.978431702	O	8.448522568	2.227753878	6.979631901	O	8.442857742	2.220560074	6.963483810
O	15.771972656	0.226582199	2.427582979	O	15.770536423	0.227876067	2.426562786	O	15.766305923	0.227341354	2.413231373
O	16.024089813	2.644974232	0.004220694	O	16.016765594	2.634074211	0.010446309	O	16.010797501	2.628791332	0.010679962
O	8.842514992	6.848793030	2.459388971	O	8.848960876	6.849151134	2.455578089	O	8.829913139	6.868849754	2.432406664
O	11.264675140	0.259845853	6.872484684	O	11.260712624	0.261402160	6.873441696	O	11.247925758	0.233422369	6.838896751
O	9.789408684	8.024812698	4.636964798	O	9.788436890	8.022651672	4.637753010	O	9.780417442	8.013684273	4.626341343
O	13.288208008	1.082437396	7.909583092	O	13.286472321	1.076220870	7.906475067	O	13.284971237	1.068397045	7.904020309
O	16.887619019	4.730539322	1.367221475	O	16.882642746	4.728168964	1.358731270	O	16.879388809	4.722977161	1.353905082

O	16.816581726	1.251566648	4.662368298	O	16.816610336	1.249222755	4.661971569	O	16.812313080	1.233496785	4.652595520
O	13.137218475	8.196124077	1.348745227	O	13.133272171	8.195259094	1.355642557	O	13.133339882	8.193893433	1.330271721
O	9.703917503	4.392506123	7.965420246	O	9.701106071	4.391911030	7.967994213	O	9.669356346	4.386172295	7.995685577
O	10.715300560	2.217634201	4.928231716	O	10.716895103	2.219249964	4.925456524	O	10.481261253	2.517775774	4.749813557
Cu	10.924994469	3.522078991	3.617620945	O	5.600300312	4.970973015	4.614342213	O	5.828547955	4.442234039	4.750952721
H	11.400354385	1.527613640	4.914074421	Cu	10.934362411	3.527806520	3.616623640	Cu	11.234521866	3.547767878	3.436433554
H	9.553892136	4.947646141	5.301989079	H	11.399142265	1.526903152	4.908138752	H	11.079216003	1.889014006	5.186916351
H	8.795764923	5.081796169	3.836091280	H	9.554700851	4.930125237	5.314408779	H	9.057832718	5.302627563	5.175220013
H	8.697529793	3.668307781	4.719500065	H	8.814937592	5.103212357	3.844578028	H	8.474986076	4.985385418	3.620271444
H	-0.648833036	6.031774521	3.196260929	H	8.702120781	3.667891741	4.691033363	H	8.764155388	3.702010155	4.720715523
H	12.758908272	2.756601572	1.805489898	H	-0.650041938	6.028357983	3.198953867	H	-0.649313688	6.019594669	3.189280510
H	13.216477394	2.314361811	3.324046850	H	12.770790100	2.770766973	1.804086447	H	12.892825127	2.255477905	1.728036523
H	12.022428513	1.490703225	2.547176600	H	13.224000931	2.318858624	3.321048260	H	13.575525284	2.241645813	3.230369806
H	10.401289940	5.716916561	2.347148657	H	12.030405998	1.501296401	2.536509037	H	12.265039444	1.294949412	2.892577648
H	12.035968781	5.671941757	2.592601299	H	10.403994560	5.720499992	2.343713284	H	10.432456017	5.714526653	2.374055624
H	11.364846230	4.802727222	1.378221631	H	12.037883759	5.683445930	2.591647863	H	12.041882515	5.850547791	2.683535576
N	9.311678886	4.438929081	4.446965694	H	11.373424530	4.811909676	1.375890255	H	11.536209106	5.023388863	1.371727109
N	12.408258438	2.428037882	2.707810402	N	9.321875572	4.442685127	4.444563866	N	8.487634659	4.684779167	4.597192764
N	11.227517128	5.091994286	2.349567652	N	12.417560577	2.436878443	2.703476906	N	12.686305046	2.215301514	2.727612734
				N	11.232964516	5.099125385	2.347425222	N	11.327293396	5.192405701	2.359288931
				N	6.398926258	5.818571091	4.703770638	N	6.615675926	5.202557564	5.148523808
Structure C				Structure D				Structure E			
Si	0.029900193	2.781871796	8.128196716	Si	0.088493943	2.789028883	8.063394547	Si	0.103443980	2.598400831	8.283793449
Si	7.804318905	0.997146428	3.039706230	Si	7.856783867	1.028435230	2.966660023	Si	7.922797203	0.800539851	3.217981577
Si	2.303669691	8.502574921	0.855787933	Si	2.368878365	8.517913818	0.796009600	Si	2.394852638	8.317947388	1.019172430
Si	5.392069817	8.612658501	1.102147698	Si	5.459936142	8.635662079	1.044549942	Si	5.516014576	8.429636002	1.256062984
Si	7.784955978	0.907568812	6.163419724	Si	7.841373444	0.947546005	6.089056492	Si	7.879184723	0.754233062	6.336932659
Si	-0.018209338	5.943210125	8.315381050	Si	0.035069227	5.955694199	8.264754295	Si	0.064849377	5.779713631	8.441279411
Si	0.020732254	8.252941132	6.210952282	Si	0.082627982	8.248436928	6.161039829	Si	0.122846663	8.068790436	6.310264587
Si	5.482818604	0.708108604	8.294873238	Si	5.543549061	0.694792151	8.231410980	Si	5.576695442	0.571571827	8.498324394
Si	2.365638971	0.683735669	8.117897987	Si	2.428148746	0.683794379	8.059189796	Si	2.425246239	0.484360099	8.297241211
Si	0.035294235	8.288537979	3.087779284	Si	0.106378451	8.291355133	3.038975239	Si	0.118214175	8.161410332	3.226610422
Si	7.876792431	3.274971247	0.882444620	Si	7.923561096	3.274873495	0.817738831	Si	7.917699337	3.133920431	1.057207108
Si	9.445979118	2.764671087	8.110436440	Si	9.505723000	2.794466972	8.027739525	Si	9.522748947	2.568040371	8.288021088
Si	17.150163651	0.986238599	3.057600975	Si	17.214017868	0.984745800	2.995972395	Si	17.370719910	0.856781542	3.221522570
Si	11.677577019	8.455774307	0.828654170	Si	11.714137077	8.505520821	0.783654273	Si	11.762069702	8.302596092	1.056973100
Si	14.767663002	8.655743599	1.158236623	Si	14.839547157	8.670214653	1.082170963	Si	14.877284050	8.518784523	1.276082397
Si	17.206672668	0.951356530	6.207890511	Si	17.273336411	0.966390252	6.145413876	Si	17.296205521	0.757620811	6.325635433
Si	9.394819260	5.929742336	8.267280579	Si	9.406698227	5.943984509	8.207329750	Si	9.495631218	5.741111279	8.491332054
Si	9.449309349	8.221694946	6.133737564	Si	9.506147385	8.257603645	6.068798065	Si	9.511697769	8.024484634	6.342342377
Si	14.875708580	0.750123501	8.330457687	Si	14.952070236	0.779672205	8.272455215	Si	14.973167419	0.542259097	8.442524910
Si	11.747802734	0.659275591	8.110320091	Si	11.810238838	0.689092994	8.022891998	Si	11.831549644	0.451329768	8.288577080
Si	9.391213417	8.230119705	3.033702135	Si	9.484243393	8.236116409	2.965137482	Si	9.515642166	8.124712944	3.243047237
Si	17.278350830	3.265042305	0.905071199	Si	17.347833633	3.275899172	0.845613778	Si	17.329345703	3.132835150	1.036930561

Al	7.723313808	6.462466240	1.060659647	Al	7.800745487	6.455641747	1.021685958	Si	-0.590847552	1.866508603	17.650913239
Al	17.094005585	6.425334454	1.020284176	Al	17.155876160	6.438167572	0.972688854	Si	7.240097523	0.048296750	12.588292122
O	1.474263310	2.043879747	8.219047546	O	1.531531096	2.043489456	8.122222900	Si	1.703048110	7.561120033	10.388338089
O	18.473268509	0.045809314	2.869754314	O	18.537441254	0.045331180	2.818430662	Si	4.839676380	7.674850464	10.651304245
O	8.013901711	2.434813261	2.297063112	O	8.145223618	2.444249392	2.214601278	Si	7.199184418	0.005538702	15.717638969
O	2.793022394	0.538094223	0.096823633	O	2.848926306	0.565056443	0.055493988	Si	-0.603231788	5.037919998	17.820571899
O	1.315354347	8.518439293	2.168212891	O	1.383101463	8.514847755	2.111214876	Si	-0.547788560	7.331662178	15.689272881
O	-0.130334809	3.191429138	0.114880875	O	-0.063891500	3.189123631	0.054031800	Si	4.871495247	-0.129451394	17.831502914
O	6.181468964	7.245570660	1.034604430	O	6.290740967	7.291400909	1.039342284	Si	1.745564580	-0.236337185	17.637390137
O	8.672338486	-0.471780509	6.222961903	O	8.736450195	-0.425618529	6.172063351	Si	-0.564061880	7.375542641	12.604829788
O	6.372809410	0.650337279	6.931296349	O	6.444426537	0.690676272	6.876168251	Si	7.244984627	2.354975462	10.438284874
O	8.038319588	6.153359413	9.067080498	O	7.960000992	6.064208508	8.872931480	Si	8.842542648	1.845905304	17.684421539
O	-0.032800615	6.793712616	6.909175396	O	-0.003604174	6.786446095	6.848771572	Si	16.697032928	0.095981300	12.593231201
O	4.822567463	8.660598755	9.036255836	O	4.880868912	8.632983208	8.943828583	Si	11.083312988	7.531321526	10.393725395
O	1.202232957	6.514676094	9.250593185	O	1.267627239	6.538713455	9.177541733	Si	14.180154800	7.765340328	10.634213448
O	18.024793625	2.210265398	6.838358879	O	18.067699432	2.240617514	6.773567677	Si	16.611774445	0.014933228	15.702773094
O	6.593291759	0.179556474	2.337502480	O	6.624074459	0.264005542	2.241774321	Si	8.769863129	5.007081032	17.827133179
O	6.067154884	1.838546753	9.291241646	O	6.106280804	1.808573961	9.260547638	Si	8.859681129	7.310242653	15.707915306
O	18.118488312	6.841592312	2.577928543	O	-0.664470851	6.851477146	2.528120756	Si	14.290815353	-0.160608649	17.817377090
O	1.863950610	-0.187162578	6.823769569	O	1.940837383	-0.215997964	6.780993938	Si	11.151473045	-0.252732635	17.681180954
O	0.387554109	8.007293701	4.629919052	O	0.454634964	8.005962372	4.582523823	Si	8.818206787	7.317611694	12.613140106
O	3.925934553	1.060533404	7.913859844	O	3.989172459	1.065363288	7.859071732	Si	16.649700165	2.359005928	10.406849861
O	7.487797737	4.763030052	1.228821635	O	7.489395618	4.759511471	1.128982186	Al	7.819621563	6.321098804	1.244905353
O	7.452307224	1.269999385	4.610695839	O	7.512917042	1.307518125	4.538617611	Al	17.377412796	6.282257080	1.277327538
O	3.801175594	8.331751823	1.404399157	O	3.871024609	8.336275101	1.323687196	Al	7.162600517	5.538650990	10.692020416
O	0.275531650	4.377082825	7.939350605	O	0.324845791	4.386440754	7.899493694	Al	16.669668198	5.513888359	10.633930206
O	10.925667763	2.053072691	8.244321823	O	10.984666824	2.080337048	8.167609215	O	1.568727255	1.875970006	8.417930603
O	9.234436035	0.227016449	2.931984186	O	9.244063377	0.178613216	2.887180567	O	0.005456865	0.197659492	3.167180538
O	17.423416138	2.362725496	2.263093710	O	17.479091644	2.359693050	2.194895267	O	7.929905415	2.182394028	2.372874737
O	12.234210014	0.529471636	0.107559055	O	11.570380211	-0.203212380	9.362278938	O	2.879973650	0.349009722	0.235179305
O	10.750994682	8.456944466	2.154468775	O	10.866440773	8.622508049	2.157258034	O	1.465752006	8.329364777	2.340161562
O	9.361030579	3.180081367	0.148047805	O	9.404646873	3.202002048	0.055008385	O	-0.051892072	3.044044256	0.281688690
O	15.667821884	7.343873978	1.184939981	O	15.715224266	7.341986179	1.110839128	O	6.231822968	7.027831078	0.980438828
O	18.088737488	-0.419222027	6.310670853	O	18.161338806	-0.399787247	6.263177872	O	8.059016228	8.773914337	6.475541592
O	15.777344704	0.720008731	6.963026524	O	15.841524124	0.741699278	6.898333549	O	6.469288349	0.563334823	7.147469997
O	17.419670105	6.122102737	9.075129509	O	17.478065491	6.149192810	9.030604362	O	8.146500587	5.949120045	9.319065094
O	9.429973602	6.771557808	6.853620052	O	9.517429352	6.828943253	6.831033230	O	0.080774724	6.618183136	7.044500351
O	14.990138054	-0.669890881	9.117084503	O	15.101519585	-0.631803036	9.063898087	O	5.039492130	8.552180290	9.282899857
O	10.670013428	6.495123386	9.170182228	O	10.590145111	6.503916740	9.223670959	O	1.306306839	6.322719574	9.394892693
O	8.638703346	2.110755444	6.858894825	O	8.715103149	2.164309025	6.751988411	O	18.112285614	2.004820824	7.010847569
O	15.835266113	0.240286455	2.443654537	O	15.897473335	0.230715930	2.389042139	O	6.803768158	-0.188356668	2.557863474
O	15.401559830	1.938971400	9.305799484	O	15.457673073	1.980155826	9.242655754	O	6.019149303	1.795622349	9.476752281
O	8.531538010	6.966316223	2.568951845	O	8.813408852	6.924409389	2.376092911	O	18.012975693	6.980975628	2.702341557
O	11.271256447	-0.198513478	6.814121246	O	11.342490196	-0.139118791	6.703734398	O	1.929674387	-0.374228358	7.020348549

O	9.924077988	8.055981636	4.581178665	O	9.977385521	8.049929619	4.524474144	O	0.562056839	7.870166779	4.769590855
O	13.332166672	1.023242235	7.878725052	O	13.401604652	1.038244963	7.833547592	O	3.998994350	0.840994179	8.135990143
O	16.905900955	4.753177166	1.351980209	O	16.997291565	4.764349937	1.303229809	O	7.555608273	4.624502659	1.434187293
O	16.884698868	1.274328709	4.637007236	O	16.943893433	1.278640985	4.574491501	O	7.521877289	1.078436375	4.781329155
O	13.203227043	8.287814140	1.373451710	O	13.265026093	8.327044487	1.237251997	O	3.925261021	8.166947365	1.494975328
O	9.706727982	4.355297089	7.908916950	O	9.781755447	4.384881973	7.836127758	O	0.365934432	4.195349693	8.114210129
O	9.640296936	3.874217987	4.232099056	O	6.017600060	4.357940674	7.266106606	O	10.982851028	1.830561638	8.405707359
O	6.554717541	4.611377716	6.372312069	Cu	12.240290642	2.027232885	3.360643148	O	9.421508789	0.169525385	3.173430681
Cu	12.488297462	2.126308680	3.308297634	H	6.558901310	5.094648838	7.615988255	O	17.380605698	2.252085686	2.408370256
H	9.048787117	4.354374409	4.860924721	H	5.491667747	4.075664520	8.034735680	O	12.336364746	0.354408890	0.306898594
H	7.427867889	6.253969193	3.898499012	H	-0.517395973	6.065629959	3.085869312	O	10.929132462	8.321471214	2.428110361
H	5.875002861	6.276739120	4.836895466	H	12.714947701	-0.117651299	4.377903461	O	9.374637604	2.997568369	0.296725363
H	9.000261307	3.459098101	3.616048336	H	14.103323936	0.437898636	3.661875725	O	15.634222984	6.992879868	1.111396313
H	-0.600330353	6.067261696	3.157372952	H	13.658393860	0.987499356	5.155946255	O	17.500528336	8.794415474	6.426871777
H	12.602232933	-0.103050843	4.317155838	H	10.459469795	3.733352423	3.104286909	O	15.884567261	0.504905283	7.102112770
H	14.103818893	0.345621824	3.776634932	H	11.760769844	4.176143169	2.206044912	O	17.500579834	5.967508793	9.195178986
H	13.531835556	0.910384893	5.223562241	H	10.728275299	3.020432234	1.661504865	O	9.469658852	6.581656933	7.086662292
H	11.013215065	4.001053333	3.074490547	N	6.644966602	6.305273056	4.782039642	O	14.435195923	8.487296104	9.212718010
H	12.341885567	4.314019680	2.088757753	N	13.298021317	0.715461493	4.236803532	O	10.794180870	6.300386429	9.372042656
H	11.158135414	3.287556410	1.583465934	N	11.207515717	3.368346214	2.505252123	O	8.718925476	2.002502918	6.979785919
N	6.824027538	5.927160740	4.670419216	N	5.616082191	6.467625141	4.388834953	O	16.257972717	-0.150825009	2.535358191
N	13.263401031	0.680369198	4.262351990					O	15.508081436	1.694065332	9.455292702
N	11.698222160	3.585485697	2.404367924					O	8.631802559	6.953074932	2.634254217
N	7.305613518	4.998450279	5.465461731					O	11.361520767	-0.430762142	7.017233372
								O	9.924253464	7.816081524	4.794208050
								O	13.418384552	0.814875424	8.090675354
								O	16.920726776	4.634794712	1.389381766
								O	16.943941116	1.113077164	4.775003433
								O	13.341905594	8.102813721	1.491052389
								O	9.781693459	4.163685799	8.141051292
								O	0.869552851	1.137289524	17.742271423
								O	-0.667989731	-0.579676628	12.543182373
								O	7.321647644	1.445871353	11.788598061
								O	2.157424212	-0.377319574	9.667330742
								O	0.799349427	7.585066319	11.736162186
								O	-0.721275866	2.291820765	9.667831421
								O	5.558794498	6.252296448	10.543885231
								O	7.349668503	7.984673977	15.814666748
								O	5.766506195	-0.229677439	16.464099884
								O	7.334833145	5.172314167	18.500282288
								O	-0.584985852	5.886337280	16.419971466
								O	4.297492504	7.872941017	18.637067795
								O	2.020155191	7.064175606	0.024733795
								O	17.425317764	1.272363544	16.359096527

		O	6.041445255	-0.875554740	11.964034081
		O	5.376565456	1.134490848	18.717947006
		O	17.351879120	6.196054935	12.051717758
		O	1.279318094	-1.084131956	16.324859619
		O	-0.122934639	7.090904236	14.141211510
		O	3.310713768	0.174362779	17.428783417
		O	6.863207340	3.840884686	10.837573051
		O	6.876394272	0.339967728	14.158023834
		O	3.236581326	7.397729874	10.858832359
		O	-0.319311559	3.460107803	17.441696167
		O	10.307548523	1.128341913	17.798013687
		O	8.693578720	-0.662245750	12.492641449
		O	16.804460526	1.506851673	11.798724174
		O	11.643891335	-0.411017716	9.664965630
		O	10.174515724	7.480918884	11.719181061
		O	8.662531853	2.209764957	9.630290031
		O	14.926988602	6.226560116	10.513902664
		O	16.828010559	8.056115150	15.786737442
		O	15.196914673	-0.237789869	16.468639374
		O	16.827182770	5.226246357	18.560567856
		O	8.813308716	5.850802898	16.412984848
		O	13.762897491	7.807005405	18.615690231
		O	11.367759705	7.075146198	0.057091448
		O	8.038363457	1.232547045	16.384290695
		O	15.589163780	-0.872790813	11.862378120
		O	16.177883148	2.520501614	0.047285683
		O	7.898204327	6.084501743	12.185411453
		O	10.641247749	-1.106467128	16.398481369
		O	9.290700912	7.126047611	14.164772034
		O	12.731734276	0.085447788	17.447649002
		O	16.223823547	3.859730244	10.749957085
		O	16.259965897	0.348310709	14.137495041
		O	12.648696899	7.379157066	10.909638405
		O	9.094875336	3.436594248	17.463418961
		O	3.290051460	3.674630165	14.435688019
		O	3.277391434	4.226616859	13.297183990
		Cu	2.704382896	2.965833664	11.278738976
		Cu	4.792230606	4.573827744	16.084466934
		H	14.992492676	6.261981010	1.017969131
		H	0.562126517	1.985247970	12.089053154
		H	1.663304329	0.802184045	11.895428658
		H	1.718308449	1.755298018	13.240267754
		H	3.188430786	4.272514820	9.271963120
		H	4.293913364	4.755646706	10.401496887

		H	4.480247498	3.307308197	9.652404785						
		H	14.275836945	5.503184319	10.423684120						
		H	4.108915806	4.421614170	18.415864944						
		H	2.943664312	3.646354675	17.507106781						
		H	4.353480339	2.880669117	17.883262634						
		H	5.094975471	5.948149681	14.028797150						
		H	6.185606956	6.399624348	15.181503296						
		H	6.461911201	5.081407547	14.242404938						
		N	1.553797960	1.766002893	12.229948997						
		N	3.768509626	3.937512398	10.046236038						
		N	3.953015804	3.786576271	17.604217529						
		N	5.725266457	5.584794998	14.750749588						
ts2			Structure F			Structure G ₁					
Si	0.106694162	2.597483158	8.224810600	Si	0.113241315	2.593125343	8.204197884	Si	0.128226638	2.641118765	8.094772339
Si	7.937908173	0.793786466	3.133752346	Si	7.947218418	0.788161516	3.104486704	Si	7.946493149	0.801704466	3.017874956
Si	2.409218550	8.295863152	0.936107814	Si	2.415416479	8.303355217	0.908805192	Si	2.397233725	8.312302589	0.805296600
Si	5.536020279	8.402371407	1.162328601	Si	5.542038918	8.399610519	1.123016596	Si	5.531002045	8.423707008	1.061376691
Si	7.868375301	0.770808220	6.253346920	Si	7.873417377	0.750676870	6.213153362	Si	7.891071320	0.785817981	6.142022133
Si	0.067876935	5.771604538	8.353042603	Si	0.056807995	5.770566940	8.324174881	Si	0.076604187	5.809980392	8.233421326
Si	0.112670511	8.068216324	6.250968933	Si	0.112224638	8.055803299	6.219524860	Si	0.171467364	8.115622520	6.119441032
Si	5.563955784	0.580065906	8.413232803	Si	5.563002586	0.535454333	8.368704796	Si	5.602866650	0.556346536	8.280424118
Si	2.423034668	0.496406496	8.248246193	Si	2.442788601	0.492925107	8.214029312	Si	2.457028866	0.535187900	8.093462944
Si	0.137524456	8.150234222	3.158304453	Si	0.148244321	8.140792847	3.131884575	Si	0.128920078	8.170985222	3.024592400
Si	7.953628063	3.111358404	0.968249619	Si	7.947379589	3.095934153	0.939974606	Si	7.939063072	3.109550953	0.857460380
Si	9.510586739	2.603721619	8.186212540	Si	9.521662712	2.586641312	8.139085770	Si	9.566884995	2.630340099	8.080398560
Si	17.409957886	0.859053552	3.133703709	Si	17.412963867	0.841201305	3.107761621	Si	17.388299942	0.875034511	3.019849300
Si	11.793038368	8.329089165	0.985493958	Si	11.794460297	8.318478584	0.949372888	Si	11.782958984	8.306073189	0.852016866
Si	14.902683258	8.525747299	1.184169054	Si	14.908071518	8.512533188	1.152361393	Si	14.895524979	8.542229652	1.084079027
Si	17.303506851	0.754037321	6.251039028	Si	17.316411972	0.753910780	6.224287510	Si	17.333702087	0.786118507	6.140125275
Si	9.488486290	5.762019634	8.412318230	Si	9.508689880	5.733061314	8.375016212	Si	9.479380608	5.749336243	8.275744438
Si	9.511271477	8.036360741	6.260894299	Si	9.520967484	8.023528099	6.218262196	Si	9.523633957	8.059145927	6.152462006
Si	14.965813637	0.592549384	8.355075836	Si	14.971373558	0.592093468	8.330510139	Si	14.999795914	0.604071796	8.238597870
Si	11.820369720	0.474431634	8.202391624	Si	11.824993134	0.454895496	8.152552605	Si	11.861186028	0.485492289	8.089511871
Si	9.525467873	8.118865967	3.158879995	Si	9.538092613	8.105528831	3.124526739	Si	9.530060768	8.101061821	3.047591925
Si	17.350719452	3.133299828	0.961270511	Si	17.357740402	3.124644279	0.931625724	Si	17.329345703	3.150425673	0.832915068
Si	-0.564164758	1.857651830	17.559371948	Si	-0.552854180	1.854959130	17.536731720	Si	-0.580240369	1.878293157	17.449512482
Si	7.239815235	0.086025476	12.499363899	Si	7.229901314	0.065305591	12.451583862	Si	7.235713959	0.081463337	12.368268967
Si	1.705144286	7.554397583	10.320032120	Si	1.721071720	7.545156956	10.289898872	Si	1.692588091	7.613454819	10.201472282
Si	4.829402924	7.708210468	10.581076622	Si	4.830380917	7.682846069	10.532166481	Si	4.825019360	7.724443436	10.447197914
Si	7.209879398	0.025722980	15.633751869	Si	7.226425171	0.018418312	15.580004692	Si	7.192201614	0.016291857	15.502179146
Si	-0.569905400	5.027551651	17.740854263	Si	-0.564493299	5.022153854	17.704174042	Si	-0.586724043	5.049484253	17.609718323
Si	-0.549661696	7.326689243	15.606463432	Si	-0.555797875	7.311682701	15.576679230	Si	-0.567999125	7.353032112	15.474547386
Si	4.893218040	-0.168289423	17.741111755	Si	4.894790649	-0.162182927	17.711082458	Si	4.877260685	-0.163268089	17.618471146
Si	1.748484373	-0.258075356	17.563072205	Si	1.756175280	-0.270345449	17.531803131	Si	1.726903200	-0.234766960	17.436134338

Si	-0.576682329	7.394970417	12.514463425	Si	-0.576653719	7.409580231	12.474743843	Si	-0.563954473	7.450529575	12.388135910
Si	7.239632130	2.384180784	10.350333214	Si	7.249102592	2.339396000	10.311308861	Si	7.301686764	2.375377893	10.245471954
Si	8.855426788	1.850215316	17.601015091	Si	8.862140656	1.834150791	17.548059464	Si	8.846595764	1.842698216	17.473157883
Si	16.703880310	0.103832006	12.498600960	Si	16.704177856	0.103978157	12.472882271	Si	16.683654785	0.145553112	12.391880035
Si	11.076328278	7.574176788	10.310716629	Si	11.079271317	7.550794601	10.275579453	Si	11.090295792	7.580374718	10.207017899
Si	14.186120987	7.787565231	10.535910606	Si	14.186339378	7.788449287	10.525035858	Si	14.193573952	7.804065704	10.445842743
Si	16.636325836	0.021370173	15.613367081	Si	16.642787933	0.022575736	15.593620300	Si	16.612094879	0.037890792	15.495829582
Si	8.803726196	5.018331528	17.749828339	Si	8.794048309	5.006546974	17.699726105	Si	8.795968056	5.006505966	17.631212234
Si	8.881694794	7.311154366	15.633065224	Si	8.884945869	7.303489685	15.586955070	Si	8.846879959	7.303496838	15.498205185
Si	14.309076309	-0.150583982	17.736642838	Si	14.312335968	-0.148643732	17.706340790	Si	14.294858932	-0.141280293	17.618480682
Si	11.183762550	-0.259342670	17.603242874	Si	11.186641693	-0.264586329	17.568750381	Si	11.155950546	-0.266466141	17.473760605
Si	8.823513985	7.332177162	12.532730103	Si	8.835038185	7.281357288	12.493397713	Si	8.847088814	7.272201061	12.392849922
Si	16.632654190	2.387267113	10.331003189	Si	16.622945786	2.388369083	10.299373627	Si	16.658006668	2.417485952	10.195950508
Al	7.829640388	6.303870201	1.152297020	Al	7.831493855	6.287640095	1.121918559	Al	7.829224110	6.288525581	1.089177847
Al	17.407335281	6.282106400	1.216091633	Al	17.412393570	6.269189358	1.186265707	Al	17.397415161	6.296235561	1.085725665
Al	7.163201809	5.551698685	10.626437187	Al	7.182383060	5.512547493	10.589039803	Al	7.162284851	5.516471863	10.492659569
Al	16.652452469	5.536844730	10.532628059	Al	16.645788193	5.539740562	10.514643669	Al	16.688165665	5.564106941	10.393072128
O	1.571708322	1.883780122	8.390739441	O	1.578478575	1.873624325	8.386984825	O	1.586040139	1.908100009	8.221147537
O	0.039375544	0.190554768	3.051134586	O	0.046026111	0.179240450	3.029484749	O	0.014113888	0.201763049	2.908282280
O	7.952309132	2.182583332	2.298901320	O	7.981773853	2.182163477	2.280243635	O	7.974298477	2.192343950	2.189173222
O	2.859741449	0.326294780	0.158391878	O	2.885604620	0.346204817	0.149739340	O	2.853516340	0.337879390	0.022357360
O	1.483441472	8.261923790	2.257719994	O	1.495098233	8.263703346	2.232272148	O	1.478452802	8.296955109	2.127908230
O	-0.050139859	3.035058498	0.173559695	O	-0.034978785	3.037947416	0.154716760	O	-0.056000847	3.060310841	0.071415260
O	6.230302334	6.987275124	0.876952469	O	6.235814095	6.982285500	0.852227509	O	6.250434875	7.015061855	0.806821048
O	8.072576523	8.807763100	6.396052837	O	8.075532913	8.784996033	6.335914612	O	8.076784134	8.813302040	6.274371147
O	6.458961487	0.557099700	7.061024189	O	6.474812031	0.531201184	7.028455734	O	6.462144852	0.567194879	6.904998302
O	8.143157005	5.944857121	9.248106956	O	8.152329445	5.881721973	9.194132805	O	8.082893372	5.816633224	9.044730186
O	0.092221141	6.600113392	6.949682236	O	0.070691764	6.585825443	6.910110474	O	0.147078335	6.663877487	6.845356941
O	5.002180099	8.552235603	9.189438820	O	4.937840939	8.483824730	9.105887413	O	5.026134014	8.504937172	9.019078255
O	1.302848339	6.334799767	9.308573723	O	1.286023617	6.358703613	9.262508392	O	1.254816413	6.362337589	9.254009247
O	18.144081116	1.979459286	6.942856312	O	-0.676182687	1.977106810	6.910648346	O	18.138198853	2.036224127	6.820571423
O	6.152285099	9.188909531	2.449599743	O	6.159743786	9.204746246	2.392273188	O	6.805514812	-0.160552710	2.344239235
O	6.020084858	1.786080599	9.407669067	O	6.044710159	1.684205055	9.406420708	O	6.143222809	1.692855954	9.307468414
O	18.017530441	6.971704006	2.657317162	O	18.036653519	6.957965851	2.622135162	O	18.024934769	6.981111050	2.520080805
O	1.897648811	-0.373180360	6.991676807	O	1.883104324	-0.387915134	6.982567310	O	1.996265531	-0.321107805	6.797049522
O	0.571257949	7.904628754	4.711052418	O	0.592476010	7.897479534	4.682855129	O	0.579496562	7.921881676	4.566991806
O	3.990329742	0.862185895	8.043936729	O	4.002629757	0.866462946	7.975359440	O	4.036131859	0.907785594	7.965703487
O	7.569894314	4.605485916	1.305368781	O	7.587290764	4.592288017	1.294600964	O	7.521044254	4.596107960	1.200231075
O	7.516455650	1.071394086	4.690182209	O	7.502732754	1.057514429	4.653627872	O	7.563891888	1.101795673	4.576336384
O	3.942631245	8.177333832	1.417220116	O	3.952066422	8.167219162	1.379840136	O	3.937601089	8.190359116	1.274438739
O	0.380367041	4.190804958	8.034775734	O	0.375045955	4.187730789	8.020207405	O	0.390149653	4.234580040	7.895515442
O	10.960966110	1.849562526	8.285571098	O	10.968607903	1.829269767	8.255583763	O	11.003133774	1.859054804	8.199783325
O	9.436562538	0.166591883	3.093045950	O	9.440736771	0.148937359	3.074465036	O	9.426925659	0.137325943	2.929950476
O	17.433361053	2.264491796	2.338132858	O	17.434122086	2.236882210	2.295861483	O	17.391357422	2.267579317	2.199330091

O	12.385639191	0.399222583	0.267135262	O	12.398277283	0.387989432	0.231260866	O	12.335880280	0.361000717	0.113763750
O	10.939471245	8.310719490	2.344240189	O	10.953097343	8.315048218	2.316690445	O	10.930792809	8.280849457	2.210024834
O	9.425814629	2.988379955	0.235637516	O	9.384381294	2.947710037	0.148018703	O	9.392908096	2.998040438	0.097540982
O	15.665347099	7.000287533	1.033481121	O	15.671476364	6.988554001	0.983505487	O	15.653676987	7.016803265	0.926737964
O	17.473955154	8.765772820	6.359292984	O	17.478887558	8.761333466	6.319530010	O	17.540010452	8.821910858	6.247086525
O	15.870876312	0.555324495	7.006906033	O	15.893105507	0.546241403	6.993683815	O	15.908634186	0.533039808	6.894815922
O	17.495105743	5.959025383	9.091143608	O	17.488378525	5.956471920	9.073261261	O	17.475971222	5.983453274	8.922439575
O	9.433494568	6.601284981	7.011949062	O	9.464722633	6.602133274	6.991835117	O	9.446343422	6.623158455	6.893806934
O	14.451212883	8.545464516	9.134867668	O	14.459527016	8.557749748	9.132142067	O	14.461838722	8.574045181	9.052978516
O	10.781217575	6.346975327	9.282412529	O	10.794085503	6.304677963	9.267713547	O	10.718181610	6.354091167	9.207145691
O	8.684234619	2.041185856	6.887460709	O	8.697238922	2.017177582	6.842280388	O	8.710231781	2.030123711	6.819457531
O	16.287425995	-0.129048631	2.431726217	O	16.299077988	-0.164515242	2.412039280	O	16.249998093	-0.123188183	2.354157686
O	15.483797073	1.758025169	9.356589317	O	15.473131180	1.779499531	9.313120842	O	15.518523216	1.795486212	9.203223228
O	8.638201714	6.957601547	2.532434702	O	8.660566330	6.946527958	2.479652405	O	8.648974419	6.901648998	2.475888252
O	11.371075630	-0.434476346	6.938610554	O	11.379152298	-0.425513387	6.867296219	O	11.375591278	-0.408719897	6.830690861
O	9.922552109	7.804679394	4.712054729	O	9.925656319	7.765242577	4.671869278	O	9.940836906	7.847593784	4.603457928
O	13.404783249	0.845233917	8.008800507	O	13.410672188	0.827745736	7.975037098	O	13.440027237	0.854311585	7.874348640
O	16.939668655	4.635949612	1.310109019	O	16.948743820	4.624336243	1.294147015	O	16.921968460	4.653570175	1.181227207
O	16.991600037	1.107097745	4.689843178	O	16.998516083	1.107402086	4.662929058	O	17.001066208	1.134479403	4.579393387
O	13.368126869	8.107819557	1.422741055	O	13.372585297	8.082330704	1.373418927	O	13.358427048	8.117926598	1.289565086
O	9.798453331	4.194105148	8.038704872	O	9.824379921	4.171925068	7.977374077	O	9.878758430	4.207892418	7.865920067
O	0.896703482	1.128858447	17.681755066	O	0.906049967	1.118632913	17.636936188	O	0.890048265	1.159795642	17.573902130
O	-0.642093778	-0.538712502	12.441525459	O	-0.631873965	-0.516762614	12.394734383	O	-0.676254988	-0.513199270	12.352249146
O	7.344827652	1.491423368	11.711544037	O	7.409752846	1.482135534	11.692032814	O	7.442642689	1.504338741	11.626441956
O	2.192784548	-0.360625535	9.633696556	O	2.277611732	-0.349277526	9.621146202	O	2.197810650	-0.339559019	9.449608803
O	0.806138873	7.552328587	11.670175552	O	0.805817723	7.548768044	11.627981186	O	0.823604763	7.701240063	11.572072029
O	-0.741094172	2.310179949	9.594202042	O	-0.752460480	2.292535782	9.559769630	O	-0.711612046	2.338850975	9.467580795
O	5.575672150	6.301169395	10.510445595	O	5.638576984	6.321399689	10.496237755	O	5.638005257	6.367874146	10.503013611
O	7.414276123	8.053325653	15.766417503	O	7.406129837	8.028156281	15.707601547	O	7.364119530	8.022976875	15.605816841
O	5.769065857	-0.269083142	16.361009598	O	5.797645569	-0.226870656	16.351665497	O	5.751709938	-0.250817180	16.238830566
O	7.357085705	5.166749477	18.412631989	O	7.330241680	5.147029877	18.352987289	O	7.359009743	5.163883209	18.337728500
O	-0.576953948	5.889139175	16.351175308	O	-0.588308990	5.857060432	16.295480728	O	-0.568722844	5.911276817	16.218591690
O	4.333792686	7.816851139	18.520029068	O	4.340986729	7.800919533	18.464260101	O	4.342903137	7.811023712	18.392105103
O	0.694468737	5.561594486	18.653621674	O	0.693179727	5.584266663	18.611600876	O	0.679470778	5.574862480	18.529697418
O	-1.356885910	1.267178535	16.247766495	O	-1.357488275	1.272162318	16.232467651	O	17.453054428	1.272758365	16.160781860
O	6.007893085	-0.788749814	11.867121696	O	5.969542503	-0.733410358	11.777253151	O	5.913779736	-0.647721887	11.707350731
O	5.430171490	1.080572724	18.625305176	O	5.373099327	1.070194483	18.647054672	O	5.401927948	1.059355617	18.540893555
O	17.314659119	6.249437809	11.941432953	O	17.299585342	6.264433384	11.923292160	O	17.378877640	6.272796631	11.792701721
O	1.285113215	-1.085719943	16.235208511	O	1.287425756	-1.131700516	16.232933044	O	1.253748775	-1.042695642	16.105119705
O	-0.148050487	7.089566231	14.053271294	O	-0.154223979	7.116622448	14.018639565	O	-0.141300261	7.128744602	13.929773331
O	3.324185610	0.129692435	17.373590469	O	3.330535889	0.111334801	17.320257187	O	3.311993599	0.114506483	17.247364044
O	6.807430744	3.860154867	10.740600586	O	6.759820938	3.816093683	10.673484802	O	6.740530014	3.819334984	10.658484459
O	6.882756233	0.368342400	14.076111794	O	6.869529247	0.349369645	14.028522491	O	6.855877876	0.362702608	13.943284035
O	3.235599995	7.391419888	10.806206703	O	3.243031502	7.304073811	10.781355858	O	3.231711626	7.445758820	10.668627739

O	-0.286229730	3.450641155	17.369173050	O	-0.247726560	3.444938660	17.352821350	O	-0.304531574	3.470864773	17.239812851
O	10.308473587	1.106181622	17.649835587	O	10.320844650	1.106264830	17.641124725	O	10.304542542	1.114464045	17.567378998
O	8.672715187	-0.660169423	12.400875092	O	8.622446060	-0.749595165	12.362064362	O	8.576639175	-0.795723498	12.250130653
O	16.733732224	1.511430383	11.706428528	O	16.701169968	1.504097462	11.670870781	O	16.708610535	1.535552740	11.570332527
O	11.617459297	-0.359522909	9.597457886	O	11.605671883	-0.404429734	9.526399612	O	11.673565865	-0.363577336	9.472350121
O	10.184858322	7.518085003	11.649194717	O	10.191425323	7.524924755	11.614081383	O	10.209811211	7.606663227	11.555350304
O	8.660017967	2.276441097	9.543103218	O	8.662128448	2.270537138	9.491073608	O	8.734530449	2.380562305	9.469331741
O	14.906842232	6.239939213	10.371016502	O	14.899803162	6.239479542	10.351051331	O	14.942222595	6.272195816	10.289994240
O	16.826570511	8.046220779	15.717903137	O	16.828594208	8.045096397	15.713972092	O	16.802068710	8.059342384	15.591176987
O	15.224949837	-0.194601893	16.395645142	O	15.225328445	-0.193767548	16.364011765	O	15.197860718	-0.198477626	16.270811081
O	16.881549835	5.222061157	18.514337540	O	16.887655258	5.201504230	18.481771469	O	16.858655930	5.245162964	18.374994278
O	8.795951843	5.831712723	16.313585281	O	8.802758217	5.832704544	16.280218124	O	8.763782501	5.847136974	16.220363617
O	13.764805794	7.797832489	18.508123398	O	13.774901390	7.807058334	18.490200043	O	13.778925896	7.828189373	18.421091080
O	10.016311646	5.644015312	18.681707382	O	9.983370781	5.637030602	18.656145096	O	10.018361092	5.601824760	18.564880371
O	7.976725578	1.292631865	16.322057724	O	8.046128273	1.268506289	16.236171722	O	7.997295380	1.256968498	16.187770844
O	15.618625641	-0.909473956	11.785571098	O	15.616722107	-0.922062099	11.784331322	O	15.583271027	-0.872580826	11.707226753
O	14.805905342	1.022749782	18.730657578	O	14.813037872	1.032415032	18.688987732	O	14.786799431	1.056085587	18.586744308
O	7.933036327	6.082605362	12.100214005	O	8.020181656	5.987713814	12.048152924	O	8.100772858	5.959792137	11.896684647
O	10.710274696	-1.188771844	16.363439560	O	10.700708389	-1.178861737	16.322439194	O	10.649750710	-1.147175789	16.210008621
O	9.302141190	7.159924507	14.086485863	O	9.328165054	7.146249294	14.048101425	O	9.286062241	7.124215126	13.960111618
O	12.753911018	0.112421155	17.358949661	O	12.757448196	0.107585549	17.328380585	O	12.730607986	0.087194443	17.246026993
O	16.219341278	3.887130022	10.689424515	O	16.227437973	3.887919426	10.677346230	O	16.238080978	3.917217016	10.550428391
O	16.285360336	0.352379322	14.051894188	O	16.306318283	0.354034305	14.030524254	O	16.257785797	0.398842931	13.944767952
O	12.647543907	7.426881790	10.806349754	O	12.647655487	7.426705837	10.788224220	O	12.659776688	7.386276722	10.687293053
O	9.134634972	3.443519115	17.411218643	O	9.134243011	3.431138992	17.389465332	O	9.111384392	3.436614990	17.276901245
O	2.696560144	3.226141691	14.775447845	O	3.081777096	3.240716934	14.567228317	O	3.837025881	2.431928635	15.138590813
O	3.326148987	3.873257875	13.724428177	O	3.844632149	4.378922462	13.978012085	O	4.393550873	4.417146683	13.832491875
Cu	3.161737442	2.930607080	11.956857681	Cu	3.286572933	3.106550217	12.652004242	O	2.655309916	5.186351299	12.747518539
Cu	4.081342697	4.142196655	15.638825417	Cu	4.065319538	4.253757954	15.878425598	Cu	3.977373362	2.610248327	13.369050980
H	15.027420044	6.267464638	0.931690276	H	15.033161163	6.257522106	0.870008051	Cu	4.372308731	4.005626202	15.928092003
H	1.457206845	1.502439737	13.119847298	H	1.451747894	1.322467923	12.613059044	H	15.014687538	6.283439636	0.835165977
H	1.961287022	0.714506209	11.760776520	H	2.374992371	1.054576159	11.287817955	H	3.679183483	0.430699468	14.248449326
H	2.891981363	0.707924843	13.120175362	H	2.919773340	0.614561677	12.768566132	H	2.748938084	0.439462066	12.860313416
H	3.054193020	4.246270657	9.832874298	H	3.379810810	3.466392279	10.106935501	H	4.394722462	0.177750230	12.743769646
H	4.338139534	4.857056141	10.676709175	H	3.689571381	4.879946232	10.898289680	H	4.086626053	2.131636858	10.851490974
H	4.475221157	3.407947302	9.942801476	H	4.866920471	3.755699635	10.793510437	H	3.411014318	3.606493950	11.147594452
H	14.253443718	5.521830559	10.262949944	H	14.242722511	5.526715279	10.231452942	H	5.066555023	3.409589291	11.236611366
H	4.073069572	4.414710045	18.231063843	H	3.864486933	4.260048866	18.404851913	H	14.296528816	5.543577194	10.205929756
H	2.772927999	3.516114235	17.704916000	H	2.605376720	3.374805927	17.749830246	H	3.901818752	4.230707645	18.434398651
H	4.262973785	2.829550028	17.828485489	H	4.104782581	2.708631039	17.911352158	H	2.711328506	3.289732933	17.698762894
H	5.790555000	5.807978630	14.735356331	H	5.810178280	6.041721821	15.480439186	H	4.199287415	2.647917271	18.043502808
H	5.454203129	6.175723076	16.304994583	H	4.863076687	6.489374638	16.748514175	H	5.688964844	6.146717548	15.588694572
H	6.473117828	4.964954376	15.965581894	H	6.060271263	5.409093380	16.991743088	H	4.723457813	6.355834007	16.902639389
N	2.278985023	1.293802023	12.546262741	N	2.417273283	1.356069088	12.269766808	H	6.089525223	5.480405807	17.050888062

N	3.811258316	3.987384319	10.473430634	N	3.839700222	3.863977909	10.930364609	N	3.659497261	0.694377303	13.256405830
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								N	5.296250820	5.666070938	16.402057648
								N	3.588595152	5.448295593	13.457756996
Structure H ₁				ts3				Structure I ₁			
Si	0.157690704	2.565630674	8.170241356	Si	0.154412985	2.559951067	8.149262428	Si	0.141878605	2.580595493	8.096383095
Si	7.986646175	0.754931152	3.076496601	Si	7.986307621	0.788917005	3.065004587	Si	7.973525047	0.769697309	3.051326752
Si	2.459908247	8.268571854	0.886128843	Si	2.444466829	8.296120644	0.860471725	Si	2.436295986	8.252837181	0.839507639
Si	5.544376850	8.347889900	1.134786606	Si	5.565512657	8.412755966	1.101354837	Si	5.570170879	8.383524895	1.089719772
Si	7.917828083	0.702827096	6.199248314	Si	7.923014641	0.726911902	6.189762115	Si	7.937303066	0.746677279	6.175219536
Si	0.124524236	5.733038902	8.283512115	Si	0.120779753	5.729834080	8.275326729	Si	0.124927580	5.748226643	8.256151199
Si	0.191374093	8.026612282	6.186892986	Si	0.162862718	8.031441689	6.160737991	Si	0.180006117	8.036613464	6.137929916
Si	5.612789631	0.491305828	8.347272873	Si	5.602289677	0.488413036	8.312781334	Si	5.615972996	0.564545453	8.317337036
Si	2.504199028	0.456802487	8.181244850	Si	2.489707947	0.460075021	8.125188828	Si	2.483977318	0.460790396	8.088500023
Si	0.159189090	8.107214928	3.102379322	Si	0.167114630	8.123444557	3.067311287	Si	0.151607513	8.078193665	3.039926767
Si	8.000976563	3.040209532	0.911744118	Si	7.978414536	3.075532198	0.904453874	Si	7.980780125	3.057545185	0.896758974
Si	9.574583054	2.548782587	8.128276825	Si	9.574945450	2.566618443	8.126190186	Si	9.571424484	2.563745499	8.118916512
Si	17.418716431	0.806806326	3.087736368	Si	17.421163559	0.815734386	3.064358473	Si	17.421371460	0.786200106	3.027476072
Si	11.820770264	8.247288704	0.913116574	Si	11.817389488	8.269162178	0.905569911	Si	11.811656952	8.273587227	0.890608430
Si	14.939582825	8.468750000	1.129404545	Si	14.932030678	8.481714249	1.109522581	Si	14.923753738	8.461726189	1.085435987
Si	17.372282028	0.730538726	6.201564312	Si	17.353466034	0.714450002	6.183293343	Si	17.335550308	0.719167948	6.154577255
Si	9.541790962	5.681144714	8.335585594	Si	9.534123421	5.700987816	8.324247360	Si	9.536041260	5.725536346	8.323762894
Si	9.565092087	7.979983807	6.186958313	Si	9.561095238	8.003641129	6.188625336	Si	9.558735847	8.013797760	6.191479206
Si	15.018927574	0.568696260	8.301446915	Si	15.013397217	0.553149164	8.287512779	Si	15.020861626	0.538515866	8.249281883
Si	11.890657425	0.417873979	8.101305962	Si	11.881127357	0.435095310	8.118272781	Si	11.882821083	0.449323416	8.131734848
Si	9.578433990	8.042692184	3.080967188	Si	9.577386856	8.061132431	3.080189466	Si	9.584230423	8.066582680	3.080217838
Si	17.386241913	3.090184927	0.900618792	Si	17.370754242	3.098549843	0.882937908	Si	17.365978241	3.082933426	0.859046102
Si	-0.517113328	1.836229444	17.515098572	Si	-0.534533620	1.851226211	17.488000870	Si	-0.530030727	1.832558393	17.478374481
Si	7.257201195	0.004977703	12.432049751	Si	7.254605770	0.021915674	12.388816833	Si	7.286270142	0.040066600	12.403183937
Si	1.768718243	7.517705441	10.271579742	Si	1.752340317	7.508475780	10.233528137	Si	1.745842695	7.556741714	10.204482079
Si	4.864164829	7.653110504	10.522834778	Si	4.854580879	7.661042213	10.482196808	Si	4.880036831	7.665311337	10.445102692
Si	7.273432732	-0.090577841	15.584084511	Si	7.251410484	-0.040876746	15.550387383	Si	7.224463940	-0.028978586	15.534107208
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Si	-0.512333512	7.304365635	15.553194046	Si	-0.520141065	7.314757347	15.534622192	Si	-0.508226812	7.298828125	15.513729095
Si	4.925330639	-0.235197902	17.695184708	Si	4.914133549	-0.190228701	17.665296555	Si	4.920918465	-0.228766561	17.676895142
Si	1.816471696	-0.288259864	17.501432419	Si	1.785797358	-0.268366456	17.485660553	Si	1.772177219	-0.305483818	17.485973358
Si	-0.526197433	7.399819374	12.443095207	Si	-0.529246092	7.398970127	12.424757957	Si	-0.526398003	7.387313843	12.411131859
Si	7.311164379	2.296704769	10.311795235	Si	7.290243626	2.303526640	10.281044006	Si	7.277621269	2.344069719	10.271551132
Si	8.912342072	1.760564446	17.529302597	Si	8.893909454	1.796867490	17.502773285	Si	8.879602432	1.793923378	17.489984512
Si	16.731750488	0.089083254	12.446344376	Si	16.739351273	0.086137295	12.426929474	Si	16.754884720	0.090776086	12.411956787
Si	11.135545731	7.516611576	10.241235733	Si	11.129720688	7.522865772	10.247166634	Si	11.132381439	7.533594131	10.245993614
Si	14.229578018	7.763235092	10.507335663	Si	14.230512619	7.754325867	10.483962059	Si	14.229035378	7.763610840	10.475517273
Si	16.679611206	0.009841323	15.570734024	Si	16.665510178	0.004511833	15.554565430	Si	16.670875549	-0.000035524	15.537531853

Si	8.827304840	4.935642719	17.656978607	Si	8.822122574	4.957914352	17.661197662	Si	8.809885979	4.956295967	17.652133942
Si	8.937134743	7.229304314	15.543010712	Si	8.884717941	7.261359215	15.544413567	Si	8.872364044	7.259376526	15.535717964
Si	14.358773232	-0.203181386	17.678356171	Si	14.335813522	-0.192801833	17.656650543	Si	14.331473351	-0.204102159	17.632734299
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Si	8.889410973	7.216984749	12.433641434	Si	8.863355637	7.236431122	12.411705017	Si	8.858989716	7.315596581	12.431436539
Si	16.656608582	2.371224642	10.266867638	Si	16.670911789	2.359625816	10.257042885	Si	16.695293427	2.361489773	10.222071648
Al	7.878773689	6.233063698	1.068233132	Al	7.868164063	6.252653599	1.099824667	Al	7.888721943	6.236546516	1.116415977
Al	17.445478439	6.230118275	1.169661045	Al	17.435907364	6.233434677	1.120150447	Al	17.429100037	6.209265709	1.100070238
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Al	16.721336365	5.512806416	10.474520683	Al	16.720029831	5.507710457	10.465997696	Al	16.709796906	5.507758141	10.449882507
O	1.606045008	1.813988209	8.341614723	O	1.617011070	1.833590865	8.332128525	O	1.594958782	1.834095478	8.211822510
O	0.048063636	0.138771176	3.018490791	O	0.052849978	0.154461443	2.982493401	O	0.049400046	0.116053089	2.935514212
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O	3.008180380	0.316466808	0.123287350	O	2.936116695	0.336251140	0.098865300	O	2.868632793	0.284139514	0.084024534
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O	6.507232666	0.473989725	6.995037556	O	6.502090931	0.495746851	6.964163303	O	6.519952297	0.580228329	6.973503590
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O	0.139592826	6.550483704	6.868112564	O	0.159285665	6.575169086	6.879099369	O	0.128627777	6.580832481	6.855785847
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O	16.965112686	4.587177277	1.264977217	O	16.947057724	4.594130516	1.251946330	O	16.929754257	4.574281216	1.228310704
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O	-0.127857625	7.123054981	13.995265007	O	-0.128794014	7.144058704	13.978064537	O	-0.115908146	7.103146553	13.955572128
O	3.381875038	0.138142347	17.273454666	O	3.356685162	0.129476905	17.287242889	O	3.348910332	0.072975159	17.353824615
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O	16.883562088	8.047971725	15.713246346	O	16.863466263	8.039159775	15.707231522	O	16.881366730	8.041914940	15.666430473
O	15.264685631	-0.246436477	16.333755493	O	15.238842010	-0.220423818	16.308055878	O	15.243556023	-0.247763276	16.288246155
O	16.937431335	5.176232815	18.475164413	O	16.910383224	5.153952599	18.409961700	O	16.914373398	5.146432400	18.403226852
O	8.889449120	5.755626202	16.234584808	O	8.841832161	5.793872356	16.249425888	O	8.811035156	5.791010857	16.240568161
O	13.839616776	7.759928226	18.472316742	O	13.813565254	7.765984535	18.444849014	O	13.803378105	7.757880688	18.427818298
O	9.994326591	5.542263031	18.657958984	O	9.998194695	5.562432289	18.649160385	O	9.986886024	5.575313568	18.627576828
O	8.107778549	1.145495534	16.236385345	O	8.078931808	1.205892682	16.204307556	O	8.033646584	1.229224324	16.198112488
O	15.619515419	-0.926389873	11.776029587	O	15.633708000	-0.919620097	11.735916138	O	15.643469810	-0.903672099	11.717457771
O	14.854433060	0.990162492	18.649389267	O	14.834125519	0.985474110	18.644477844	O	14.833055496	0.979299545	18.611980438
O	8.160645485	5.877761364	11.975873947	O	8.122718811	5.910780907	11.933556557	O	7.968234539	6.097036839	11.932290077
O	10.736894608	-1.219298959	16.259880066	O	10.706776619	-1.191853046	16.237998962	O	10.702566147	-1.212887645	16.241430283
O	9.358185768	7.110720634	13.993397713	O	9.274999619	7.123951912	13.989422798	O	9.295410156	7.093825340	13.991868973
O	12.802568436	0.028904438	17.295513153	O	12.778420448	0.047817826	17.279155731	O	12.774398804	0.042909741	17.257284164
O	16.255163193	3.871109247	10.640014648	O	16.259872437	3.861316204	10.610188484	O	16.256698608	3.855204582	10.575916290
O	16.349664688	0.341191411	14.008551598	O	16.342674255	0.314960241	13.987218857	O	16.355655670	0.334612370	13.968648911
O	12.697165489	7.354255199	10.753611565	O	12.698159218	7.351940155	10.738615036	O	12.701000214	7.366395950	10.748070717
O	9.158030510	3.360220194	17.346004486	O	9.168089867	3.391542912	17.323102951	O	9.160457611	3.389821768	17.317071915
O	3.419155598	2.625018597	14.784612656	O	3.255440235	2.496142387	15.141964912	O	3.052519321	2.136080980	15.367260933
O	3.858996868	4.872868061	13.808044434	O	3.787655830	4.759634972	13.643229485	O	3.558753252	5.399379253	12.833864212
O	1.912453890	5.047742844	12.929388046	O	1.761515975	4.911731720	12.983296394	O	1.831581116	4.365546227	13.446640015
O	5.349241734	2.310561180	15.653528214	O	5.345645428	2.670404911	14.728036880	O	4.681835175	2.973093510	14.327753067
Cu	3.507591724	3.104664803	12.786688805	Cu	3.352058172	3.166862965	12.486997604	Cu	2.782019377	3.836768389	11.758883476
Cu	4.057523727	4.320100307	15.795119286	Cu	4.180913448	3.977098465	16.102079391	Cu	4.164439678	3.622136116	16.183683395
H	15.070737839	6.212933540	0.882529914	H	15.056666374	6.226898670	0.869918764	H	15.060294151	6.210575581	0.827013850
H	2.790054560	0.677224994	13.009591103	H	2.118809223	1.004640341	12.804940224	H	1.555800438	1.753422022	12.433420181
H	2.758248806	0.989921689	11.395278931	H	2.027525425	1.302433729	11.190746307	H	0.896117926	2.228268385	10.993851662
H	4.188611507	0.694550097	12.156795502	H	3.420381069	0.727252305	11.850726128	H	2.287530661	1.372705936	11.012315750
H	3.471057177	3.342577457	10.230289459	H	3.381340027	3.554211140	9.949062347	H	3.191884041	4.031538010	9.274621010
H	3.735444069	4.813724518	10.932100296	H	3.811941624	4.937481880	10.757737160	H	4.403497219	4.808230400	10.131905556
H	4.980138302	3.735426664	10.836653709	H	4.917432785	3.732388258	10.614765167	H	4.452078819	3.171259880	9.913695335
H	14.338412285	5.507515907	10.235764503	H	14.335924149	5.498112679	10.221385956	H	14.321624756	5.511590958	10.193636894
H	3.931666374	4.316020966	18.363080978	H	3.678100586	4.311088562	18.587814331	H	2.449641705	3.729655504	18.049076080
H	2.420419216	4.008684635	17.751407623	H	2.491670132	3.327531338	17.893781662	H	3.640296459	2.623885632	18.390014648
H	3.552598476	2.805066586	17.777265549	H	4.000865459	2.730678320	18.245233536	H	3.918482542	4.238762379	18.669403076
H	5.672595024	6.256839275	15.576481819	H	5.600210190	5.952535629	15.564022064	H	5.706182480	5.457108498	15.397386551
H	4.787760258	6.475465775	16.947496414	H	4.747217655	6.320727825	16.931390762	H	4.759333134	6.070332050	16.601806641
H	6.027356625	5.412021160	16.958545685	H	6.065190792	5.354248047	17.050661087	H	6.062261105	5.153923988	16.998987198
N	3.281280279	1.173461676	12.259926796	N	2.643177748	1.377313614	12.007077217	N	1.784198046	2.119036436	11.503945351
N	3.949285984	3.812344074	11.003808022	N	3.897727074	3.913887024	10.756193161	N	3.806412697	3.953301907	10.090205193
N	3.418178082	3.808268785	17.615779877	N	3.490106106	3.557669640	17.906616211	N	3.461512566	3.565267086	18.022895813
N	5.246739388	5.762513638	16.364873886	N	5.243141174	5.564485550	16.441926956	N	5.286275864	5.241264343	16.306324005
N	2.711929798	5.587451935	13.673810959	N	2.644819021	5.421991825	13.676408768	N	2.680146217	5.285883904	13.747051239
N	4.497304440	1.814838052	14.929115295	N	4.257807732	2.164036274	14.378039360	N	3.718160152	2.128387451	14.278986931

Structure J ₁				ts4			Structure K ₁				
Si	0.176622808	2.736840248	7.981910229	Si	0.324798524	2.695982218	7.938202858	Si	0.336640835	2.532080173	7.922616959
Si	8.013886452	0.882080972	2.926664114	Si	8.172534943	0.829279125	2.860108614	Si	8.123180389	0.722459614	2.855218410
Si	2.463600159	8.441513062	0.722073853	Si	2.615341902	8.395687103	0.697816551	Si	2.608494759	8.246497154	0.646501005
Si	5.557578087	8.509619713	0.969049513	Si	5.705466747	8.442656517	0.924635708	Si	5.745401382	8.365392685	0.914079547
Si	7.945574284	0.773625851	6.061697006	Si	8.102632523	0.721678555	5.993236065	Si	8.105870247	0.659124851	5.976205349
Si	0.156810462	5.907711029	8.137963295	Si	0.309068263	5.863626003	8.102870941	Si	0.286746204	5.700842857	8.058463097
Si	0.222632736	8.191230774	6.020177364	Si	0.381397963	8.158519745	5.977129459	Si	0.398293465	8.008832932	5.927561283
Si	5.619066238	0.665376425	8.192033768	Si	5.780601501	0.526769221	8.115844727	Si	5.805505753	0.555338264	8.107803345
Si	2.513947487	0.621843457	7.990544319	Si	2.678586006	0.577924609	7.948013783	Si	2.666698694	0.429130733	7.883606911
Si	0.178255588	8.243289948	2.932508945	Si	0.321704805	8.206347466	2.893285275	Si	0.360269964	8.070349693	2.829085112
Si	8.033355713	3.177922487	0.803323746	Si	8.210344315	3.088116884	0.732016146	Si	8.182676315	3.055549622	0.672645092
Si	9.599954605	2.614192724	8.013240814	Si	9.749432564	2.579927444	7.930378914	Si	9.787907600	2.503299713	7.927194595
Si	17.438589096	0.958248377	2.922320127	Si	17.576366425	0.910165489	2.873212337	Si	17.590183258	0.761191487	2.839955568
Si	11.854112625	8.333729744	0.734037220	Si	11.979206085	8.314987183	0.671438038	Si	11.985960960	8.239990234	0.666256964
Si	14.953008652	8.603214264	0.984164953	Si	15.096663475	8.567300797	0.924345553	Si	15.105954170	8.425743103	0.897911906
Si	17.386610031	0.890707850	6.037328720	Si	17.533210754	0.860020638	5.984782696	Si	17.554395676	0.662105918	5.960968971
Si	9.570430756	5.784199715	8.172175407	Si	9.673960686	5.732131004	8.090364456	Si	9.700202942	5.650629520	8.056097984
Si	9.618370056	8.073569298	6.044198990	Si	9.788548470	8.020440102	5.958975315	Si	9.757648468	7.971960545	5.939297676
Si	15.067571640	0.650286436	8.146378517	Si	15.215159416	0.627383411	8.095908165	Si	15.230977058	0.468029082	8.056882858
Si	11.933256149	0.492418587	7.980286598	Si	12.078428268	0.454377770	7.895365238	Si	12.083141327	0.391860783	7.877719402
Si	9.562895775	8.147277832	2.927594185	Si	9.746497154	8.067604065	2.848590136	Si	9.768041611	8.073486328	2.830835342
Si	17.406425476	3.225535393	0.731963634	Si	17.549362183	3.190429926	0.683027923	Si	17.553642273	3.040141582	0.656342149
Al	7.874330044	6.375791073	0.949587405	Al	8.030879021	6.276447296	0.868808329	Al	8.070604324	6.251982212	0.822365522
Al	17.464431763	6.362595558	0.996013403	Al	17.602212906	6.324791908	0.946484506	Al	17.602643967	6.174968243	0.861679077
O	1.625518680	1.984760404	8.062265396	O	1.770472765	1.930218101	8.027459145	O	1.810730457	1.819056749	8.053981781
O	0.055248335	0.271425456	2.845230579	O	0.201955184	0.233164743	2.814469814	O	0.206560940	0.077500194	2.727599621
O	8.103090286	2.338029385	2.204633713	O	8.316002846	2.280955791	2.145954609	O	8.159696579	2.083406210	1.973784924
O	2.324085712	-0.229507029	9.363285065	O	2.491117001	-0.289937347	9.312790871	O	2.415573120	-0.486904979	9.203911781
O	1.501806259	8.409220695	2.013704062	O	1.658175349	8.382044792	1.991933227	O	1.736308217	8.306748390	1.999868751
O	-0.664817333	2.421062469	9.348318100	O	-0.515716314	2.397423267	9.306575775	O	-0.502426028	2.247609615	9.295739174
O	6.324238300	7.131591320	0.697838068	O	6.462532520	7.049768925	0.738094687	O	6.497071266	6.979804516	0.651624560
O	8.188529968	8.850344658	6.239371300	O	8.352434158	8.801095963	6.142748833	O	8.280929565	8.665095329	6.088442326
O	6.518955708	0.578767896	6.827048302	O	6.656602383	0.435689270	6.726488590	O	6.669486046	0.418510854	6.729066372
O	8.170615196	5.969062328	8.910784721	O	8.224757195	5.859477043	8.749941826	O	8.222429276	5.751053333	6.668963432
O	0.124393523	6.729164124	6.722607136	O	0.297093064	6.705951214	6.701813221	O	0.387942225	6.578303337	6.691993237
O	4.985228539	8.625444412	8.926307678	O	5.060618401	8.468540192	8.825061798	O	5.278766155	8.607316017	8.986205101
O	1.410317183	6.503032207	9.028261185	O	1.552258372	6.447908401	9.017428398	O	1.475049496	6.212008953	9.095474243
O	-0.676809192	2.166002512	6.700767517	O	-0.538711309	2.139758587	6.657678604	O	-0.491810739	1.914818287	6.653758049
O	6.872514725	0.001621276	2.189601183	O	6.993334293	-0.015681133	2.118186951	O	6.280784607	9.128589630	2.261695385
O	6.195403099	1.829284430	9.161702156	O	6.421965122	1.617535830	9.113965988	O	6.340609550	1.852575064	8.946713448
O	18.072237015	7.044176102	2.444665194	O	-0.613779783	7.011848927	2.381541252	O	-0.518948972	6.865591526	2.248505354
O	2.073861361	-0.290372103	6.717685699	O	2.234093189	-0.321483403	6.669069767	O	2.192356110	-0.360725343	6.554136753
O	0.649479508	8.001188278	4.472082615	O	0.794181645	7.942582607	4.429070473	O	0.761550426	7.774590969	4.374633312

O	4.085314274	1.047967911	7.771959305	O	4.253361702	1.007195950	7.738623619	O	4.238489628	0.856399894	7.750551224
O	7.645032883	4.675228596	1.141910672	O	7.705384254	4.572854042	0.966562569	O	7.852231503	4.546446323	1.138622880
O	7.641248703	1.142026305	4.504488945	O	7.758409500	1.050837278	4.434691906	O	7.793876648	1.033079863	4.424221039
O	3.981632710	8.249737740	1.236786366	O	4.126015663	8.180271149	1.240922809	O	4.154876709	8.041339874	1.071054220
O	0.463711977	4.329392910	7.797219276	O	0.639314950	4.288568974	7.749894619	O	0.618050337	4.125131607	7.715012074
O	11.036441803	1.849025965	8.045832634	O	11.183298111	1.810388088	7.938919544	O	11.247768402	1.776798248	8.023059845
O	9.483030319	0.192631364	2.843590260	O	9.602614403	0.081938773	2.788866520	O	9.610927582	0.071011707	2.779054403
O	17.471149445	2.351891994	2.106282949	O	17.613687515	2.292953014	2.040739775	O	17.598247528	2.156567574	2.025024414
O	11.711556435	-0.355390310	9.359492302	O	11.842776299	-0.385461032	9.274827003	O	11.851105690	-0.488356888	9.229817390
O	10.942946434	8.286605835	2.062638760	O	11.145238876	8.347908974	2.044443846	O	11.182418823	8.343094826	2.059059858
O	9.484463692	3.042559624	0.027743708	O	8.971944809	2.266548634	9.325885773	O	8.957883835	2.208726883	9.302725792
O	15.716614723	7.083803654	0.841627061	O	15.860107422	7.043356419	0.782105148	O	15.852434158	6.892518997	0.777129412
O	18.310567856	-0.445497930	6.158804893	O	-0.369260758	-0.469237834	6.093497753	O	-1.083915710	8.700828552	6.070345879
O	15.967506409	0.599229872	6.798647404	O	16.120908737	0.564677894	6.750798225	O	16.125152588	0.403289855	6.706617355
O	17.607088089	6.070388317	8.923812866	O	-1.086182833	6.020695686	8.876159668	O	17.681997299	5.850652695	8.740583420
O	9.537555695	6.600662231	6.740373135	O	9.711712837	6.565066338	6.676039696	O	9.798029900	6.519200325	6.669044495
O	14.508313179	8.605515480	8.936684608	O	14.684916496	8.594623566	8.898560524	O	14.702049255	8.435976982	8.863950729
O	10.828747749	6.364156723	9.073576927	O	10.878114700	6.332911491	9.059477806	O	10.840682983	6.241871834	9.100951195
O	8.701863289	2.090851068	6.725189209	O	8.815052032	2.035067081	6.674695969	O	8.932018280	1.888831973	6.671648026
O	16.301364899	-0.033157766	2.238708973	O	16.445131302	-0.089891449	2.195943117	O	15.759816170	9.161488533	2.171479940
O	15.572723389	1.832479239	9.122769356	O	15.715433121	1.826687336	9.058212280	O	15.739010811	1.659171343	9.021102905
O	8.632081032	6.946561813	2.422642946	O	8.933402061	6.851406574	2.231797218	O	8.974323273	6.861537457	2.170181990
O	11.489724159	-0.427412719	6.715734959	O	11.656369209	-0.459823489	6.621458530	O	11.576656342	-0.435518682	6.576223373
O	9.978996277	7.866762161	4.482777596	O	10.148276329	7.786598682	4.406378269	O	10.141896248	7.720438957	4.385752678
O	13.498788834	0.896300137	7.788921833	O	13.649695396	0.860988379	7.735236645	O	13.668914795	0.716859639	7.692868233
O	16.960237503	4.721357346	1.075341582	O	17.119590759	4.684225559	1.047658205	O	17.109132767	4.535867214	0.999579251
O	17.032207489	1.217136621	4.477823734	O	17.174564362	1.194306970	4.426672459	O	17.214588165	1.017774463	4.404429913
O	13.415617943	8.169985771	1.221571684	O	13.558135033	8.136209488	1.110581875	O	13.561454773	8.015795708	1.084930897
O	9.870617867	4.206979752	7.802778244	O	10.028637886	4.166530132	7.719449043	O	10.080682755	4.090954304	7.714226246
O	5.923511505	7.350802422	4.812540531	O	4.720882416	7.162135124	5.184523106	O	4.001214981	6.688839912	6.501922131
O	4.443537712	6.006611824	4.046345711	O	4.542089939	5.729879856	3.333850145	O	6.849084854	4.080982685	4.499454975
H	15.087619781	6.341481686	0.752417743	H	15.223229408	6.307922363	0.690055609	H	15.214742661	6.157020569	0.697569609
H	4.507741451	7.206781387	6.926865578	H	3.849439144	6.649628639	7.367105007	H	3.604585409	5.403781414	0.153090239
H	3.816229105	5.719283104	7.029798985	H	3.573785782	5.042508602	7.546277523	H	3.473122358	3.265915871	8.828706741
H	5.018662930	6.163820267	8.088964462	H	4.728211403	5.789726257	8.481122971	H	5.159274101	4.908951759	0.457179636
H	8.483139992	4.986487389	5.162581444	H	8.018827438	5.721102715	5.209501266	H	9.721738815	5.097853661	4.377639771
H	7.515495300	4.219760895	4.067851543	H	7.118174553	4.926033497	4.111205578	H	8.638136864	4.568202496	3.049659491
H	7.842517376	5.819992542	3.900952578	H	5.243699074	7.989636898	5.244915485	H	4.642278671	7.414975166	6.416667461
H	5.429880142	3.099997044	6.154030800	H	5.469689846	2.990307570	6.404456615	H	6.067914009	4.197409153	6.110543251
H	6.980667114	3.295090199	6.658100605	H	7.065472126	3.383385420	6.534878254	H	6.791567326	4.937640667	7.411068439
H	5.741236210	3.725980997	7.636450768	H	6.057866573	3.569615126	7.826508522	H	6.055837154	3.479929686	7.629148483
Cu	6.062911987	5.569371223	5.773085594	Cu	5.715399265	5.530017853	6.149652481	Cu	4.359689713	5.353893757	7.622206211
N	4.704522610	6.220857620	7.107060432	N	4.308662891	5.753447056	7.537946224	N	3.739278793	4.214298248	9.107113838
N	7.632918835	5.088287354	4.599581242	N	7.064426422	5.646729469	4.835875988	N	8.882087708	4.627640724	4.050558090

N	4.944732666	7.147092342	3.985617161	N	5.145931721	6.689080238	3.592375994	N	7.950919151	4.475815296	4.949643135
N	6.053668976	3.734758854	6.661411285	N	6.120704174	3.670690536	6.807754040	N	5.975327492	4.372772217	7.133934498

Structure L ₁				Structure A			
Si	0.344252110	2.507693052	7.947758198	Si	0.082571745	2.671322107	8.037472725
Si	8.145228386	0.693387091	2.867711067	Si	7.870397091	0.855011404	3.000867367
Si	2.623173714	8.203776360	0.680256426	Si	2.365613699	8.359323502	0.764512300
Si	5.743941784	8.348475456	0.932881713	Si	5.501899242	8.511999130	1.069970012
Si	8.114080429	0.648447692	6.005602837	Si	7.850375175	0.825757861	6.114461422
Si	0.310952485	5.665275574	8.097093582	Si	0.055215299	5.829790592	8.200046539
Si	0.387456059	7.966569901	5.969029427	Si	0.119889230	8.143510818	6.067290783
Si	5.798166275	0.499621928	8.117413521	Si	5.548678875	0.684216142	8.247546196
Si	2.669386148	0.395143092	7.933836937	Si	2.404592991	0.553648055	8.028228760
Si	0.363924384	8.035750389	2.882694006	Si	0.097282872	8.198137283	2.982678413
Si	8.173163414	3.029016972	0.720750272	Si	7.890789032	3.197973251	0.810515642
Si	9.784402847	2.482158899	7.968711853	Si	9.527779579	2.647067785	8.100582123
Si	17.615589142	0.736100018	2.885472775	Si	17.355733871	0.908293366	2.980627060
Si	12.015176773	8.169704437	0.717839420	Si	11.744167328	8.354942322	0.811327398
Si	15.117057800	8.397954941	0.950680315	Si	14.851133347	8.570522308	1.035558701
Si	17.550422668	0.645701289	5.993849277	Si	17.282201767	0.819376111	6.083781242
Si	9.751897812	5.609043121	8.131250381	Si	9.452945709	5.807182789	8.245150566
Si	9.753562927	7.930821419	6.021000385	Si	9.486872673	8.103783607	6.105915546
Si	15.229272842	0.455977201	8.110417366	Si	14.962629318	0.618885756	8.204342842
Si	12.088043213	0.341863513	7.973119259	Si	11.818367004	0.534840941	8.084904671
Si	9.741707802	7.945148945	2.913956404	Si	9.466479301	8.162605286	3.019550800
Si	17.570529938	3.018510103	0.700918972	Si	17.300975800	3.184768915	0.797843516
Al	8.071905136	6.176043034	0.979470372	Al	7.792209148	6.358871460	1.069876075
Al	17.611293793	6.148739815	0.926126540	Al	17.342044830	6.316263199	1.031764984
O	1.816954374	1.787644148	8.071962357	O	1.541470766	1.937211514	8.165376663
O	0.239630744	0.062080175	2.811242342	O	-0.017184079	0.232500196	2.917158842
O	8.240512848	2.106011391	2.064887285	O	7.862960339	2.187500477	2.089058876
O	2.447467327	-0.503667653	9.272014618	O	2.152827978	-0.359137118	9.350070000
O	1.725210071	8.237092018	2.017741442	O	1.454871893	8.361573219	2.102689028
O	-0.495546341	2.228694916	9.320097923	O	-0.087842070	3.135429382	0.034331582
O	6.554544449	6.991638184	0.738675714	O	6.230596542	7.110515594	0.821882069
O	8.293234825	8.668647766	6.139335632	O	7.990444660	8.805073738	6.166611671
O	6.660667896	0.414939642	6.729151249	O	6.421625614	0.589280665	6.862112522
O	8.346324921	5.690530777	8.900897980	O	8.058469772	5.941717148	9.006511688
O	0.337269276	6.529574394	6.718331337	O	0.069413066	6.715001106	6.831441879
O	5.227582455	8.506758690	8.932893753	O	5.782104015	-0.608583748	9.185853004
O	1.529927969	6.194223881	9.083587646	O	1.294368505	6.347942829	9.164402962
O	-0.484786630	1.895902872	6.677072048	O	18.087167740	2.071126461	6.761351109
O	6.232544422	9.212098122	2.240824223	O	6.715524673	-0.173350036	2.468158245
O	6.365132332	1.729941368	9.013400078	O	6.087315083	2.011400938	9.039411545
O	-0.560797572	6.852216721	2.329630613	O	17.987474442	7.027421951	2.445378304

O	2.191821814	-0.435409367	6.631294250	O	1.927423000	-0.245214522	6.699535370
O	0.787019491	7.738043785	4.422278404	O	0.544518352	7.907811165	4.522287846
O	4.236807346	0.837330937	7.759239674	O	3.982251644	0.962466598	7.881797791
O	7.683042049	4.488478661	1.127904534	O	7.526241302	4.663521290	1.290146589
O	7.830113411	1.015466928	4.442069530	O	7.524732590	1.241940856	4.567539215
O	4.165188313	7.993936062	1.120940924	O	3.909008265	8.233305931	1.239015698
O	0.637286842	4.095538616	7.729260445	O	0.370193660	4.261023045	7.817825317
O	11.215549469	1.707135201	8.077679634	O	10.988291740	1.928237200	8.207122803
O	9.580533981	-0.058702722	2.747017384	O	9.357587814	0.200971797	2.949158192
O	17.639791489	2.122795343	2.059088945	O	17.388605118	2.302442551	2.166466475
O	11.882517815	-0.517160177	9.349055290	O	12.301293373	0.414534539	0.087354898
O	11.119093895	8.136240005	2.055237532	O	10.832489967	8.321606636	2.135818958
O	8.949061394	2.242572308	9.351234436	O	9.375411987	3.099874258	0.094497755
O	15.864307404	6.869554043	0.785174131	O	15.589963913	7.037829876	0.885573745
O	-1.084064960	8.684729576	6.086439133	O	17.483150482	8.852722168	6.164237022
O	16.130563736	0.386404455	6.762089729	O	15.865661621	0.564765751	6.859990597
O	-1.109295607	5.818329334	8.829826355	O	17.480512619	5.980514050	8.943924904
O	9.689268112	6.483919621	6.749528408	O	9.389904976	6.650104046	6.830941677
O	14.679961205	8.421506882	8.917539597	O	14.413451195	8.573599815	8.990653038
O	10.973886490	6.202885628	9.066943169	O	10.711482048	6.401458740	9.135478973
O	8.908948898	1.892738819	6.710084438	O	8.701085091	2.026499748	6.818941593
O	15.799265862	9.126276970	2.211522102	O	16.231733322	-0.086522691	2.284570217
O	15.742185593	1.650068283	9.072220802	O	15.461460114	1.796617150	9.191384315
O	8.884101868	6.676320076	2.440454960	O	8.540099144	6.961946011	2.525276899
O	10.904287338	8.858511925	6.703601837	O	11.265906334	-0.326903462	6.824713707
O	10.167805672	7.733423233	4.471084595	O	9.936620712	7.909464836	4.567448139
O	13.663834572	0.705148637	7.752186298	O	13.394645691	0.861679316	7.838939667
O	17.132160187	4.508553028	1.072429299	O	16.852931976	4.676007271	1.158832550
O	17.206241608	1.007594109	4.438378334	O	16.921844482	1.171617270	4.529961109
O	13.578661919	7.985656738	1.192764640	O	13.308407784	8.173120499	1.286789298
O	10.097787857	4.059324265	7.724758625	O	9.766206741	4.239987850	7.847235203
O	4.114908695	6.558527470	6.334192276	O	3.726181984	7.159702778	6.729632854
O	7.783275604	4.597748756	4.446848869	H	14.951359749	6.303038120	0.805379391
H	15.222576141	6.136224270	0.711798966	H	3.108416080	5.372612000	8.102687836
H	4.015838623	5.424667835	0.103501514	H	3.883536339	3.902480125	8.122495651
H	3.565804958	3.266056538	8.654651642	H	4.519310951	5.212402821	8.938459396
H	5.483227730	4.660662174	0.210104704	H	3.606349468	7.750836372	5.967262745
H	8.139060020	5.331068516	3.901540756	H	5.271135807	7.287295341	4.387693405
H	7.790809631	3.832153082	3.844606400	H	6.558032036	7.411735058	5.395066261
H	4.595330238	7.403825283	6.350542545	H	6.492193699	6.199664116	4.290284634
H	6.684600830	4.574057102	6.012951374	H	6.216609955	3.637762070	5.612728119
H	7.071214676	4.939056873	7.585971832	H	7.294341087	4.592564106	6.392873764
H	6.418904781	3.467969179	7.232008934	H	6.267564774	3.648768187	7.254272461
Cu	4.627903938	5.266340256	7.437070370	Cu	4.961165905	5.787171841	6.501441479

N	4.017401695	4.140221119	8.941965103	N	4.024553299	4.914298058	8.082682610
N	11.652682304	4.598212719	4.195065975	N	5.922279358	6.736082077	4.952722073
N	12.162637711	4.583230019	5.184813976	N	6.329616547	4.250650406	6.426143169
N	6.369838238	4.461822510	6.995263577				

Table S6. Cartesian coordinates of RC, TS, IM, and PC for cycle II. The structures from A to F are the same as those in Table S5.

Structure G ₁				Structure H ₂				ts3			
Si	0.127521813	2.641449928	8.094452858	Si	0.113862276	2.664176941	8.092165947	Si	0.136661828	2.695935726	8.102260590
Si	7.945889950	0.802341163	3.017595291	Si	7.921969891	0.813450456	3.029660940	Si	7.974413395	0.836480618	3.021285772
Si	2.398298740	8.311174393	0.805331171	Si	2.384796143	8.307554245	0.817342281	Si	2.409290791	8.346792221	0.818703234
Si	5.531866074	8.424050331	1.060423255	Si	5.518944740	8.439457893	1.082177758	Si	5.555300713	8.464070320	1.058762550
Si	7.890388966	0.785078645	6.141847610	Si	7.873642445	0.807511806	6.153990269	Si	7.910598278	0.800507069	6.148369789
Si	0.076506793	5.810199261	8.233730316	Si	0.054988325	5.830817223	8.248012543	Si	0.067258477	5.864031315	8.241390228
Si	0.172180235	8.115809441	6.119307518	Si	0.135983139	8.134983063	6.126774311	Si	0.193655163	8.161922455	6.142655373
Si	5.602657795	0.555753767	8.280886650	Si	5.583258152	0.567475736	8.292941093	Si	5.612228394	0.589678526	8.275927544
Si	2.456231356	0.535198867	8.094388008	Si	2.424611092	0.548247993	8.093068123	Si	2.494445801	0.592446804	8.097721100
Si	0.129724219	8.171380043	3.024477482	Si	0.112738669	8.178673744	3.028048992	Si	0.143415958	8.194975853	3.035605907
Si	7.938280582	3.110564947	0.856769025	Si	7.918601513	3.115142822	0.867269695	Si	7.957462788	3.135267258	0.867346108
Si	9.565783501	2.629895687	8.080441475	Si	9.534361839	2.654852629	8.087147713	Si	9.580582619	2.644783735	8.059148788
Si	17.390504837	0.875877738	3.019397020	Si	17.383039474	0.884857059	3.018907309	Si	17.405334473	0.899498224	3.020066261
Si	11.784244537	8.306998253	0.850756168	Si	11.769152641	8.314283371	0.875273347	Si	11.783845901	8.331174850	0.866253197
Si	14.896564484	8.541965485	1.083332896	Si	14.882542610	8.549106598	1.089660048	Si	14.903870583	8.562890053	1.087159753
Si	17.333742142	0.786396384	6.139757156	Si	17.312789917	0.806720972	6.145930767	Si	17.355165482	0.842094779	6.157843113
Si	9.478164673	5.751043320	8.277019501	Si	9.449849129	5.771248817	8.302216530	Si	9.504235268	5.764867306	8.289351463
Si	9.524212837	8.059147835	6.151535034	Si	9.505778313	8.082924843	6.171383381	Si	9.560045242	8.070333481	6.156640053
Si	14.999542236	0.604417562	8.237822533	Si	14.978718758	0.615506411	8.248372078	Si	15.022272110	0.635859668	8.252821922
Si	11.860951424	0.486040533	8.089275360	Si	11.834476471	0.514015019	8.103273392	Si	11.883734703	0.498922706	8.065793037
Si	9.530570984	8.101600647	3.047048569	Si	9.519702911	8.102743149	3.066443920	Si	9.562565804	8.113262177	3.046588659
Si	17.329494476	3.150858164	0.832517147	Si	17.313720703	3.160943985	0.835009098	Si	17.333320618	3.178730488	0.841761589
Si	-0.580068111	1.878814936	17.449310303	Si	-0.587179899	1.879572511	17.453897476	Si	-0.561923742	1.914010286	17.466516495
Si	7.235664368	0.081426084	12.367868423	Si	7.225497246	0.092192709	12.373921394	Si	7.252897739	0.103415191	12.364221573
Si	1.692112327	7.612586498	10.201599121	Si	1.678682923	7.632678986	10.198249817	Si	1.723731756	7.682274342	10.217260361
Si	4.824754715	7.724151134	10.447592735	Si	4.822053432	7.738743782	10.446078300	Si	4.837999821	7.747031212	10.442342758
Si	7.191559792	0.016529799	15.501686096	Si	7.179361820	0.025730491	15.508445740	Si	7.209509373	0.038675308	15.498338699
Si	-0.585471272	5.049666405	17.610336304	Si	-0.592184782	5.047805309	17.615421295	Si	-0.568102121	5.081943989	17.627441406
Si	-0.567244112	7.353618145	15.475489616	Si	-0.575327456	7.354780674	15.479228973	Si	-0.567707539	7.394595623	15.488675117
Si	4.877169132	-0.163051605	17.617805481	Si	4.867454529	-0.160755515	17.634204865	Si	4.904014111	-0.156509995	17.631669998
Si	1.726982117	-0.234724879	17.436784744	Si	1.714589953	-0.235379577	17.448474884	Si	1.735169411	-0.206805348	17.459300995
Si	-0.564395785	7.449433327	12.388731956	Si	-0.558355629	7.450049400	12.396733284	Si	-0.533629000	7.488828182	12.392742157
Si	7.301724434	2.375024319	10.245479584	Si	7.255785942	2.390320539	10.254504204	Si	7.340648174	2.391684294	10.236006737
Si	8.846237183	1.842924118	17.472997665	Si	8.827312469	1.850344896	17.479745865	Si	8.863300323	1.871499658	17.464794159
Si	16.684932709	0.145282447	12.391274452	Si	16.688381195	0.150591791	12.394954681	Si	16.685016632	0.178511620	12.406288147

Si	11.090305328	7.581309319	10.207044601	Si	11.067398071	7.608956337	10.228223801	Si	11.092682838	7.613831043	10.211513519
Si	14.193628311	7.804907799	10.445056915	Si	14.180397034	7.819093704	10.439955711	Si	14.200818062	7.841723442	10.450541496
Si	16.612499237	0.038130879	15.496424675	Si	16.604028702	0.035938144	15.496818542	Si	16.616802216	0.076467991	15.506402969
Si	8.797756195	5.006911278	17.631359100	Si	8.774433136	5.012767315	17.655368805	Si	8.784024239	5.019185066	17.628450394
Si	8.846472740	7.303588867	15.498037338	Si	8.829564095	7.310780048	15.514770508	Si	8.854075432	7.325966835	15.500854492
Si	14.294882774	-0.140645862	17.618694305	Si	14.280259132	-0.133850455	17.621976852	Si	14.302556992	-0.128010392	17.627090454
Si	11.156090736	-0.266124010	17.472776413	Si	11.141576767	-0.260725975	17.481939316	Si	11.161530495	-0.247353673	17.475694656
Si	8.847249031	7.272301674	12.392818451	Si	8.837316513	7.287775993	12.407427788	Si	8.862709045	7.293050766	12.395380974
Si	16.657714844	2.417724371	10.195647240	Si	16.650514603	2.426042557	10.209268570	Si	16.676479340	2.453310728	10.215730667
Al	7.829936981	6.289256573	1.090146899	Al	7.823277473	6.291426659	1.119182348	Al	7.841563225	6.300868511	1.077635646
Al	17.397768021	6.296285629	1.086720943	Al	17.381267548	6.305082321	1.084198594	Al	17.409002304	6.321401596	1.104626775
Al	7.161921024	5.516276836	10.493220329	Al	7.135018349	5.519825935	10.503577232	Al	7.182792187	5.528826714	10.484352112
Al	16.687337875	5.564199924	10.393264771	Al	16.668054581	5.572212696	10.408635139	Al	16.700344086	5.593777657	10.400674820
O	1.584988594	1.908146143	8.220268250	O	1.571992636	1.935569882	8.219713211	O	1.579485178	1.939890146	8.204733849
O	0.016741350	0.203496233	2.908845901	O	0.011149421	0.216985926	2.901675940	O	0.031397596	0.226233095	2.884867191
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O	-0.055666447	3.060804605	0.071480133	O	-0.073711000	3.074959755	0.068254702	O	-0.046476994	3.113893747	0.084503636
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O	6.461098671	0.566003799	6.904736042	O	6.446641922	0.602660358	6.920375824	O	6.485369682	0.562565267	6.907545567
O	8.081654549	5.818824291	9.045756340	O	8.043326378	5.829184055	9.048929214	O	8.100785255	5.838373184	9.035154343
O	0.147232831	6.664258957	6.845800877	O	0.121217191	6.690767288	6.865157604	O	0.136262357	6.697854042	6.842180729
O	5.026005745	8.504185677	9.019417763	O	5.040391922	8.512898445	9.016763687	O	4.972777843	8.532234192	9.007409096
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Cu	4.371337891	4.005622387	15.927210808	Cu	4.242485523	3.985267878	16.004680634	Cu	4.120201111	3.895426750	15.956869125
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H	4.393152237	0.175751328	12.744760513	H	4.408132076	0.175374627	12.866440773	H	4.356326103	-0.168783545	13.198037148
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H	5.066645622	3.409034014	11.238844872	H	4.949577808	3.344071150	11.379609108	H	5.203957081	3.192833424	11.709412575
H	14.295889854	5.543984890	10.206672668	H	14.273372650	5.553753853	10.235590935	H	14.305377007	5.579109192	10.261755943
H	3.900544405	4.232096195	18.433048248	H	3.852585077	4.230273247	18.527223587	H	3.901286125	4.303956509	18.496042252
H	2.709102631	3.292888641	17.696979523	H	2.640096664	3.292879820	17.828243256	H	2.658793211	3.347896576	17.866432190
H	4.196083546	2.649182796	18.042297363	H	4.134171963	2.646677732	18.134351730	H	4.163675308	2.711285591	18.121433258
H	5.690219879	6.147171497	15.589425087	H	5.635514259	6.067522049	15.614225388	H	5.594046116	5.722259998	15.377493858
H	4.723668575	6.355746269	16.902591705	H	4.710593224	6.334905624	16.945196152	H	4.722327232	6.250638008	16.697069168
H	6.089727402	5.480978489	17.051719666	H	6.052170753	5.423370361	17.082944870	H	6.018779755	5.273122787	16.939783096
N	3.657546520	0.691838622	13.257436752	H	1.013434768	3.812061787	13.078677177	H	0.749398112	5.079603195	14.192132950
N	4.143379688	2.955512285	11.452692986	H	0.674073040	2.238707542	12.772926331	H	0.331780791	3.527529001	13.712169647
N	3.710928917	3.499692440	17.726648331	H	1.046580434	2.722868443	14.300580025	H	1.858978391	3.790423393	14.403359413
N	5.296934605	5.666071892	16.402307510	N	3.645653725	0.618842363	13.400144577	N	3.568409443	0.327274799	13.633620262

N	3.588671684	5.447719574	13.458477974	N	4.011248589	2.923527479	11.551472664	N	4.467829227	2.477720022	11.845652580
				N	3.642365932	3.496953011	17.829563141	N	3.659640312	3.556568384	17.820592880
				N	5.250997543	5.617288589	16.448232651	N	5.223302841	5.451862335	16.292469025
				N	3.705100536	5.546702385	13.589482307	N	1.886989594	4.784618378	12.061031342
				N	1.286419868	2.855016470	13.314598083	N	1.099042773	4.190732956	13.828644753
Structure I₂				Structure J₂				Structure K₂			
Si	0.114353955	2.576234579	8.107199669	Si	0.138006389	2.575533390	8.109479904	Si	0.161789894	2.483213902	8.244474411
Si	7.933447838	0.774565578	3.050510406	Si	7.955383778	0.755113661	3.040444851	Si	7.964020729	0.709188223	3.119638920
Si	2.398762226	8.279253006	0.835182428	Si	2.407428265	8.250000954	0.854557157	Si	2.430744171	8.225805283	0.937309444
Si	5.534419060	8.399662971	1.073971868	Si	5.537412643	8.375576973	1.081123710	Si	5.540681839	8.331542969	1.143465877
Si	7.871357918	0.741406083	6.159420967	Si	7.902341366	0.729922891	6.168125153	Si	7.910173416	0.650286376	6.244731903
Si	0.076393604	5.755684853	8.255202293	Si	0.034062207	5.724943161	8.262047768	Si	0.108595431	5.660794735	8.366298676
Si	0.134841710	8.044327736	6.147884846	Si	0.149053216	8.034913063	6.172341347	Si	0.191598773	7.956430435	6.258005619
Si	5.579485893	0.485553205	8.316109657	Si	5.601061344	0.481622159	8.307661057	Si	5.618750095	0.420867801	8.402459145
Si	2.449145555	0.464724958	8.131926537	Si	2.468043804	0.452297688	8.140509605	Si	2.491956472	0.389931440	8.258201599
Si	0.123984680	8.112533569	3.052030802	Si	0.129032180	8.094319344	3.071542025	Si	0.167732790	8.033579826	3.165659428
Si	7.952534199	3.076209068	0.877379358	Si	7.941955566	3.059737682	0.873763144	Si	7.950688362	3.015347004	0.965817750
Si	9.532183647	2.590085030	8.092337608	Si	9.561138153	2.579181671	8.086791992	Si	9.581661224	2.483796835	8.164203644
Si	17.379241943	0.807827473	3.028508663	Si	17.387834549	0.774516404	3.045849323	Si	17.414482117	0.737912476	3.152249336
Si	11.770188332	8.281758308	0.866858721	Si	11.788785934	8.267256737	0.862755537	Si	11.810280800	8.199529648	0.971316040
Si	14.885997772	8.483849525	1.078653336	Si	14.906289101	8.460580826	1.101985455	Si	14.918556213	8.403651237	1.204310060
Si	17.316766739	0.746697307	6.146199703	Si	17.326675415	0.726274967	6.173738003	Si	17.371986389	0.633134961	6.268459320
Si	9.439719200	5.718677044	8.288399696	Si	9.502962112	5.712804317	8.304958344	Si	9.535199165	5.633670330	8.373044014
Si	9.521191597	8.017477036	6.148968220	Si	9.577177048	8.016801834	6.164053917	Si	9.560892105	7.928607464	6.237905979
Si	14.973387718	0.565813124	8.249279022	Si	15.011102676	0.526333749	8.288496971	Si	15.026371956	0.441021264	8.359509468
Si	11.840020180	0.458482027	8.083025932	Si	11.878085136	0.443817616	8.086259842	Si	11.887553215	0.346095145	8.169554710
Si	9.539746284	8.068822861	3.062639475	Si	9.547158241	8.051956177	3.058906794	Si	9.544859886	8.010298729	3.140154839
Si	17.323398590	3.100268841	0.849060535	Si	17.328731537	3.079186678	0.872100353	Si	17.344097137	3.000986576	0.970237195
Si	-0.576502442	1.842734933	17.452186584	Si	-0.574194074	1.810484886	17.493921280	Si	-0.590971768	1.761179090	17.584011078
Si	7.215449333	0.040135980	12.384590149	Si	7.211209297	0.025487125	12.385264397	Si	7.257372379	-0.035971940	12.480513573
Si	1.706730008	7.530303955	10.204945564	Si	1.699531317	7.528904915	10.244129181	Si	1.744072795	7.445607662	10.341554642
Si	4.802049160	7.673729420	10.502605438	Si	4.817595959	7.649731636	10.484228134	Si	4.857499123	7.564995766	10.560863495
Si	7.197623730	-0.016645312	15.522971153	Si	7.190361500	-0.025817871	15.519854546	Si	7.217034817	-0.081989527	15.607365608
Si	-0.574112058	5.009280205	17.632160187	Si	-0.574186742	4.970986843	17.671264648	Si	-0.584792554	4.960112095	17.764993668
Si	-0.544428647	7.316533566	15.500369072	Si	-0.563137770	7.268290520	15.527132988	Si	-0.530302763	7.224626541	15.620460510
Si	4.886500359	-0.184878945	17.642700195	Si	4.877366543	-0.210433125	17.642091751	Si	4.876574516	-0.233738422	17.722919464
Si	1.739955068	-0.276699424	17.467115402	Si	1.736441016	-0.310079455	17.475036621	Si	1.757414579	-0.328698039	17.559476852
Si	-0.582998812	7.338862419	12.405643463	Si	-0.547473013	7.319505692	12.425389290	Si	-0.538961172	7.282245159	12.520730019
Si	7.271718979	2.326436996	10.267612457	Si	7.310795307	2.306335211	10.255462646	Si	7.335505486	2.230987072	10.335669518
Si	8.853284836	1.810830355	17.482397079	Si	8.849707603	1.800140262	17.477840424	Si	8.875698090	1.734507442	17.585002899
Si	16.667966843	0.054076195	12.387693405	Si	16.703456879	0.056254864	12.427917480	Si	16.712282181	-0.016658485	12.512484550
Si	11.066193581	7.545109749	10.207041740	Si	11.096884727	7.551953316	10.225615501	Si	11.109118462	7.448568344	10.300696373
Si	14.168087006	7.743916988	10.436861038	Si	14.207682610	7.728609085	10.476080894	Si	14.210672379	7.653832436	10.558144569
Si	16.624567032	0.006627917	15.504987717	Si	16.627088547	-0.023008585	15.539101601	Si	16.646326065	-0.073731780	15.632391930

Si	8.779386520	4.970070839	17.631195068	Si	8.793025017	4.960558891	17.632308960	Si	8.823517799	4.900131702	17.742460251
Si	8.849736214	7.274026394	15.510065079	Si	8.849477768	7.267470837	15.510642052	Si	8.866339684	7.207209110	15.609059334
Si	14.297386169	-0.182738900	17.632179260	Si	14.300169945	-0.187326431	17.647003174	Si	14.316840172	-0.285382509	17.747846603
Si	11.161156654	-0.295395017	17.477844238	Si	11.164351463	-0.305710673	17.482299805	Si	11.182273865	-0.367605090	17.587673187
Si	8.844010353	7.232450962	12.398024559	Si	8.853157043	7.232627392	12.400427818	Si	8.851976395	7.155153275	12.510357857
Si	16.641372681	2.342571259	10.209116936	Si	16.700876236	2.322953224	10.252583504	Si	16.678812027	2.251924992	10.336015701
Al	7.834729195	6.256321430	1.082709551	Al	7.838945866	6.236322403	1.092390060	Al	7.841637611	6.198902607	1.164149761
Al	17.393115997	6.242081165	1.106289148	Al	17.389739990	6.214727402	1.160589337	Al	17.430133820	6.171752453	1.235007524
Al	7.162414551	5.470023632	10.517419815	Al	7.201918125	5.469099998	10.500729561	Al	7.227138042	5.410394669	10.577301979
Al	16.677703857	5.491075993	10.446356773	Al	16.627700806	5.485655785	10.432098389	Al	16.710475922	5.404091835	10.543385506
O	1.564890265	1.833749294	8.239006996	O	1.582698464	1.820200682	8.249347687	O	1.629283071	1.769585371	8.409207344
O	0.011342019	0.143853247	2.935503006	O	0.026614517	0.130513445	2.937975168	O	0.033738866	0.052546889	3.053220510
O	7.999539375	2.156492949	2.208983898	O	7.996672630	2.144648075	2.208061218	O	7.993312836	2.118900776	2.319762468
O	2.837096453	0.306130230	0.055918451	O	2.868127584	0.280305535	0.075678274	O	2.933940411	0.269319504	0.174045503
O	1.471889734	8.245355606	2.152533293	O	1.478869200	8.205710411	2.171423912	O	1.498959064	8.204664230	2.251540661
O	-0.073683098	3.028588772	0.058490131	O	-0.053854156	2.995124578	0.113954723	O	-0.058391072	2.860374451	0.191061929
O	6.256660461	6.992055893	0.839602947	O	6.264376640	6.973214149	0.826457441	O	6.279931545	6.942551136	0.851189256
O	8.080723763	8.782917023	6.254266739	O	8.143289566	8.794975281	6.311964035	O	8.121107101	8.693073273	6.380405426
O	6.471730232	0.483997524	6.960076809	O	6.483010769	0.472451746	6.946428299	O	6.499896049	0.418150127	7.040824413
O	8.041954994	5.815178394	9.050152779	O	8.089262962	5.809168816	9.043842316	O	8.158815384	5.783435822	9.165056229
O	0.048830807	6.578674316	6.844849110	O	0.083879292	6.571004391	6.869393349	O	0.153706372	6.492145538	6.962519646
O	4.955005646	8.428961754	9.054755211	O	4.989373207	8.428970337	9.054451942	O	5.003120422	8.365369797	9.139396667
O	1.316888094	6.340605736	9.167243004	O	1.195436001	6.325350761	9.273630142	O	1.318424225	6.239612103	9.335687637
O	18.127399445	1.998639107	6.814951897	O	18.132551193	1.987141728	6.839266777	O	-0.633251786	1.865965605	6.951976299
O	6.797965527	-0.171043456	2.350475073	O	6.127151966	9.201839447	2.350185156	O	6.159328938	9.146049500	2.407114506
O	6.107376099	1.610238314	9.359012604	O	6.136229992	1.614247680	9.341943741	O	6.148854733	1.555659294	9.434440613
O	18.021415710	6.922982693	2.539991140	O	18.014736176	6.900433540	2.594951868	O	18.078990936	6.820110798	2.680985928
O	1.960312366	-0.429068655	6.869114876	O	1.987447023	-0.441766560	6.879682064	O	1.982766390	-0.486650854	6.998325825
O	0.567469954	7.872102261	4.597589493	O	0.570443511	7.872210979	4.621070862	O	0.637874901	7.801891804	4.711273193
O	4.020900726	0.847359955	7.959173679	O	4.038223267	0.846425831	7.969201088	O	4.057991982	0.782710373	8.066923141
O	7.549391747	4.563232422	1.227618456	O	7.536746025	4.544621468	1.230440736	O	7.552794933	4.507760525	1.297310472
O	7.513873100	1.073431492	4.601600647	O	7.563693523	1.035565138	4.600596905	O	7.558299065	0.954431772	4.683320045
O	3.939483166	8.161859512	1.292622924	O	3.947920561	8.133519173	1.322814703	O	3.962470055	8.066269875	1.427609324
O	0.355328321	4.173535347	7.931277752	O	0.412520409	4.164333344	7.920307159	O	0.422123969	4.079000950	8.057745934
O	10.980876923	1.831402063	8.204867363	O	10.994780540	1.802253246	8.166221619	O	11.022324562	1.717640996	8.256756783
O	9.404308319	0.088119730	3.004868269	O	9.429604530	0.081151605	2.969744921	O	9.446107864	0.049503699	3.055781603
O	17.400936127	2.193585873	2.196393251	O	17.367156982	2.156060219	2.210949659	O	17.418077469	2.143388271	2.354697704
O	12.351942062	0.333365053	0.118902199	O	12.353390694	0.322656810	0.120186962	O	12.378629684	0.249016285	0.222029403
O	10.943321228	8.310817719	2.241565466	O	10.944792747	8.268987656	2.225487232	O	10.953330040	8.215059280	2.326931477
O	9.399510384	2.951809645	0.102987394	O	9.387203217	2.945218325	0.092402734	O	9.399056435	2.877337694	0.191463530
O	15.651023865	6.962313175	0.918101907	O	15.677977562	6.959483624	0.901617706	O	15.680874825	6.877617359	1.078056335
O	17.517827988	8.782996178	6.256320000	O	17.535650253	8.770225525	6.323146343	O	17.556251526	8.654973984	6.363333702
O	15.899008751	0.504946649	6.918861866	O	15.903953552	0.491975188	6.934098244	O	15.945825577	0.393686831	7.023399830
O	17.520883560	5.969321251	9.032734871	O	17.427852631	5.838721752	8.948580742	O	17.527038574	5.841671944	9.089746475

O	9.440158844	6.590288639	6.905602932	O	9.513617516	6.590066910	6.925489426	O	9.503291130	6.493454933	6.985199451
O	14.444447517	8.526357651	9.053317070	O	14.470685959	8.479211807	9.065093994	O	14.473893166	8.392266273	9.144571304
O	10.679304123	6.315172672	9.223601341	O	10.728175163	6.297872543	9.260722160	O	10.793871880	6.216021538	9.287359238
O	8.681840897	1.996391773	6.824771404	O	8.673840523	2.011568785	6.830819607	O	8.718624115	1.921393156	6.890119553
O	15.557168961	9.205653191	2.349242687	O	15.580478668	9.141440392	2.391578674	O	15.592262268	9.145009995	2.463210583
O	15.468943596	1.750689507	9.240014076	O	15.553192139	1.685649872	9.286992073	O	15.540022850	1.608362436	9.356550217
O	8.704155922	6.865715504	2.440664291	O	8.687872887	6.852577209	2.460086346	O	8.665119171	6.828360081	2.539236069
O	11.364241600	-0.429221004	6.816409588	O	11.450431824	-0.445641428	6.800982952	O	11.424140930	-0.537691593	6.894548893
O	9.950492859	7.764840126	4.609288216	O	9.952217102	7.767124653	4.609641075	O	9.950596809	7.704065323	4.686738968
O	13.420993805	0.825684309	7.869699955	O	13.460072517	0.825844109	7.933402061	O	13.472521782	0.705312073	7.982456684
O	16.922840118	4.598614216	1.219529033	O	16.929306030	4.569729328	1.261607766	O	16.966165543	4.520544052	1.284527421
O	16.970525742	1.076986313	4.582581997	O	17.001302719	1.040033460	4.604698658	O	17.027538300	0.986659229	4.714125633
O	13.351781845	8.049498558	1.275707364	O	13.362853050	8.047365189	1.278576136	O	13.379599571	7.985813141	1.419447422
O	9.827726364	4.172660351	7.887124538	O	9.870815277	4.160485744	7.909765244	O	9.868938446	4.071588516	7.997759819
O	0.881353140	1.109461427	17.575080872	O	0.887020588	1.077433944	17.604164124	O	0.878171325	1.041897416	17.669778824
O	-0.705461502	-0.638155580	12.324455261	O	-0.686703086	-0.663082004	12.369122505	O	-0.655160248	-0.687792063	12.424305916
O	7.451413631	1.457561731	11.646808624	O	7.443519115	1.443727016	11.643425941	O	7.456626415	1.385620832	11.731641769
O	2.240357399	-0.382870853	9.519211769	O	2.266846895	-0.396180451	9.530144691	O	2.302937746	-0.467299283	9.645905495
O	0.763264894	7.528346539	11.529687881	O	0.859079421	7.593658447	11.636513710	O	0.852908432	7.484818459	11.694026947
O	-0.746455193	2.256057739	9.463706970	O	-0.692791164	2.307550430	9.496185303	O	-0.691719174	2.167710781	9.604595184
O	5.653945446	6.345893383	10.591638565	O	5.676033020	6.321893692	10.567149162	O	5.676565170	6.209513664	10.572948456
O	7.366735935	7.986672401	15.642412186	O	7.363281727	7.977553368	15.624768257	O	7.369504929	7.906079769	15.690503120
O	5.758514404	-0.276153922	16.262859344	O	5.758012772	-0.301578104	16.264741898	O	5.780893326	-0.314793408	16.359590530
O	7.326840401	5.104948521	18.305376053	O	7.348737240	5.088126659	18.323144913	O	7.376134872	5.055044651	18.418788910
O	-0.585838735	5.868263721	16.233810425	O	-0.598557532	5.834047794	16.280389786	O	-0.580341637	5.776142597	16.347923279
O	4.336215019	7.779781818	18.403047562	O	4.333410263	7.756573677	18.406490326	O	4.284049988	7.722057343	18.469833374
O	0.682322145	5.546416283	18.547670364	O	0.693199396	5.521867752	18.569137573	O	0.699794888	5.508305550	18.645366669
O	17.466211319	1.269166231	16.131185532	O	17.443975449	1.226918459	16.201387405	O	17.445833206	1.205174327	16.266658783
O	5.868328571	-0.665641487	11.739880562	O	5.869352818	-0.692350447	11.733864784	O	5.969923496	-0.811619103	11.807218552
O	5.401036263	1.037227631	18.570898056	O	5.391835213	1.016212106	18.566089630	O	5.407529354	0.971584678	18.658506393
O	17.344684601	6.099981308	11.926458359	O	17.447164536	6.116373062	11.808820724	O	17.403842926	6.090521812	11.950323105
O	1.296122313	-1.110493422	16.134504318	O	1.281944633	-1.150815725	16.151786804	O	1.315208197	-1.208275080	16.262601852
O	-0.126991272	7.073798180	13.950494766	O	-0.156645536	7.013326168	13.979181290	O	-0.123884380	7.002125740	14.069184303
O	3.315004587	0.086519957	17.286897659	O	3.311798811	0.065164685	17.272993088	O	3.322804451	0.102235198	17.342271805
O	6.725277901	3.779914856	10.645770073	O	6.778434753	3.769388437	10.638133049	O	6.835209846	3.709126711	10.688201904
O	6.863813400	0.315022707	13.964197159	O	6.848668098	0.314104080	13.960775375	O	6.874197006	0.263327122	14.048738480
O	3.218044281	7.334125042	10.750447273	O	3.236361027	7.273322582	10.698515892	O	3.275826931	7.218042374	10.824041367
O	-0.285647869	3.435987473	17.225290298	O	-0.275782645	3.399369001	17.287454605	O	-0.343004942	3.363255024	17.477611542
O	10.317064285	1.089256525	17.573982239	O	10.311822891	1.075826287	17.571975708	O	10.336163521	1.014737487	17.707679749
O	8.536729813	-0.866580606	12.245507240	O	8.538704872	-0.869933426	12.257242203	O	8.616702080	-0.890212476	12.376537323
O	16.715530396	1.444563866	11.574231148	O	16.814735413	1.460496902	11.632246017	O	16.738378525	1.390018344	11.720886230
O	11.674983025	-0.404860586	9.459272385	O	11.654295921	-0.413043112	9.455817223	O	11.675281525	-0.500880420	9.553773880
O	10.205205917	7.604387283	11.565629005	O	10.206546783	7.607362747	11.570034981	O	10.197875977	7.442549706	11.631106377
O	8.698982239	2.311985731	9.470235825	O	8.740058899	2.287422657	9.476248741	O	8.762884140	2.178028345	9.549192429

O	14.935760498	6.213983059	10.298928261	O	14.927382469	6.215487003	10.409854889	O	14.959733963	6.116705418	10.428395271
O	16.837013245	8.046000481	15.612092972	O	16.819133759	8.002263069	15.649498940	O	16.863681793	7.971834183	15.752757072
O	15.218952179	-0.226583481	16.290746689	O	15.206891060	-0.260540247	16.301940918	O	15.234719276	-0.322175145	16.410497665
O	16.872150421	5.172238350	18.399644852	O	16.881206512	5.128963470	18.456169128	O	16.873121262	5.202558041	18.541610718
O	8.787164688	5.813269138	16.222610474	O	8.785036087	5.805523872	16.222967148	O	8.810256004	5.756991863	16.340103149
O	13.783555984	7.779322624	18.421968460	O	13.780707359	7.793186188	18.460836411	O	13.786461830	7.664305210	18.523181915
O	9.969164848	5.578271866	18.599081039	O	9.996643066	5.571160793	18.577032089	O	10.034605980	5.491582870	18.692983627
O	8.010643959	1.224658012	16.196113586	O	8.007671356	1.218012094	16.187665939	O	8.062204361	1.143342495	16.276338577
O	14.858247757	8.453282356	11.711705208	O	15.546584129	-0.868382573	11.730690002	O	14.908691406	8.385428429	11.811606407
O	14.775817871	1.016341448	18.605117798	O	14.788373947	1.028836012	18.592691422	O	16.160144806	2.376061916	0.024750326
O	8.148743629	5.894092560	11.897950172	O	8.155759811	5.894668579	11.899825096	O	8.057016373	5.849903584	12.052513123
O	10.661139488	-1.179310918	16.215908051	O	10.657746315	-1.185263395	16.218542099	O	10.645749092	-1.214422822	16.312604904
O	9.281062126	7.112944126	13.968521118	O	9.286478996	7.106082439	13.971096992	O	9.305001259	7.007604599	14.071940422
O	12.740459442	0.050159693	17.250841141	O	12.740706444	0.049595356	17.256835938	O	12.761147499	-0.045412302	17.346940994
O	16.241359711	3.840702295	10.606422424	O	16.209814072	3.804724693	10.652781487	O	16.259441376	3.755267620	10.671651840
O	16.274541855	0.337414742	13.945236206	O	16.292474747	0.327899575	13.981549263	O	16.296419144	0.220855713	14.067390442
O	12.639936447	7.319380760	10.672021866	O	12.653512001	7.391990185	10.731127739	O	12.669663429	7.271425247	10.809412956
O	9.122172356	3.403634071	17.288183212	O	9.133334160	3.392765522	17.282796860	O	9.138629913	3.329612970	17.388843536
O	3.807020426	2.346048355	15.164534569	O	3.842041016	2.371280909	15.096754074	O	3.400085926	2.485580683	14.895490646
O	4.681992531	4.211413860	13.866741180	O	4.755072594	4.253518105	13.879437447	O	4.861024857	4.206180573	13.883729935
O	1.329900026	4.048902988	11.693029404	O	13.576369286	4.226506233	10.990174294	O	1.508221507	3.467371941	15.345993042
Cu	3.991906881	2.554156303	13.406276703	Cu	4.060196877	2.618953705	13.342731476	Cu	4.067602158	2.722496986	12.989680290
Cu	4.357861519	3.990958691	15.831714630	Cu	4.388909340	3.996376514	15.818567276	Cu	4.364698887	4.041385651	15.755184174
H	15.011323929	6.227602005	0.839345515	H	15.107432365	6.303232670	0.435309887	H	15.048567772	6.141510963	0.965257287
H	3.506906033	0.416920781	14.249056816	H	3.529768944	0.472390890	14.146821976	H	3.015178919	0.478680015	13.319391251
H	2.647739172	0.521985531	12.814534187	H	2.701215506	0.568112850	12.697657585	H	2.872694731	0.781826198	11.709354401
H	4.280547619	0.139495015	12.771540642	H	4.333451271	0.205379248	12.688133240	H	4.315006256	0.261368871	12.319087982
H	4.035911560	2.118106127	10.880875587	H	4.006791115	2.298765898	10.785174370	H	3.710410595	4.503634930	11.227144241
H	3.155843735	3.468839645	11.298613548	H	3.490385771	3.806862831	11.183539391	H	5.040621758	3.609614134	10.855175018
H	4.868209839	3.488772154	11.240872383	H	5.118442535	3.450035095	11.208368301	H	3.517846823	3.056009769	10.448927879
H	14.288899422	5.486795425	10.204560280	H	14.222352982	5.429628849	10.653306961	H	14.318098068	5.387358665	10.320956230
H	3.920503616	4.245009899	18.377887726	H	3.922675610	4.207515240	18.343978882	H	4.029031754	4.239252567	18.332490921
H	2.729977846	3.308234692	17.656354904	H	2.727056265	3.296050072	17.596519470	H	2.695697784	3.553182125	17.608932495
H	4.213743687	2.668145657	17.984796524	H	4.198373795	2.629067183	17.938344955	H	4.046828270	2.650213718	17.887485504
H	5.725839615	6.131068230	15.539864540	H	5.748958111	6.150432110	15.599141121	H	5.829761505	6.161754131	15.653814316
H	4.717743397	6.365595341	16.819292068	H	4.727047920	6.336277008	16.875755310	H	4.785531044	6.286251545	16.911819458
H	6.050505161	5.447469711	17.003597260	H	6.066276550	5.422216415	17.041788101	H	6.122589111	5.368835449	17.072925568
H	-0.289133906	3.256293058	14.176177979	H	13.145631790	4.215776443	11.862882614	H	5.692852497	4.585545540	13.550615311
H	-0.684208214	4.446481705	12.882553101	H	14.424530029	3.711222410	11.054140091	N	3.505188942	0.873153925	12.510990143
H	4.283193111	4.944628239	13.359234810	H	4.457312584	5.027762890	13.364368439	N	4.051103592	3.538036108	11.176505089
N	3.554017305	0.688201427	13.260085106	N	3.595329762	0.754768252	13.161429405	N	3.719640017	3.579077721	17.596000671
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N	1.078590512	3.429271698	12.752414703	N	12.569107056	3.330790997	16.754503250				
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Structure L₂				ts4				Structure M₂			
Si	0.115482330	2.480034351	8.279045105	Si	0.134475172	2.517123222	8.287724495	Si	0.119776368	2.501265526	8.221027374
Si	7.932430267	0.684162259	3.140663862	Si	7.941755295	0.684119821	3.141234636	Si	7.944416046	0.734181583	3.123152733
Si	2.406986237	8.168911934	1.004136324	Si	2.406871080	8.218574524	0.990130424	Si	2.423340559	8.248470306	0.949544847
Si	5.523061275	8.295531273	1.162333608	Si	5.526451588	8.294761658	1.170020819	Si	5.525856972	8.351650238	1.150067091
Si	7.876119137	0.645816326	6.274670124	Si	7.898660183	0.658155620	6.274918556	Si	7.887881756	0.659878731	6.241838932
Si	0.081055343	5.649220467	8.401958466	Si	0.075547934	5.684193611	8.410698891	Si	0.095345676	5.690226078	8.371236801
Si	0.112494797	7.945050240	6.299650669	Si	0.159835428	7.981597424	6.309101105	Si	0.149304569	7.974666595	6.245423794
Si	5.567118168	0.436994433	8.418512344	Si	5.592057228	0.439840317	8.425511360	Si	5.574357986	0.439947665	8.391364098
Si	2.443474293	0.377683818	8.268396378	Si	2.473443985	0.414117575	8.292976379	Si	2.468825817	0.407278299	8.223978996
Si	0.119263157	8.029959679	3.192473412	Si	0.139376298	8.049061775	3.218000174	Si	0.143402040	8.063338280	3.164836168
Si	7.941005707	3.002303839	0.996906102	Si	7.949779510	2.992784977	0.985780597	Si	7.959906578	3.032463074	0.964835942
Si	9.528903961	2.487664461	8.184808731	Si	9.562632561	2.490707159	8.188062668	Si	9.550640106	2.480286121	8.168644905
Si	17.381208420	0.729511380	3.190067530	Si	17.387552261	0.738271058	3.212716579	Si	17.386655807	0.760194898	3.154954910
Si	11.773186684	8.183693886	0.989908099	Si	11.782464027	8.188848495	0.996413767	Si	11.800987244	8.224415779	0.971231580
Si	14.886039734	8.401659966	1.249837995	Si	14.899401665	8.419156075	1.258678913	Si	14.905604362	8.421990395	1.186671853
Si	17.317548752	0.629667997	6.321491241	Si	17.344598770	0.664952874	6.328642845	Si	17.325483322	0.672949255	6.255105019
Si	9.513522148	5.643819809	8.402518272	Si	9.543129921	5.647839546	8.416502953	Si	9.503908157	5.635839939	8.366359711
Si	9.540100098	7.933703899	6.276125431	Si	9.547253609	7.934626579	6.279181004	Si	9.534489632	7.927870750	6.239320278
Si	14.978878975	0.494225919	8.423706055	Si	15.003166199	0.501656771	8.433137894	Si	14.995194435	0.447637737	8.378806114
Si	11.844256401	0.354086816	8.211498260	Si	11.863356590	0.354435563	8.208352089	Si	11.850406647	0.339397490	8.196851730
Si	9.511877060	7.992676735	3.168668270	Si	9.516000748	7.986993790	3.170635939	Si	9.535379410	8.028600693	3.144182920
Si	17.291284561	3.006833315	1.016737342	Si	17.323440552	3.030075312	1.046045661	Si	17.367439270	3.040442705	0.969139576
Si	-0.606515527	1.730541825	17.649854660	Si	-0.583455682	1.780761123	17.661264420	Si	-0.562252700	1.799655437	17.583597183
Si	7.218449593	-0.015354216	12.506414413	Si	7.259541035	-0.024523318	12.499311447	Si	7.248407841	-0.037550271	12.472746849
Si	1.721595168	7.433481216	10.369016647	Si	1.735504150	7.471879005	10.389790535	Si	1.744769216	7.466176033	10.318245888
Si	4.827447891	7.594869614	10.602990150	Si	4.848695755	7.588732243	10.577672958	Si	4.832819462	7.584134579	10.561035156
Si	7.182569504	-0.080259681	15.637860298	Si	7.208170414	-0.097097397	15.640188217	Si	7.235817909	-0.058744311	15.607893944
Si	-0.609174848	4.917747974	17.792234421	Si	-0.607529044	4.948904514	17.798774719	Si	-0.576244473	4.957860947	17.743162155
Si	-0.552689612	7.209880352	15.664806366	Si	-0.583689630	7.244981766	15.672468185	Si	-0.516747057	7.252688408	15.618978500
Si	4.855112553	-0.256840229	17.754566193	Si	4.876517296	-0.274059534	17.744991302	Si	4.894696236	-0.222627163	17.718450546
Si	1.725873232	-0.364482045	17.645833969	Si	1.744508266	-0.336323619	17.624864578	Si	1.783447981	-0.323159337	17.553474426
Si	-0.556979299	7.301544189	12.565274239	Si	-0.553211272	7.339256763	12.573160172	Si	-0.541451514	7.252864838	12.516427994
Si	7.272509098	2.248299360	10.348610878	Si	7.319162846	2.237355947	10.364338875	Si	7.289008617	2.232533693	10.334939003
Si	8.853867531	1.734706640	17.619646072	Si	8.854372978	1.731465220	17.607667923	Si	8.871747971	1.757150888	17.576068878
Si	16.692337036	-0.020443678	12.567124367	Si	16.700588226	0.023751676	12.578320503	Si	16.679477692	-0.019558609	12.511246681
Si	11.081599236	7.454920292	10.328356743	Si	11.099836349	7.465063095	10.335279465	Si	11.085974693	7.435347080	10.301255226
Si	14.186536789	7.670821190	10.614487648	Si	14.203767776	7.700817585	10.629292488	Si	14.187573433	7.666128159	10.578964233
Si	16.624086380	-0.108046293	15.682991028	Si	16.613704681	-0.043457747	15.691096306	Si	16.643791199	-0.045113921	15.633484840
Si	8.809682846	4.892390251	17.750345230	Si	8.814997673	4.892147064	17.764587402	Si	8.827311516	4.924024105	17.746242523
Si	8.841738701	7.213314056	15.633559227	Si	8.880373001	7.203989983	15.650051117	Si	8.898227692	7.223125935	15.610109329
Si	14.287893295	-0.284918308	17.789531708	Si	14.303978920	-0.250029683	17.815746307	Si	14.330343246	-0.268292308	17.723024368

Si	11.147983551	-0.375574231	17.627706528	Si	11.167928696	-0.375403762	17.633762360	Si	11.193281174	-0.350831270	17.577470779
Si	8.822120667	7.174859524	12.535997391	Si	8.846679688	7.160576820	12.542605400	Si	8.831214905	7.154314995	12.507973671
Si	16.636497498	2.274142265	10.387777328	Si	16.645389557	2.306616783	10.393523216	Si	16.646495819	2.252105236	10.329908371
Al	7.830226421	6.180408478	1.186844110	Al	7.820686817	6.176936150	1.188817501	Al	7.841575623	6.223735809	1.164476991
Al	17.381357193	6.164767742	1.240428686	Al	17.387460709	6.163547039	1.302853465	Al	17.400264740	6.167927265	1.217880964
Al	7.209494114	5.430332661	10.613772392	Al	7.229218483	5.422849655	10.621322632	Al	7.187767506	5.416747093	10.571565628
Al	16.680271149	5.425747871	10.589423180	Al	16.676643372	5.446161747	10.590081215	Al	16.717071533	5.401562214	10.572280884
O	1.573575854	1.750034928	8.447566032	O	1.587874174	1.779972315	8.459847450	O	1.574773908	1.768274307	8.377218246
O	0.010597736	0.065310434	3.062578678	O	0.017802283	0.077783614	3.114636898	O	0.013885051	0.088238493	3.109139442
O	7.966183186	2.094535351	2.341101646	O	7.976822853	2.087937832	2.331895590	O	8.000733376	2.143151045	2.322337866
O	2.910420895	0.211815894	0.243759334	O	2.900109768	0.269447267	0.239840657	O	2.963545322	0.293182552	0.177716061
O	1.495423079	8.155695915	2.337109089	O	1.479119539	8.184214592	2.310346127	O	1.476229548	8.256625175	2.254095316
O	-0.109368600	2.883914948	0.247429624	O	-0.065007851	2.955102444	0.270134181	O	0.004090166	3.019950628	0.238785878
O	6.271038532	6.915634155	0.857359529	O	6.244266987	6.893975735	0.895872056	O	6.275550842	6.967092514	0.875549078
O	8.101377487	8.699844360	6.444577217	O	8.106903076	8.699185371	6.442361355	O	8.099370003	8.701883316	6.361026764
O	6.461787701	0.411345065	7.064900875	O	6.483633995	0.442708731	7.069899082	O	6.487470150	0.422111094	7.048573017
O	8.149659157	5.818853378	9.210639954	O	8.185323715	5.820210457	9.231376648	O	8.136500359	5.799707890	9.167220116
O	0.110972345	6.479061604	6.998142719	O	0.117053628	6.517290115	7.009309292	O	0.083222508	6.517296791	6.964589596
O	4.951604843	8.396179199	9.180594444	O	4.943500519	8.372573853	9.140089989	O	4.918394089	8.384909630	9.130417824
O	1.296893120	6.224541664	9.363528252	O	1.268087626	6.272879601	9.392425537	O	1.335207939	6.265293598	9.294532776
O	-0.682088733	1.864154816	6.990651608	O	-0.665893257	1.906952024	6.998557568	O	-0.688308239	1.924696326	6.915185928
O	6.127967834	9.120042801	2.428253651	O	6.132550716	9.119890213	2.436906576	O	6.124203205	9.196926117	2.400512934
O	6.072584152	1.593091846	9.440994263	O	6.120347977	1.555095434	9.477403641	O	6.089229584	1.572518587	9.430771828
O	18.018932343	6.843227863	2.673197031	O	18.029184341	6.857400417	2.725539923	O	18.055473328	6.870188713	2.632298946
O	1.910679102	-0.484671742	7.009106159	O	1.959672570	-0.464280695	7.035743713	O	1.949834108	-0.473701060	6.968681335
O	0.529531121	7.782853603	4.749214649	O	0.601197958	7.814889431	4.763037682	O	0.600595832	7.779899597	4.703292370
O	4.004620552	0.774922252	8.059342384	O	4.032183170	0.819926560	8.082531929	O	4.024056435	0.815780282	7.999077320
O	7.535740376	4.491885662	1.328909993	O	7.550101280	4.483302116	1.317603469	O	7.565136909	4.528655529	1.281898856
O	7.529031754	0.925972581	4.707268238	O	7.546896935	0.939161658	4.708532810	O	7.520726681	0.969840527	4.683289528
O	3.949780703	8.005064011	1.453376293	O	3.941238880	8.049921036	1.451306939	O	3.948724985	8.057991028	1.437412381
O	0.389624178	4.071195126	8.081775665	O	0.408774316	4.108395100	8.090744019	O	0.375233412	4.101785183	8.069655418
O	10.968693733	1.719013810	8.271367073	O	11.006015778	1.729100227	8.275176048	O	10.998922348	1.720054626	8.268901825
O	9.418566704	0.034016609	3.066769838	O	9.426963806	0.031347215	3.070991039	O	9.419422150	0.058214217	3.057667255
O	17.357553482	2.135950804	2.394180775	O	17.398235321	2.131298542	2.397261143	O	17.425642014	2.149804354	2.329962730
O	12.311039925	0.236178532	0.253807455	O	12.335365295	0.248286515	0.268830419	O	12.379188538	0.272380084	0.216903299
O	10.916909218	8.164022446	2.343680382	O	10.923597336	8.164076805	2.347600222	O	10.942625046	8.242148399	2.324908495
O	9.404148102	2.891841173	0.246791899	O	9.410868645	2.870047331	0.233443037	O	9.406189919	2.886292458	0.188150197
O	15.633338928	6.873032570	1.105835676	O	15.649895668	6.888971806	1.119534135	O	15.666156769	6.896152973	1.031061411
O	17.476209641	8.636258125	6.453539371	O	17.529026031	8.687767029	6.434019566	O	17.528110504	8.706027985	6.332733631
O	15.886840820	0.429871976	7.080439091	O	15.927469254	0.444232166	7.103345394	O	15.923073769	0.416482687	7.048725605
O	17.502132416	5.826191902	9.131834984	O	17.481472015	5.839052677	9.118814468	O	17.540300369	5.893236160	9.148284912
O	9.484626770	6.487260342	7.003601551	O	9.493039131	6.494384766	7.019566059	O	9.465208054	6.482058525	6.966565609
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O	10.782304764	6.228364468	9.303460121	O	10.824485779	6.231503487	9.308474541	O	10.774970055	6.225335598	9.262605667

O	8.664789200	1.936442018	6.905468464	O	8.711964607	1.937654257	6.899796963	O	8.711192131	1.926598787	6.874467850
O	15.557847023	9.123621941	2.521353483	O	15.564790726	9.138067245	2.535349846	O	15.591376305	9.156890869	2.441850662
O	15.472856522	1.690609217	9.398748398	O	15.487817764	1.694939375	9.417722702	O	15.472198486	1.630334377	9.381684303
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O	10.727962494	8.845125198	6.937193871	O	11.426348686	-0.543056369	6.932513237	O	10.702005386	8.837118149	6.932581425
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O	13.423330307	0.740909576	8.053672791	O	13.448865891	0.725825131	8.049906731	O	13.440391541	0.677601695	7.997921944
O	16.903764725	4.520658493	1.340863943	O	16.911104202	4.523031712	1.424291492	O	16.903863907	4.527673721	1.326350331
O	17.004539490	0.966656387	4.757104874	O	16.997621536	1.004141927	4.770549297	O	16.945976257	1.019967794	4.703127861
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O	-0.657808423	-0.657112122	12.502125740	O	-0.639356136	-0.602410078	12.534916878	O	-0.739156902	-0.781304598	12.397070885
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O	16.122457504	2.395099878	0.045299876	O	16.169395447	2.429577112	0.056269825	O	14.891010284	0.905872464	18.678932190
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O	4.757224560	4.423737049	13.763305664	O	4.715037346	4.519016743	13.734504700	O	4.625803471	4.532703400	13.876693726
O	1.689139247	2.480835438	15.700318336	O	1.309312701	4.511401653	14.748249054	O	0.771939516	1.831836939	13.943786621
Cu	3.999077797	2.936799765	12.805821419	Cu	3.942098141	2.954027176	12.883110046	Cu	3.934052467	2.900642157	13.080323219
Cu	4.447317123	4.064069748	15.644113541	Cu	4.384681702	3.979948044	15.585240364	Cu	4.452426910	4.032320023	15.755614281
H	14.996109009	6.138527393	1.013542295	H	15.006848335	6.162452221	1.004136086	H	15.024759293	6.162827969	0.950779378
H	2.791259766	0.766912818	12.941082954	H	3.150395870	0.556626678	13.134336472	H	2.272908211	1.071688771	12.987510681
H	2.975819349	1.008753896	11.324773788	H	2.888530493	0.889030337	11.538458824	H	3.035114527	0.951624632	11.516652107
H	4.249001026	0.454918385	12.213718414	H	4.397108078	0.528687596	12.079939842	H	3.785497427	0.358844519	12.854166031
H	3.693429470	4.788002968	11.101910591	H	3.731964111	4.718452930	11.059046745	H	3.719762087	4.711521626	11.312222481
H	4.890792370	3.759967804	10.638895035	H	4.949950218	3.691566467	10.690808296	H	4.902513981	3.668345451	10.875200272
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H	4.078220844	4.217507362	18.225896835	H	3.915074587	4.126757145	18.185327530	H	3.986375332	4.245899677	18.330316544
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H	4.353069782	2.655053139	17.803436279	H	4.321311951	2.594420910	17.784217834	H	4.203680038	2.669623613	17.926939011
H	5.885241985	6.213190556	15.648062706	H	5.882385731	6.071799278	15.627096176	H	5.789135933	6.208860397	15.664011002
H	4.785612106	6.286004066	16.859252930	H	4.785818100	6.191486359	16.831754684	H	4.751648426	6.298108101	16.927326202
H	6.130001068	5.386314392	17.056600571	H	6.116801739	5.284001827	17.056701660	H	6.129765511	5.441708565	17.089439392
H	5.580153942	4.817147732	13.423875809	H	5.604264736	4.782821655	13.436532021	H	5.496014595	4.809517860	13.536605835
H	0.093630791	4.329583645	14.018201828	H	0.780085802	1.531858325	13.537920952	H	-0.754648089	4.409028530	13.208500862
H	-0.863456130	3.692195892	12.872473717	H	2.226041317	2.010936260	14.722305298	H	3.253265619	1.825021386	15.314662933
H	-0.223096848	2.733993530	14.026260376	H	0.297147274	2.066608429	15.053491592	H	-0.894943833	3.328698635	14.647850037
N	3.448211432	1.103765845	12.228557587	N	3.535323858	1.040807962	12.319398880	N	3.193228245	1.120905995	12.513106346
N	3.928173780	3.793092728	11.021236420	N	3.970211744	3.722079515	11.025936127	N	3.937132597	3.711469650	11.252268791
N	3.885759830	3.515909672	17.489835739	N	3.792843580	3.411495686	17.452125549	N	3.768257618	3.542659998	17.604082108
N	5.409706116	5.646196365	16.353816986	N	5.401042938	5.528724194	16.346738815	N	5.369801998	5.658840179	16.416088104
N	2.348624706	1.979320645	14.823780060	N	1.615556359	3.728873730	13.941346169	N	0.485817015	2.845491409	13.258993149
N	-0.008782864	3.516867876	13.405039787	N	1.077118158	1.992815971	14.399336815	N	-0.460527301	3.589919329	13.754899979

Structure N ₂				Structure O ₂			Structure P ₂				
Si	0.130352736	2.512420654	8.197725296	Si	0.114696443	2.468727589	8.182585716	Si	0.111344039	2.443337202	8.249779701
Si	7.952978134	0.735113561	3.111871481	Si	7.931901455	0.723283291	3.105977058	Si	7.950971127	0.683286905	3.169215918
Si	2.446456194	8.227173805	0.902027845	Si	2.424883604	8.196546555	0.904668450	Si	2.419319868	8.218028069	0.950245500
Si	5.536282063	8.344120979	1.143295646	Si	5.511710167	8.326664925	1.136605024	Si	5.530155659	8.295038223	1.184905887
Si	7.891477108	0.668753743	6.224248886	Si	7.860537529	0.653152645	6.223788738	Si	7.855834484	0.619890094	6.277751446
Si	0.089865208	5.698505402	8.312045097	Si	0.061341703	5.640662193	8.305376053	Si	0.053642452	5.616729259	8.341883659
Si	0.154376090	7.987277985	6.206350803	Si	0.139259964	7.947826385	6.201116562	Si	0.121147633	7.915413857	6.251277924
Si	5.579743862	0.444205821	8.375821114	Si	5.574618340	0.393805981	8.387970924	Si	5.570557117	0.380983055	8.431371689
Si	2.470530748	0.415346265	8.203131676	Si	2.438155651	0.357910931	8.215163231	Si	2.441074848	0.338625968	8.260749817
Si	0.152915314	8.079949379	3.115981102	Si	0.126014963	8.040218353	3.109357595	Si	0.144371107	8.038809776	3.164861679
Si	7.966885567	3.025698185	0.946572661	Si	7.943994522	3.006068230	0.945806324	Si	7.979905128	2.983993053	1.012683153
Si	9.553073883	2.495210409	8.151535988	Si	9.526038170	2.488716125	8.148837090	Si	9.509654999	2.456408739	8.222276688
Si	17.407178879	0.775431395	3.106680155	Si	17.375539780	0.734485269	3.097322464	Si	17.384641647	0.728411436	3.171834707
Si	11.828331947	8.219242096	0.961227000	Si	11.781563759	8.195757866	0.932431221	Si	11.794302940	8.182131767	1.018428922
Si	14.918011665	8.422485352	1.173078060	Si	14.892510414	8.398731232	1.142660022	Si	14.904443741	8.378021240	1.225553393
Si	17.336641312	0.681060195	6.221400738	Si	17.321788788	0.638053894	6.207583427	Si	17.301963806	0.598798394	6.278441429
Si	9.515592575	5.640215874	8.352197647	Si	9.464817047	5.631284237	8.350779533	Si	9.464082718	5.594532967	8.434246063
Si	9.540044785	7.935642719	6.218698978	Si	9.520882607	7.928667545	6.211384773	Si	9.499467850	7.880397797	6.286867619
Si	15.006360054	0.457326412	8.331088066	Si	14.973586082	0.450791597	8.309293747	Si	14.960297585	0.427137554	8.378615379
Si	11.854789734	0.349606812	8.174569130	Si	11.843508720	0.356768787	8.142406464	Si	11.816622734	0.316723406	8.227049828
Si	9.548726082	8.030695915	3.123834372	Si	9.534432411	8.011036873	3.116848946	Si	9.537428856	7.987633228	3.196099758
Si	17.388355255	3.041061640	0.910179734	Si	17.329238892	3.017307997	0.910140991	Si	17.374763489	2.993640184	0.978765190
Si	-0.535605013	1.775643110	17.530279160	Si	-0.578164220	1.754514694	17.517448425	Si	-0.566888571	1.748795152	17.583673477
Si	7.269649029	-0.053793430	12.454180717	Si	7.196374416	-0.059327960	12.441770554	Si	7.191082954	-0.096291304	12.518802643
Si	1.737619281	7.471636772	10.281531334	Si	1.707958460	7.404892445	10.279767990	Si	1.708262205	7.390047073	10.323700905
Si	4.835537910	7.574391365	10.534492493	Si	4.817097187	7.567820549	10.553808212	Si	4.817150593	7.545325756	10.612080574
Si	7.258540154	-0.086144567	15.593147278	Si	7.211692810	-0.110671163	15.586790085	Si	7.234954834	-0.113325000	15.661707878
Si	-0.535439909	4.952492714	17.712442398	Si	-0.565994442	4.917221069	17.699090958	Si	-0.570926368	4.919941902	17.752683640
Si	-0.498747349	7.225736618	15.558060646	Si	-0.538036227	7.210618973	15.566229820	Si	-0.516364336	7.205481529	15.613725662
Si	4.907024384	-0.232898712	17.701848984	Si	4.865252495	-0.260298967	17.703891754	Si	4.891149521	-0.270316720	17.775306702
Si	1.798049808	-0.326072216	17.493013382	Si	1.765698671	-0.356092691	17.503477097	Si	1.780503750	-0.361819386	17.540512085
Si	-0.557118714	7.280365467	12.464865685	Si	-0.576834559	7.261595726	12.462653160	Si	-0.576385856	7.251837730	12.508466721
Si	7.287685871	2.237386227	10.326229095	Si	7.276339531	2.217948437	10.329031944	Si	7.250479221	2.196605206	10.394701004
Si	8.884553909	1.733279228	17.556243896	Si	8.851483345	1.720941424	17.540714264	Si	8.892760277	1.709705114	17.628629684
Si	16.711048126	-0.006884038	12.470926285	Si	16.697975159	-0.031781077	12.451489449	Si	16.694967270	-0.035761654	12.516998291
Si	11.102359772	7.442449093	10.276663780	Si	11.071802139	7.456654549	10.278009415	Si	11.056739807	7.421366692	10.340324402
Si	14.210269928	7.668696880	10.510771751	Si	14.173239708	7.646264553	10.498358727	Si	14.161502838	7.642454147	10.581047058
Si	16.672300339	-0.090524554	15.595727921	Si	16.634458542	-0.093799710	15.575478554	Si	16.643014908	-0.093538642	15.642925262
Si	8.847839355	4.903630733	17.725671768	Si	8.799714088	4.887957096	17.692884445	Si	8.798598289	4.885544777	17.779745102
Si	8.923949242	7.191486835	15.592132568	Si	8.855919838	7.189713478	15.574999809	Si	8.880965233	7.178039074	15.660260201
Si	14.343059540	-0.255001307	17.695680618	Si	14.303132057	-0.276811004	17.685922623	Si	14.335027695	-0.314149022	17.757045746
Si	11.228502274	-0.370680928	17.549936295	Si	11.168274879	-0.382471561	17.538850784	Si	11.199228287	-0.391416550	17.636827469
Si	8.855527878	7.141119003	12.492360115	Si	8.825441360	7.139856339	12.460900307	Si	8.814754486	7.094375134	12.560658455

Si	16.664699554	2.267887354	10.301002502	Si	16.632085800	2.247522593	10.286477089	Si	16.628005981	2.239156961	10.342350006
Al	7.859497547	6.219502449	1.136362314	Al	7.846866131	6.197506905	1.130818963	Al	7.830529213	6.183343410	1.186918378
Al	17.442802429	6.193457127	1.181466699	Al	17.398155212	6.155226707	1.164327502	Al	17.416494370	6.143757820	1.218324065
Al	7.196174622	5.409053802	10.571673393	Al	7.188706875	5.377821445	10.574520111	Al	7.177722454	5.336668491	10.689601898
Al	16.690620422	5.423986435	10.496042252	Al	16.655279160	5.397583008	10.492576599	Al	16.650865555	5.388442039	10.533980370
O	1.588801980	1.782778263	8.349723816	O	1.566168070	1.733154178	8.360699654	O	1.571112871	1.715153933	8.412319183
O	0.035162106	0.109079301	3.018809557	O	0.004150152	0.066412777	3.026890278	O	0.009797081	0.058641851	3.094059706
O	8.006445885	2.142693520	2.308244944	O	8.006422043	2.137528896	2.315480471	O	8.027534485	2.083492756	2.357418299
O	2.990192890	0.260884225	0.099770173	O	2.985732794	0.234895229	0.114628874	O	2.940117359	0.248394042	0.157881171
O	1.477746606	8.241789818	2.188698292	O	1.452788830	8.218683243	2.188366890	O	1.478057623	8.234743118	2.260495186
O	0.014755426	2.945805788	0.165786698	O	-0.057783622	2.955021620	0.139510453	O	-0.000372691	2.913976908	0.232115313
O	6.291099072	6.963498116	0.852259338	O	6.283632278	6.953882694	0.875516653	O	6.246261120	6.890712738	0.931225598
O	8.104091644	8.711157799	6.334733486	O	8.083238602	8.700817108	6.336760044	O	8.065317154	8.659618378	6.393823147
O	6.495277405	0.425748587	7.037115574	O	6.452578068	0.410494328	7.020626545	O	6.446435928	0.375112176	7.067065239
O	8.152727127	5.775998592	9.169630051	O	8.073603630	5.751581669	9.121137619	O	8.111882210	5.708634377	9.273675919
O	0.094606817	6.512793541	6.893924236	O	0.086392105	6.483488560	6.906248093	O	0.075323403	6.438859463	6.931295395
O	4.938931465	8.390646935	9.118389130	O	4.966655731	8.328737259	9.107241631	O	4.982490540	8.331982613	9.182977676
O	1.319164753	6.286612511	9.247383118	O	1.273977518	6.202771664	9.272516251	O	1.269386292	6.206485748	9.293549538
O	-0.688318253	1.926003575	6.905050755	O	18.156185150	1.875526071	6.883062363	O	18.136438370	1.821001410	6.978196621
O	6.142914772	9.184788704	2.391914606	O	6.107033730	9.204864502	2.364674568	O	6.150236607	9.130885124	2.438373327
O	6.087295532	1.577051759	9.423541069	O	6.096674919	1.524346471	9.425649643	O	6.086316109	1.528536797	9.455801964
O	18.056020737	6.873311043	2.630313635	O	18.033031464	6.845671654	2.592648983	O	18.056882858	6.841137886	2.643147230
O	1.945983171	-0.470886886	6.956796646	O	1.935750961	-0.495717824	6.931857586	O	1.904849768	-0.540866435	7.014984131
O	0.619177997	7.847470760	4.661296844	O	0.581637681	7.777438641	4.652047157	O	0.593652487	7.775584221	4.710914135
O	4.031113148	0.814435124	7.980750561	O	4.006785393	0.740577161	8.050650597	O	4.007366657	0.717038929	8.061719894
O	7.580860615	4.524902821	1.263038635	O	7.546439171	4.505185604	1.249356866	O	7.608590126	4.482977390	1.334174514
O	7.525259495	0.991452336	4.667679310	O	7.499138355	0.964308143	4.662193775	O	7.506724358	0.948945045	4.720660210
O	3.961239100	8.063685417	1.439563513	O	3.940304279	8.010297775	1.431583166	O	3.942911863	8.059656143	1.455104709
O	0.388893902	4.109798431	8.026412010	O	0.374874771	4.061719418	7.985930443	O	0.372811615	4.034074783	8.038392067
O	10.991579056	1.722723961	8.265545845	O	10.970426559	1.721852779	8.242994308	O	10.954042435	1.689931393	8.303243637
O	9.426630020	0.058070675	3.055372953	O	9.399049759	0.031415284	3.046617508	O	9.436300278	0.026391357	3.156548262
O	17.425367355	2.164959908	2.283581495	O	17.402240753	2.123583555	2.270291805	O	17.413085938	2.122594595	2.355656385
O	12.452067375	0.270500004	0.203877434	O	12.363956451	0.244234398	0.179282755	O	12.387689590	0.240091801	0.278317690
O	10.953782082	8.262387276	2.306238651	O	10.942443848	8.241622925	2.300563574	O	10.948354721	8.209370613	2.381399870
O	9.405533791	2.862012863	0.160063848	O	9.379707336	2.857728720	0.151828945	O	9.427452087	2.835175514	0.233569905
O	15.703131676	6.913168907	0.994032145	O	15.659901619	6.879224300	0.969923913	O	15.665854454	6.853440762	1.081079364
O	17.529115677	8.707927704	6.323296070	O	17.508419037	8.660363197	6.304626942	O	17.482997894	8.616518974	6.354936123
O	15.916377068	0.432899773	6.987681866	O	15.906649590	0.408516586	6.983171463	O	15.877760887	0.368932843	7.041743279
O	17.526737213	5.888805389	9.069762230	O	17.486829758	5.816699505	9.047403336	O	17.477827072	5.795647144	9.081356049
O	9.456135750	6.495129585	6.958541393	O	9.449193954	6.493185043	6.958920002	O	9.393088341	6.448383331	7.040678978
O	14.490749359	8.405403137	9.102159500	O	14.423955917	8.401376724	9.093179703	O	14.422573090	8.385919571	9.172210693
O	10.791511536	6.227820396	9.242594719	O	10.711914063	6.222177029	9.283413887	O	10.741539955	6.198544025	9.315542221
O	8.706752777	1.934049368	6.866792679	O	8.667437553	1.922430992	6.872034550	O	8.649980545	1.881669044	6.952726841
O	15.597061157	9.160241127	2.430206776	O	15.564512253	9.125949860	2.411043406	O	15.574899673	9.123870850	2.482866526

O	15.517469406	1.614620447	9.341858864	O	15.484915733	1.612857103	9.316273689	O	15.487759590	1.597960234	9.367609024
O	8.686884880	6.841413498	2.510853529	O	8.688081741	6.812399864	2.501472950	O	8.664664268	6.824737549	2.553855896
O	11.399897575	-0.543026865	6.901663303	O	11.382432938	-0.541455686	6.877219200	O	10.667411804	8.792171478	6.978607178
O	9.955462456	7.720686436	4.670441151	O	9.939681053	7.706472874	4.663827896	O	9.936866760	7.659338474	4.744895935
O	13.442399025	0.703460097	7.986910343	O	13.424689293	0.729801476	7.927635193	O	13.400886536	0.685023606	8.024623871
O	16.981618881	4.543733120	1.259101033	O	16.909696579	4.515202045	1.272196412	O	16.951194763	4.495398998	1.317321301
O	17.003566742	1.040981412	4.663185120	O	16.965522766	0.993028104	4.652854443	O	16.965694427	0.977756202	4.727652073
O	13.391619682	7.975537300	1.419220924	O	13.358862877	7.966012955	1.354302883	O	13.369242668	7.951583385	1.445741057
O	9.856308937	4.079753399	7.975487232	O	9.827634811	4.074377537	7.970126629	O	9.816245079	4.040112972	8.039938927
O	0.937848210	1.055398464	17.612043381	O	0.866781712	0.995148778	17.632263184	O	0.879034877	0.991691828	17.626968384
O	-0.658139586	-0.678140402	12.394019127	O	-0.656563044	-0.686474562	12.380579948	O	-0.664616406	-0.699464440	12.423409462
O	7.443952560	1.375063896	11.711623192	O	7.442986012	1.367920399	11.718592644	O	7.419145584	1.322426796	11.773230553
O	2.309608459	-0.433319479	9.601346016	O	2.212682724	-0.512181461	9.591215134	O	2.259338856	-0.514006615	9.652029991
O	0.809434831	7.485631943	11.608587265	O	0.816964209	7.403994560	11.638901711	O	0.812279463	7.396999836	11.675289154
O	-0.710789263	2.181097984	9.564067841	O	-0.744140506	2.168951511	9.546491623	O	-0.736877799	2.169985056	9.623703957
O	5.649565220	6.215636253	10.515083313	O	5.672448635	6.239252567	10.636471748	O	5.672977448	6.215983391	10.690925598
O	7.454431534	7.932198524	15.714583397	O	7.365422249	7.885042191	15.721282005	O	7.395217896	7.888098717	15.770208359
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O	-0.511892676	5.787531376	16.305450439	O	-0.563282132	5.762127399	16.296079636	O	-0.571909249	5.759380341	16.345891953
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O	0.732349873	5.490308762	18.625715256	O	0.684044600	5.475796223	18.616199493	O	0.667200804	5.495517254	18.672367096
O	-1.342753291	1.165614843	16.238801956	O	17.446550369	1.178145528	16.214523315	O	17.409524918	1.196942925	16.297948837
O	5.977203369	-0.822371900	11.784839630	O	5.860245705	-0.764092684	11.783612251	O	5.864640713	-0.819433331	11.868150711
O	5.409366608	0.973569393	18.652898788	O	5.379929543	0.920568824	18.677902222	O	5.429352283	0.921329975	18.724143982
O	17.355175018	6.097359657	11.926532745	O	17.331909180	6.084905148	11.913471222	O	17.336744308	6.077773571	11.946578979
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O	6.798563004	3.711437225	10.705823898	O	6.764170647	3.686147690	10.692111015	O	6.730102539	3.651984930	10.799439430
O	6.907404423	0.207057714	14.031888008	O	6.871466637	0.199048162	14.028709412	O	6.878292561	0.222294807	14.103117943
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O	10.215366364	7.376232147	11.618525505	O	10.182744026	7.493932247	11.619027138	O	10.148071289	7.398311615	11.669163704
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O	16.922504425	5.170948029	18.489652634	O	16.875644684	5.086067200	18.458887100	O	16.860893250	5.088375568	18.499027252
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O	14.867302895	0.932931423	18.652431488	O	14.799607277	0.914684176	18.656394958	O	14.859825134	0.870171666	18.720441818
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O	16.313777924	0.248508215	14.033669472	O	16.285932541	0.200313449	14.009300232	O	16.302112579	0.214127302	14.076193810
O	12.670065880	7.299818039	10.775102615	O	12.639867783	7.260784149	10.777069092	O	12.624206543	7.258323193	10.846737862
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Cu	3.984358788	2.755017757	13.139677048	Cu	4.166997910	3.989632130	15.842043877	Cu	4.452998638	3.974565983	15.557523727
Cu	4.444670677	3.988030910	15.801182747	H	15.022108078	6.142329216	0.894624949	H	15.027941704	6.116863251	1.007752061
H	15.077764511	6.181427956	0.825132906	H	2.616444111	0.761920750	11.810546875	H	2.636858940	0.885026574	11.504433632
H	2.878077030	0.424337029	13.222229958	H	4.109550476	0.410040021	12.401116371	H	4.039515972	0.538554072	12.282845497
H	2.922656536	0.849650204	11.640965462	H	2.796611071	0.364787698	13.387845993	H	2.621033192	0.557307363	13.108481407
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H	3.673667908	4.559518814	11.393726349	H	4.900244236	3.516510248	11.086779594	H	4.715044498	3.634561539	10.874207497
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H	3.987903118	4.244822025	18.364658356	H	2.667843342	3.325773716	17.792539597	H	2.939704657	3.147670746	17.439096451
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H	13.979005814	2.244091511	15.202795029	H	1.338249207	4.671142578	13.308171272	H	1.094788313	4.515533447	13.394546509
H	3.565178871	1.570167780	15.483825684	H	0.548673451	3.459720135	12.535553932	H	0.308598936	3.287231445	12.634838104
H	15.359213829	2.586005449	14.623626709	H	0.940171003	3.313606739	14.122540474	H	0.885004163	3.090602160	14.159233093
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			N 6.562563419 3.442371845 14.683748245		
ts5			Structure A		
Si 0.092674077	2.443238974	8.288076401	Si 0.062787652	2.488001347	8.345581055
Si 7.922149658	0.706389308	3.207546711	Si 7.904357910	0.665149331	3.259986162
Si 2.398022175	8.198570251	0.980299294	Si 2.393449068	8.193976402	1.060106397
Si 5.523376942	8.325926781	1.238930583	Si 5.480361462	8.289840698	1.301761866
Si 7.859600544	0.657290280	6.327646732	Si 7.845445633	0.622872889	6.378610611
Si 0.051336288	5.605600834	8.400504112	Si 0.008716166	5.645285606	8.477866173
Si 0.127619952	7.916281223	6.278968811	Si 0.099183977	7.963845730	6.343591690
Si 5.550834179	0.418547869	8.472402573	Si 5.519732475	0.438694954	8.529117584
Si 2.421811104	0.339958906	8.248893738	Si 2.402659893	0.385964811	8.302776337
Si 0.123156190	8.017143250	3.199718237	Si 0.090992168	8.029586792	3.257080078
Si 7.927308559	3.013962269	1.049927354	Si 7.942065239	2.954846859	1.130996823
Si 9.515876770	2.487674952	8.274030685	Si 9.493626595	2.459733963	8.312067986
Si 17.397975922	0.736850381	3.216431856	Si 17.347429276	0.731312215	3.280567169
Si 11.790156364	8.216218948	1.062097073	Si 11.755349159	8.166297913	1.134072661
Si 14.891875267	8.404489517	1.267266154	Si 14.869935036	8.384332657	1.336425543
Si 17.289239883	0.583748043	6.321117401	Si 17.260391235	0.630059958	6.387560844
Si 9.473568916	5.630197525	8.485372543	Si 9.481692314	5.572020531	8.533293724
Si 9.496741295	7.926910877	6.347669601	Si 9.475055695	7.891253471	6.418738842
Si 14.958713531	0.428103566	8.423170090	Si 14.938700676	0.439409137	8.513181686
Si 11.819630623	0.348475933	8.304536819	Si 11.788895607	0.310288310	8.387834549
Si 9.511537552	7.992911339	3.257338762	Si 9.501029015	7.912405968	3.323530436
Si 17.345785141	3.007602692	1.033086896	Si 17.318237305	3.007810831	1.083491921
Si -0.583715439	1.749697804	17.629241943	Si -0.598461330	1.759216070	17.685394287
Si 7.176504135	-0.070585191	12.553318977	Si 7.214650631	-0.120704710	12.618648529
Si 1.674832702	7.380191803	10.356374741	Si 1.670297146	7.440359116	10.426955223
Si 4.788566589	7.567880630	10.639564514	Si 4.795577526	7.525369167	10.652233124
Si 7.201005936	-0.044030190	15.702010155	Si 7.185035706	-0.129016280	15.755331039
Si -0.596585631	4.913640499	17.780757904	Si -0.609851599	4.920304775	17.840480804
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Si 4.864687920	-0.235906124	17.832666397	Si 4.849269867	-0.309078574	17.889318466
Si 1.741668463	-0.363812804	17.600294113	Si 1.752624273	-0.353188992	17.674568176
Si -0.597113013	7.273500919	12.559950829	Si -0.579921186	7.315291405	12.626973152
Si 7.230921268	2.224476814	10.429654121	Si 7.205162525	2.209357262	10.513438225
Si 8.851428986	1.755967259	17.649139404	Si 8.839946747	1.696177721	17.711147308
Si 16.676624298	-0.024270773	12.575532913	Si 16.642980576	-0.008229971	12.652489662
Si 11.058732986	7.430991650	10.407912254	Si 11.051852226	7.387017250	10.464423180
Si 14.151811600	7.642010689	10.648439407	Si 14.143799782	7.648802757	10.716362000
Si 16.618064880	-0.101257205	15.690223694	Si 16.598596573	-0.086684227	15.758796692
Si 8.840837479	4.912421227	17.858530045	Si 8.792438507	4.852350235	17.933084488
Si 8.866517067	7.217937469	15.718034744	Si 8.846116066	7.150432110	15.771381378
Si 14.305416107	-0.287519336	17.803174973	Si 14.290580750	-0.305965662	17.875734329
Si 11.179194450	-0.361166954	17.665798187	Si 11.148553848	-0.418692946	17.727550507

Si	8.780017853	7.116415501	12.607361794	Si	8.792591095	7.094665527	12.677877426
Si	16.627431870	2.247542858	10.384926796	Si	16.598367691	2.267534971	10.469292641
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O	2.875792980	0.232911557	0.208103240	O	2.951462030	0.241259620	0.288322270
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O	4.947702408	8.369419098	9.220874786	O	4.888851166	8.384223938	9.260931969
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O	6.079005241	9.178920746	2.515785456	O	6.716623783	-0.173386633	2.527254581
O	6.047424793	1.564057708	9.509658813	O	5.993186474	1.568361878	9.605660439
O	18.000165939	6.851620674	2.676028013	O	17.990669250	6.849648952	2.725703001
O	1.925085068	-0.483704388	6.950272560	O	1.903815389	-0.434426606	7.001310825
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O	3.988112211	0.742031336	8.097841263	O	3.965786934	0.799546599	8.145747185
O	7.556887627	4.499518394	1.416295409	O	7.528587818	4.437982082	1.466683865
O	7.517448902	0.981969833	4.769423485	O	7.485420227	0.919118583	4.822362423
O	3.931730986	8.056652069	1.459013224	O	3.902847052	7.988768101	1.588823557
O	0.353059411	4.030331135	8.053055763	O	0.356957793	4.077155113	8.133161545
O	10.958853722	1.722231627	8.410418510	O	10.916325569	1.674154520	8.491912842
O	9.394384384	0.019198090	3.168912649	O	9.337552071	-0.092976391	3.211038351
O	17.426761627	2.141820908	2.414849281	O	17.375583649	2.119210720	2.452460766
O	12.366312027	0.262654841	0.302325428	O	12.299944878	0.204812974	0.360675693
O	10.894424438	8.205072403	2.389812708	O	10.896884918	8.162428856	2.487365484
O	9.366935730	2.892827988	0.239784583	O	9.380914688	2.847896576	0.319146454
O	15.631031036	6.871645927	1.106727481	O	15.618841171	6.860562325	1.150111198
O	17.491569519	8.615682602	6.405500412	O	17.461502075	8.659483910	6.476651669
O	15.866005898	0.324849188	7.080271244	O	15.849179268	0.381774664	7.170710564
O	17.467826843	5.792974472	9.123995781	O	17.401119232	5.785383224	9.156559944
O	9.413784027	6.489364147	7.097070694	O	9.379164696	6.457493782	7.167256355
O	14.399377823	8.403333664	9.248293877	O	14.411875725	8.400829315	9.314313889
O	10.753302574	6.216537476	9.372056961	O	10.753680229	6.177575588	9.420546532
O	8.677800179	1.910820961	6.994006634	O	8.684231758	1.876819611	7.017032623

O	15.593361855	9.141472816	2.509391069	O	15.542992592	9.111302376	2.602317572
O	15.511801720	1.610540390	9.381879807	O	15.466710091	1.625966311	9.481356621
O	8.647593498	6.776566505	2.713736534	O	8.698725700	6.660965919	2.761269808
O	11.339835167	-0.543356419	7.044828415	O	10.626194000	8.806616783	7.132326126
O	9.948025703	7.726581573	4.807545662	O	9.934947968	7.692188740	4.883290768
O	13.400747299	0.712988913	8.077539444	O	13.370738983	0.683208466	8.179618835
O	16.899425507	4.505011559	1.363749623	O	16.885728836	4.503923416	1.440737009
O	16.960317612	0.969771147	4.770473957	O	16.913040161	0.993800640	4.834878922
O	13.353630066	8.017324448	1.529229403	O	13.330970764	7.984356403	1.571419835
O	9.814126968	4.074120522	8.092780113	O	9.846035004	4.030799389	8.105545998
O	0.860886574	1.000380158	17.711269379	O	0.839610457	0.991482258	17.777023315
O	-0.677088797	-0.670958638	12.501336098	O	-0.720451593	-0.674926400	12.571162224
O	7.409839630	1.346232533	11.804912567	O	7.411533356	1.294117928	11.855890274
O	2.189311504	-0.573377609	9.593417168	O	2.202559948	-0.537291050	9.638712883
O	0.777363718	7.433203697	11.703974724	O	0.816927791	7.566390038	11.809601784
O	-0.726230085	2.188136339	9.684372902	O	-0.775485456	2.232262135	9.726887703
O	5.620834351	6.220472813	10.679704666	O	5.589262009	6.158610821	10.561838150
O	7.400169373	7.974071980	15.844092369	O	7.363609314	7.871572495	15.859002113
O	5.778454304	-0.279832602	16.463647842	O	5.769753456	-0.364932775	16.526836395
O	7.442889214	5.057085037	18.615839005	O	7.364951134	4.995116234	18.633602142
O	-0.601939976	5.753002167	16.372358322	O	-0.611351669	5.761419296	16.430587769
O	4.312677383	7.724873543	18.576070786	O	4.177014828	7.626693249	18.591548920
O	0.650053382	5.479296684	18.694341660	O	2.009108067	6.979711056	0.024574205
O	17.406646729	1.170002580	16.346574783	O	17.385810852	1.184988022	16.407264709
O	5.868091583	-0.817574143	11.899833679	O	5.982715130	-0.938703358	11.923905373
O	6.747320175	2.456291199	0.041938826	O	6.793066025	2.317112446	0.139438123
O	17.310369492	6.104959965	11.993322372	O	17.415681839	6.105160713	12.006479263
O	1.298260331	-1.229341388	16.288124084	O	1.297186732	-1.230408788	16.372274399
O	-0.157370210	6.973182678	14.097828865	O	-0.163268864	6.998690605	14.167121887
O	3.311468124	0.030728698	17.423248291	O	3.316215515	0.080674529	17.448719025
O	6.730240822	3.684698343	10.841099739	O	6.709825516	3.650521994	10.995944023
O	6.862586975	0.251707077	14.133939743	O	6.837810040	0.187307596	14.188613892
O	3.205436468	7.195729733	10.855579376	O	3.201747417	7.196983337	10.901348114
O	-0.298443437	3.339515209	17.414875031	O	-0.311242819	3.347859621	17.477350235
O	10.297505379	1.001437545	17.739986420	O	10.299122810	0.963809013	17.798362732
O	8.521178246	-0.954566598	12.428144455	O	8.620874405	-0.915879667	12.561883926
O	16.687709808	1.374693155	11.765061378	O	16.677022934	1.383712292	11.838445663
O	11.644643784	-0.501308799	9.695552826	O	11.600119591	-0.536561012	9.777459145
O	10.121909142	7.383249760	11.719717026	O	10.143995285	7.307928085	11.793705940
O	8.657678604	2.202010155	9.634700775	O	8.594793320	2.220791578	9.658160210
O	14.887053490	6.103578568	10.467456818	O	14.890156746	6.114633083	10.575103760
O	16.834838867	7.941482544	15.792005539	O	16.830898285	7.965075970	15.853729248
O	15.197727203	-0.359980583	16.448705673	O	15.192747116	-0.374175847	16.530324936
O	16.841892242	5.082013607	18.540416718	O	16.821086884	5.087303162	18.590785980

O	8.769054413	5.760876656	16.442134857	O	8.762115479	5.704441071	16.515838623
O	13.750613213	7.668427467	18.587825775	O	13.761410713	7.661030769	18.671712875
O	11.464014053	6.994421959	0.021800289	O	11.401996613	6.930263042	0.119536616
O	8.024350166	1.228838921	16.315370560	O	8.023675919	1.125329614	16.389213562
O	14.888858795	8.351646423	11.892377853	O	14.849636078	8.370195389	11.969321251
O	16.199825287	2.363811970	0.058395058	O	16.165740967	2.379336834	0.101538517
O	7.986401081	5.781263828	12.209441185	O	7.912887096	5.830381870	12.235190392
O	10.700778961	-1.253025293	16.395324707	O	10.659942627	-1.293318987	16.445589066
O	9.252119064	7.006239891	14.167435646	O	9.262313843	6.892387867	14.231850624
O	12.749572754	0.004346609	17.434333801	O	12.725867271	-0.078077197	17.510068893
O	16.200166702	3.746021271	10.737154961	O	16.173009872	3.762680531	10.845801353
O	16.266952515	0.227283239	14.127977371	O	16.223566055	0.243182540	14.201877594
O	12.616642952	7.261251450	10.937559128	O	12.613851547	7.238230228	10.979442596
O	9.138857841	3.350231171	17.444812775	O	9.103116989	3.295286655	17.503252029
O	3.360630512	1.856170416	14.692348480	O	1.777390957	2.318921089	14.088196754
O	3.779129982	4.389168262	13.870284081	O	4.556569099	3.454470158	13.394040108
Cu	3.277640820	2.721256733	12.964651108	Cu	2.677429914	2.846337318	12.454368591
Cu	4.926688194	4.315089226	15.435473442	Cu	5.137386799	4.044002533	15.082732201
H	14.987795830	6.140803337	1.024574161	H	14.981025696	6.121601105	1.105644584
H	2.574284077	0.778698683	11.265543938	H	2.727821827	0.218674779	12.253082275
H	3.913603783	0.343982041	12.126559258	H	4.055840492	0.802155495	11.466639519
H	2.446578979	0.403378010	12.862707138	H	3.981712341	0.881324649	13.103547096
H	3.388665438	4.568046570	11.073401451	H	3.417993069	4.509672165	10.564827919
H	4.722359657	3.625264645	10.968785286	H	4.349170685	3.181472301	10.433148384
H	3.294237852	3.118529558	10.321811676	H	2.825994015	3.168472290	9.808106422
H	14.239446640	5.379302025	10.363499641	H	14.245891571	5.382223606	10.515015602
H	2.832025051	4.095561504	17.050146103	H	2.992787600	3.855490685	16.606418610
H	3.303471088	2.732440472	16.131874084	H	2.853926659	2.806046724	15.304514885
H	4.055290222	3.148234606	17.602636337	H	3.801737309	2.447566986	16.634788513
H	6.054082394	6.498834610	16.134298325	H	5.870811939	6.291631699	16.103712082
H	4.787674904	6.195238113	17.128379822	H	4.584180355	5.781249046	16.969776154
H	6.214873791	5.446644306	17.377424240	H	6.065061569	5.171180725	17.267433167
H	4.109513760	5.053655624	13.241319656	H	5.261848450	3.557558537	12.726560593
H	3.861404419	1.024471164	14.740251541	H	1.423112750	1.415213704	14.117414474
H	0.930503428	4.186769485	13.413660049	H	2.096892118	5.383769035	12.846555710
H	0.336224377	3.123414516	12.308079720	H	0.853407502	4.739593506	11.976714134
H	0.647339582	2.636290073	13.843120575	H	1.066279650	4.271606922	13.548661232
H	6.513153553	3.019134998	13.889140129	H	7.274782181	3.017839193	14.146211624
H	7.057615280	4.561184883	13.820543289	H	7.312821388	4.600936890	13.694919586
H	7.426541328	3.611109257	15.114291191	H	7.786073685	4.170490265	15.212389946
N	3.036504745	0.873185396	12.172863007	N	3.423493862	0.967912376	12.250971794
N	3.702230215	3.594930172	11.129523277	N	3.385302544	3.487119436	10.605302811
N	3.624996185	3.524674892	16.753118515	N	3.529016972	3.216273308	16.014595032
N	5.563373089	5.749633789	16.630516052	N	5.430476189	5.452748299	16.496908188

N	0.997485638	3.221643448	13.081256866	N	1.557324409	4.531137466	12.686299324
N	6.672725677	3.852992535	14.463729858	N	7.095664501	3.967529297	14.483567238

Table S7. Cartesian coordinates of RC, TS, IM, and PC for cycle III. The structures from A to F are the same as those in Table S5.

Structure G ₃				Structure H ₃				ts3			
Si	0.123453081	2.551858425	8.111183167	Si	0.177241921	2.514806032	8.104107857	Si	0.160102844	2.532066584	8.098523140
Si	7.967732430	0.764650047	3.051858425	Si	8.002029419	0.746678829	3.012587547	Si	7.996063232	0.738525391	3.026687622
Si	2.426109314	8.263879776	0.842182159	Si	2.468835115	8.224849701	0.838591516	Si	2.457997084	8.213848114	0.842463017
Si	5.543925285	8.379703522	1.100468755	Si	5.585228920	8.351881981	1.071654797	Si	5.569439411	8.350424767	1.122260571
Si	7.906554222	0.712535620	6.172687054	Si	7.961997509	0.719059110	6.155089378	Si	7.966343880	0.706351399	6.166296482
Si	0.086347997	5.721328735	8.247645378	Si	0.145122111	5.674674511	8.231168747	Si	0.132212400	5.686505795	8.238596916
Si	0.166939735	8.011688232	6.134830475	Si	0.206307024	7.979840279	6.131366730	Si	0.202882320	7.985532761	6.124999046
Si	5.599462032	0.494137943	8.297962189	Si	5.642168045	0.493661046	8.278084755	Si	5.624126911	0.517491639	8.266117096
Si	2.463080168	0.447828472	8.103330612	Si	2.514201641	0.410481870	8.080696106	Si	2.501889706	0.422937095	8.067117691
Si	0.142084837	8.078055382	3.052813053	Si	0.175567731	8.038078308	3.020790577	Si	0.167017221	8.029564857	3.025006533
Si	7.984808922	3.053752899	0.895925820	Si	8.042730331	3.019817114	0.866111934	Si	8.016327858	3.022387981	0.871402740
Si	9.563755035	2.555931091	8.108778000	Si	9.606044769	2.544958115	8.084616661	Si	9.621704102	2.523897409	8.108431816
Si	17.396528244	0.780701101	3.042559385	Si	17.445590973	0.753614426	3.012705564	Si	17.440536499	0.753061652	3.017544746
Si	11.800999641	8.259466171	0.882205665	Si	11.824940681	8.254827499	0.851670206	Si	11.831986427	8.218605995	0.852357507
Si	14.912207603	8.452354431	1.085201025	Si	14.943882942	8.425400734	1.059517741	Si	14.944368362	8.420000076	1.068040967
Si	17.329513550	0.698024392	6.156201363	Si	17.377920151	0.654309928	6.153488159	Si	17.368200302	0.666862130	6.148520470
Si	9.499400139	5.696785927	8.312355042	Si	9.550491333	5.690045834	8.277235031	Si	9.572996140	5.681411743	8.276158333
Si	9.546391487	7.991321087	6.171287537	Si	9.592739105	7.985008717	6.155695438	Si	9.579841614	7.982595444	6.170449734
Si	15.002559662	0.519597292	8.265663147	Si	15.056890488	0.515261412	8.244553566	Si	15.061734200	0.488111377	8.252871513
Si	11.867694855	0.428871453	8.094962120	Si	11.915354729	0.411994278	8.088548660	Si	11.916623116	0.403539181	8.117074013
Si	9.569233894	8.050765038	3.067092657	Si	9.598686218	8.006521225	3.029397726	Si	9.597142220	8.002154350	3.047344208
Si	17.360994339	3.072592258	0.866120636	Si	17.415203094	3.037233353	0.856540501	Si	17.388607025	3.035037279	0.852311254
Si	-0.550966859	1.824732304	17.471601486	Si	-0.501120567	1.800375223	17.476198196	Si	-0.511272371	1.796177030	17.478235245
Si	7.231354237	0.028194308	12.375006676	Si	7.288428307	0.022102594	12.347828865	Si	7.285436630	-0.006444037	12.356319427
Si	1.721456766	7.514912128	10.199491501	Si	1.778851032	7.471978188	10.185462952	Si	1.767619371	7.490539074	10.183023453
Si	4.836488724	7.668545246	10.462121964	Si	4.897340775	7.658051491	10.419574738	Si	4.885972023	7.627461433	10.373682022
Si	7.232455730	-0.036310673	15.529719353	Si	7.269396782	-0.032752991	15.517605782	Si	7.245082855	-0.081964254	15.514797211
Si	-0.545034766	4.985081673	17.622400284	Si	-0.520388186	4.966518879	17.615516663	Si	-0.527912855	4.952273846	17.606952667
Si	-0.521057963	7.285541534	15.507168770	Si	-0.478702128	7.258184433	15.495958328	Si	-0.486664534	7.248373508	15.491283417
Si	4.907711506	-0.213830352	17.668262482	Si	4.951847076	-0.277975082	17.636957169	Si	4.931371212	-0.264915228	17.656139374
Si	1.772494197	-0.293378830	17.473367691	Si	1.814063191	-0.321928501	17.488193512	Si	1.795574784	-0.334222078	17.490596771
Si	-0.551558971	7.355919838	12.397030830	Si	-0.480968177	7.335830212	12.391600609	Si	-0.484657347	7.331267357	12.398406029
Si	7.291827679	2.321026802	10.265928268	Si	7.331803799	2.305595875	10.248451233	Si	7.331534863	2.289466858	10.250739098
Si	8.875808716	1.788234472	17.480844498	Si	8.916183472	1.788286805	17.445335388	Si	8.897630692	1.752494097	17.442815781
Si	16.712305069	0.046801090	12.398929596	Si	16.767475128	0.027708113	12.390089989	Si	16.763986588	0.031308651	12.403696060
Si	11.095910072	7.526996613	10.231547356	Si	11.156374931	7.510150433	10.206433296	Si	11.161891937	7.487190247	10.214297295
Si	14.197494507	7.719558716	10.468673706	Si	14.265302658	7.711928844	10.454962730	Si	14.265552521	7.699479103	10.467160225

Si	16.654642105	-0.019381046	15.528623581	Si	16.705886841	-0.039411783	15.512459755	Si	16.693073273	-0.048267961	15.513179779
Si	8.789159775	4.955136299	17.639379501	Si	8.812446594	4.944681644	17.608234406	Si	8.833670616	4.908627033	17.629997253
Si	8.872405052	7.253904343	15.525839806	Si	8.926251411	7.247819901	15.513798714	Si	8.901662827	7.206863880	15.509549141
Si	14.324600220	-0.211690664	17.637491226	Si	14.382701874	-0.264352322	17.615587234	Si	14.365444183	-0.274117947	17.613063812
Si	11.194895744	-0.319970846	17.488788605	Si	11.241753578	-0.338852406	17.463960648	Si	11.225608826	-0.372572660	17.455303192
Si	8.850977898	7.226494789	12.405306816	Si	8.907485008	7.220188618	12.377635002	Si	8.885468483	7.219710350	12.385290146
Si	16.660232544	2.333043814	10.223222733	Si	16.722368240	2.314937592	10.210435867	Si	16.714923859	2.313047409	10.218982697
Al	7.868486404	6.242813110	1.085924506	Al	7.908563614	6.199452400	1.064178467	Al	7.916794777	6.195985794	1.115226865
Al	17.425664902	6.207215786	1.098917603	Al	17.445194244	6.177782536	1.070824385	Al	17.437282562	6.161940098	1.068781376
Al	7.189087868	5.461379051	10.506150246	Al	7.247276783	5.449582100	10.467441559	Al	7.220732689	5.451813698	10.430738449
Al	16.691558838	5.475813389	10.443247795	Al	16.760744095	5.447362900	10.432477951	Al	16.749670029	5.437986374	10.439112663
O	1.578349233	1.812860489	8.237711906	O	1.623983145	1.766747236	8.224165916	O	1.601056099	1.772341847	8.206293106
O	0.021645918	0.104435787	2.960823536	O	0.059705630	0.063369110	2.869813681	O	0.055157915	0.059386179	2.890532255
O	8.053741455	2.169305325	2.248001099	O	8.128029823	2.165022612	2.238450766	O	8.105597496	2.143519878	2.226806164
O	2.945804596	0.316986531	0.087514758	O	2.964578629	0.279311955	0.093322605	O	2.973527908	0.273524731	0.104216374
O	1.477877140	8.241568565	2.140623093	O	1.544300199	8.176791191	2.154463768	O	1.532148838	8.176759720	2.155996561
O	-0.021210913	3.018578291	0.100832745	O	0.041392043	2.989836454	0.110886894	O	0.015163763	3.005443335	0.107332610
O	6.286009789	6.981593132	0.887641132	O	6.329580307	6.950034142	0.927581847	O	6.350207329	6.970888615	0.939860106
O	8.092825890	8.736882210	6.301512718	O	8.155307770	8.753131866	6.332117558	O	8.119555473	8.711375237	6.328605175
O	6.478250504	0.498177469	6.935673714	O	6.531237602	0.531529427	6.923170567	O	6.525316238	0.551662743	6.919128418
O	8.102745056	5.831633568	9.066297531	O	8.156789780	5.834102154	9.034842491	O	8.196292877	5.848418236	9.052554131
O	0.101691008	6.552257538	6.842149734	O	0.175010502	6.517233849	6.833349705	O	0.149987876	6.534845352	6.845480442
O	4.991161823	8.434436798	9.021662712	O	5.031284809	8.416704178	8.976316452	O	5.008608818	8.447648048	8.964708328
O	1.306943655	6.304705620	9.196140289	O	1.350229740	6.248170853	9.207296371	O	1.338659048	6.259281158	9.211505890
O	18.126968384	1.954493761	6.836158276	O	-0.676969886	1.910438180	6.844198704	O	18.139272690	1.929781914	6.842410088
O	6.799195766	-0.142083943	2.347460985	O	6.803947926	-0.101938114	2.287876368	O	6.774230480	-0.122870699	2.354961157
O	6.126739979	1.610237122	9.347691536	O	6.146633148	1.600893855	9.350380898	O	6.138260841	1.615565419	9.342021942
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O	1.987524748	-0.438752741	6.835137367	O	2.040768147	-0.469244033	6.806823730	O	2.043359995	-0.462800264	6.790728569
O	0.609093904	7.824488163	4.589729309	O	0.596026003	7.809369087	4.572982788	O	0.594288230	7.778974533	4.571238041
O	4.032511234	0.841979802	7.953307629	O	4.076882362	0.823443830	7.919940472	O	4.061137676	0.856060863	7.906440735
O	7.580556393	4.547219753	1.213091373	O	7.578627586	4.504695892	1.147276044	O	7.577087402	4.507686138	1.184829712
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O	3.956864119	8.104620934	1.326083302	O	4.001735210	8.064916611	1.305091500	O	3.988563538	8.028696060	1.317066193
O	0.390925586	4.143905640	7.919016838	O	0.452512026	4.101796627	7.890596390	O	0.441797554	4.117534637	7.884013176
O	11.014392853	1.803558946	8.214452744	O	11.047242165	1.777845740	8.194217682	O	11.078031540	1.787127733	8.237383842
O	9.424465179	0.060937896	2.967667341	O	9.431516647	-0.001151010	2.884270668	O	9.421292305	-0.013719067	2.871371269
O	17.438037872	2.171583414	2.220484972	O	17.483242035	2.172409296	2.236234903	O	17.477828979	2.162734985	2.225609303
O	12.401494980	0.314370990	0.136119291	O	12.410547256	0.319291323	0.122074597	O	12.405768394	0.270214707	0.104568683
O	10.977499962	8.296900749	2.259513617	O	11.011774063	8.265645981	2.235343456	O	10.993984222	8.240715027	2.219657183
O	9.409646988	2.909579992	0.090458952	O	9.476630211	2.905194759	0.070514344	O	9.443978310	2.898554087	0.066359922
O	15.688942909	6.936845303	0.927836001	O	15.704607964	6.896981239	0.931938469	O	15.703983307	6.894369602	0.928991556
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O	15.916079521	0.435251474	6.926341534	O	15.940647125	0.407588243	6.885076523	O	15.939562798	0.397656798	6.888946056

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O	10.744943619	6.282868385	9.249278069	O	10.794898033	6.284194469	9.206578255	O	10.833034515	6.272029877	9.188112259
O	8.719432831	1.967583179	6.831205368	O	8.776082993	1.991049290	6.783232212	O	8.817538261	1.948255777	6.802747250
O	15.577708244	9.182798386	2.354088545	O	15.607123375	9.180021286	2.318756580	O	15.606342316	9.173649788	2.325967789
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Cu	3.528106689	2.034630775	13.275177002	Cu	3.386468172	1.723541617	13.407551765	Cu	3.476269960	2.010141373	13.281156540
Cu	3.798881531	4.095111370	16.202470779	Cu	3.540853024	3.790989161	16.355604172	Cu	3.749348640	4.054553032	16.294998169
H	15.052636147	6.198997974	0.845786035	H	15.064523697	6.161781311	0.862000704	H	15.063087463	6.159840107	0.856548429
H	3.483928680	0.036086321	14.967981339	H	2.759057283	-0.483549178	14.699774742	H	3.170166969	-0.042406201	14.954348564
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H	3.828649282	2.402935028	10.727108955	H	3.909941912	2.246777058	10.922019005	H	4.111442566	2.202306509	10.744360924
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H	14.298059464	5.454320431	10.211042404	H	14.377660751	5.459324360	10.174777985	H	14.363562584	5.437904358	10.228506088
H	3.821820021	4.104275703	18.713718414	H	5.118918896	5.450336456	0.119608559	H	5.116427422	5.488824368	0.091711774
H	2.569951296	3.138068438	18.161527634	H	2.505806208	2.902138948	18.457654953	H	2.518634319	3.023734093	18.230976105
H	4.115457058	2.555687189	18.238454819	H	4.087237358	2.413751602	18.436294556	H	4.076443195	2.478024960	18.324346542
H	5.542275906	5.847059250	15.513910294	H	5.155699253	5.496398926	15.436424255	H	5.467074871	5.967790604	15.760963440
H	4.769284725	6.347102165	16.879915237	H	4.526354790	6.072372437	16.889261246	H	4.687079430	6.248760700	17.167264938
H	5.966294765	5.254765511	17.001113892	H	5.732550144	4.992207527	16.941755295	H	5.919919968	5.191069603	17.133985519
N	3.512106419	0.105968952	13.947065353	H	5.927656651	7.021480560	14.000061989	H	5.144566059	6.435273647	13.254623413
N	3.682190895	1.601681828	11.349081993	H	5.111617565	6.079979897	12.951617241	H	5.250520229	5.075920105	14.236439705
N	3.552696943	3.387251139	18.018428802	H	6.582163811	5.635905266	13.464156151	H	6.494591713	5.434337139	13.125395775
N	5.157958508	5.523110390	16.404502869	N	3.438124657	-0.233851850	13.972869873	N	3.529293060	0.072404981	14.004307747
N	4.159368515	3.904015541	12.952972412	N	3.696470737	1.409053087	11.472200394	N	3.771157742	1.476151347	11.381359100
				N	3.457058191	3.196970701	18.223783493	N	3.497498512	3.299190044	18.111137390

	N	4.876689434	5.231275558	16.417798996	N	5.090983868	5.498698235	16.590049744			
	N	3.881922722	3.637487411	13.175972939	N	3.692519903	3.970337391	12.767795563			
	N	5.699466705	6.049354553	13.787545204	N	5.497673988	5.486206532	13.348015785			
Structure I₃			Structure J₃			Structure K₃					
Si	0.195088983	2.442432642	8.170463562	Si	0.131778061	2.546823025	8.149000168	Si	0.080103815	2.549339533	8.228446960
Si	8.001094818	0.657417059	3.095283747	Si	7.960992813	0.722699463	3.076645136	Si	7.889608383	0.737042248	3.144510031
Si	2.467935801	8.158400536	0.881959558	Si	2.417836666	8.247150421	0.882945180	Si	2.353227854	8.259913445	0.931133628
Si	5.574268341	8.286371231	1.127954125	Si	5.557272911	8.352200508	1.105158806	Si	5.470675945	8.360114098	1.183571696
Si	7.939347267	0.594998479	6.215335846	Si	7.904254436	0.690327466	6.200273037	Si	7.850917816	0.710954785	6.267478466
Si	0.154631197	5.606751919	8.280663490	Si	0.036174953	5.700570583	8.285870552	Si	0.030784011	5.719343185	8.347519875
Si	0.215866536	7.922725677	6.190635204	Si	0.168601334	8.007802010	6.198464870	Si	0.099641502	8.005869865	6.231440544
Si	5.639523983	0.331313610	8.369127274	Si	5.592991352	0.473073900	8.331377029	Si	5.538071632	0.476634800	8.419378281
Si	2.523791552	0.324892819	8.204174995	Si	2.470142365	0.431374669	8.180324554	Si	2.407482147	0.432448089	8.217355728
Si	0.177398905	8.006809235	3.092792034	Si	0.158232555	8.091576576	3.113214254	Si	0.080159724	8.083694458	3.145882368
Si	7.988520145	2.968465090	0.932593822	Si	7.958281994	3.024487019	0.892306149	Si	7.904130936	3.033893108	0.981443465
Si	9.609317780	2.433345079	8.124233246	Si	9.580055237	2.530915499	8.122852325	Si	9.499331474	2.552332401	8.195314407
Si	17.419975281	0.693684638	3.076284885	Si	17.400676727	0.759489596	3.102735758	Si	17.346702576	0.797132611	3.144150019
Si	11.831039429	8.135890961	0.914238453	Si	11.815764427	8.234712601	0.922813833	Si	11.733841896	8.240540504	0.996694803
Si	14.942379951	8.350714684	1.122837543	Si	14.923616409	8.426327705	1.137622833	Si	14.853000641	8.464833260	1.209070206
Si	17.394594193	0.605144322	6.199900150	Si	17.328859329	0.682358861	6.218909740	Si	17.281047821	0.713882208	6.255029678
Si	9.545036316	5.559192657	8.331313133	Si	9.551727295	5.662056923	8.348631859	Si	9.426774025	5.658132076	8.393923759
Si	9.584769249	7.866414547	6.201995850	Si	9.560767174	7.970204830	6.203587532	Si	9.482190132	7.984944820	6.273242474
Si	15.049073219	0.435713768	8.296165466	Si	15.025692940	0.445385516	8.357272148	Si	14.942153931	0.536658049	8.356185913
Si	11.918719292	0.293498218	8.126800537	Si	11.860781670	0.372462809	8.146159172	Si	11.809796333	0.407983124	8.206110001
Si	9.593745232	7.974207878	3.095729589	Si	9.556553841	8.040042877	3.100870371	Si	9.478333473	8.030642509	3.169258356
Si	17.365943909	2.970328569	0.890752971	Si	17.377582550	3.042736292	0.924264491	Si	17.300336838	3.077462435	0.945418954
Si	-0.538917243	1.710927844	17.519968033	Si	-0.542849302	1.790034413	17.543815613	Si	-0.615569770	1.824123383	17.556011200
Si	7.282764912	-0.126029670	12.408767700	Si	7.237599373	-0.023856878	12.395155907	Si	7.189210415	-0.014727890	12.504117966
Si	1.785218239	7.379333019	10.280164719	Si	1.709509134	7.495733738	10.275862694	Si	1.673157215	7.511747360	10.323999405
Si	4.881000996	7.511042118	10.534277916	Si	4.827402592	7.607025146	10.484686852	Si	4.785431385	7.627321243	10.592333794
Si	7.263226986	-0.169599652	15.569425583	Si	7.222465515	-0.052046061	15.542670250	Si	7.164525032	-0.057705641	15.633836746
Si	-0.514315128	4.888490677	17.696521759	Si	-0.568921030	4.954563141	17.711675644	Si	-0.621342957	4.988180161	17.724418640
Si	-0.494685173	7.182897568	15.556928635	Si	-0.548323572	7.242616653	15.557049751	Si	-0.590244889	7.288870811	15.591825485
Si	4.921396732	-0.271420717	17.685680389	Si	4.901033878	-0.226500154	17.655206680	Si	4.837954044	-0.230111957	17.746339798
Si	1.801333785	-0.387817204	17.496330261	Si	1.757446289	-0.329363585	17.492656708	Si	1.700850248	-0.295046568	17.547574997
Si	-0.507267892	7.247766495	12.449432373	Si	-0.543917239	7.293276787	12.453993797	Si	-0.607977986	7.368032932	12.501673698
Si	7.340656757	2.161778688	10.304518700	Si	7.315031052	2.271838665	10.282567978	Si	7.207719326	2.301019907	10.388636589
Si	8.906858444	1.655722141	17.532440186	Si	8.865668297	1.757213473	17.509679794	Si	8.812963486	1.764097333	17.602918625
Si	16.764322281	-0.052676141	12.436676979	Si	16.710315704	0.051511467	12.477983475	Si	16.638902664	0.050028086	12.504042625
Si	11.157953262	7.394046783	10.262632370	Si	11.097802162	7.476138115	10.265676498	Si	11.046347618	7.500098228	10.343743324
Si	14.257394791	7.620621681	10.482641220	Si	14.211887360	7.709600449	10.554325104	Si	14.145970345	7.717738628	10.559436798
Si	16.683143616	-0.128885031	15.564201355	Si	16.650039673	-0.041140437	15.587870598	Si	16.576801300	-0.028945088	15.615402222
Si	8.814607620	4.811117649	17.666187286	Si	8.828825951	4.926329136	17.684900284	Si	8.752172470	4.935192108	17.778102875
Si	8.890970230	7.110894203	15.558211327	Si	8.893397331	7.234818459	15.562740326	Si	8.819259644	7.226298332	15.627306938

Si	14.348778725	-0.319554687	17.662776947	Si	14.326618195	-0.230155587	17.687076569	Si	14.264160156	-0.220133066	17.738052368
Si	11.222500801	-0.455682278	17.518058777	Si	11.202323914	-0.347059846	17.526205063	Si	11.120148659	-0.342246890	17.593753815
Si	8.910148621	7.072644234	12.423856735	Si	8.829589844	7.164805889	12.452085495	Si	8.827072144	7.198531628	12.514980316
Si	16.700483322	2.240841150	10.272669792	Si	16.687984467	2.295587063	10.296756744	Si	16.597648621	2.335608244	10.322115898
Al	7.870059967	6.146567822	1.100967050	Al	7.859054565	6.218310356	1.123553634	Al	7.766290665	6.227789879	1.192856669
Al	17.463575363	6.121360779	1.161341667	Al	17.416597366	6.190114975	1.200386524	Al	17.351598740	6.214952946	1.191835523
Al	7.243206501	5.302536964	10.540950775	Al	7.206485748	5.429361343	10.547513008	Al	7.127559662	5.422499657	10.587123871
Al	16.744997025	5.373085976	10.462660789	Al	16.642967224	5.465748787	10.449428558	Al	16.639339447	5.478033066	10.526939392
O	1.637173176	1.689906240	8.351858139	O	1.571454525	1.789728999	8.305042267	O	1.535333157	1.804977059	8.360777855
O	0.050570816	0.031006560	2.973692417	O	0.043893203	0.123267084	3.016573429	O	-0.028647080	0.118963063	3.068048000
O	8.030592918	2.048700094	2.267130613	O	7.964579105	2.102872372	2.223085642	O	7.947466850	2.135309219	2.330057383
O	2.983661652	0.187749177	0.094927989	O	2.878276587	0.273314774	0.099623039	O	2.832341433	0.287582278	0.141316816
O	1.511390686	8.154654503	2.175900221	O	1.501854777	8.234107971	2.207401752	O	1.415743232	8.241031647	2.239483833
O	-0.016819498	2.867411375	0.137835801	O	0.003813471	2.952591419	0.177933902	O	-0.081503287	3.020263195	0.188103482
O	6.293493271	6.885103226	0.824967563	O	6.280921936	6.947267532	0.819077313	O	6.187345505	6.953141689	0.934433460
O	8.148562431	8.635232925	6.344691277	O	8.113018990	8.729568481	6.328571320	O	8.035495758	8.739353180	6.411464691
O	6.534159660	0.358256280	7.012989521	O	6.482413292	0.452993751	6.971577168	O	6.449353695	0.503875256	7.083115578
O	8.146124840	5.647655010	9.092571259	O	8.177767754	5.784129620	9.152340889	O	7.998098850	5.674253464	9.102796555
O	0.181229770	6.451222420	6.880634785	O	0.099914432	6.540081501	6.888679504	O	0.054390788	6.545496941	6.940514088
O	5.009308338	8.259028435	9.077963829	O	4.970086098	8.420841217	9.069948196	O	4.951261520	8.433113098	9.170928001
O	1.348906517	6.178725243	9.265742302	O	1.189888716	6.296128273	9.304286957	O	1.226729512	6.311026573	9.323076248
O	-0.614677370	1.839103937	6.879994392	O	18.138488770	1.945700169	6.874507904	O	18.092380524	1.955286503	6.948283195
O	6.190502167	9.088257790	2.395214319	O	6.154359818	9.131626129	2.398925066	O	6.055687428	9.192873955	2.454106092
O	6.177222252	1.435319781	9.426488876	O	6.142677784	1.607417345	9.352748871	O	6.001449585	1.628052115	9.484335899
O	18.079729080	6.800561905	2.606798172	O	18.045635223	6.901435852	2.619310141	O	17.980447769	6.894837856	2.629832745
O	2.017287731	-0.536988080	6.927709579	O	1.988966703	-0.457119435	6.913528919	O	1.913755417	-0.456633091	6.960270405
O	0.648398995	7.783998013	4.635374546	O	0.619580925	7.848342896	4.651972294	O	0.538261712	7.817968845	4.686829567
O	4.089775085	0.710269392	8.004488945	O	4.032517433	0.843369067	7.988683701	O	3.979526281	0.811721802	8.043120384
O	7.604309082	4.457408428	1.299689651	O	7.582546711	4.521702766	1.233806729	O	7.518461227	4.529017925	1.308149934
O	7.587931156	0.912448168	4.652055264	O	7.571665287	1.014875889	4.631612301	O	7.491804123	1.009245634	4.706840515
O	3.995830059	8.012533188	1.392228007	O	3.965799332	8.119642258	1.325498462	O	3.880268097	8.135109901	1.435364842
O	0.485160470	4.029677391	7.958216190	O	0.406380594	4.136509418	7.952056885	O	0.359236002	4.140839577	8.039768219
O	11.040740013	1.651818752	8.243503571	O	11.016647339	1.757995129	8.222903252	O	10.916800499	1.754321456	8.362176895
O	9.488677979	0.010826200	3.028727531	O	9.447948456	0.074821934	3.004510641	O	9.361711502	0.057683557	3.070541382
O	17.406522751	2.089666367	2.261700869	O	17.404823303	2.153093815	2.286017656	O	17.374156952	2.175933123	2.300735235
O	12.433589935	0.187210247	0.167846844	O	12.393225670	0.283845276	0.168396741	O	12.281717300	0.277218848	0.226627961
O	11.014743805	8.178111076	2.295913219	O	10.963338852	8.256114006	2.280845881	O	10.891192436	8.251061440	2.361189842
O	9.433315277	2.833370447	0.146952167	O	9.409041405	2.878409624	0.124545477	O	9.353606224	2.881807804	0.214197651
O	15.720573425	6.836879730	0.967971861	O	15.698859215	6.923638344	0.959914207	O	15.607398987	6.939350605	1.037118316
O	17.583015442	8.631136894	6.310753345	O	17.543956757	8.726322174	6.327666283	O	17.484231949	8.746938705	6.341591835
O	15.968078613	0.384534419	6.960348129	O	15.919391632	0.433649123	7.001079082	O	15.862724304	0.452278733	7.020905495
O	17.570129395	5.769005299	9.005017281	O	17.419467926	5.821311474	8.959300041	O	17.447086334	5.890635967	9.066769600
O	9.528605461	6.428377151	6.945332050	O	9.510839462	6.545891285	6.971697807	O	9.434742928	6.555067062	7.028171062
O	14.503382683	8.393376350	9.087971687	O	14.535684586	8.394087791	9.122329712	O	14.403972626	8.507198334	9.174515724

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O	8.760496140	1.861958265	6.845695972	O	8.705927849	1.954079866	6.860429764	O	8.676474571	1.971850395	6.903789520
O	15.597289085	9.090853691	2.394671917	O	15.604420662	9.142949104	2.402955770	O	15.521034241	9.186609268	2.484409332
O	15.560101509	1.609452724	9.288404465	O	15.540880203	1.612771988	9.362310410	O	15.458200455	1.731671691	9.319081306
O	8.727519989	6.817638874	2.432042837	O	8.689528465	6.853427887	2.484136581	O	8.619741440	6.836187840	2.562764168
O	10.759595871	8.795264244	6.859366894	O	11.423305511	-0.475459039	6.833546638	O	11.334697723	-0.462894231	6.926612854
O	9.968364716	7.641992092	4.644879341	O	9.945974350	7.725928783	4.647597790	O	9.874368668	7.746013165	4.724303722
O	13.493671417	0.686718464	7.917064667	O	13.459802628	0.697266936	8.027770042	O	13.384356499	0.799708307	7.986856461
O	16.970315933	4.479977131	1.232216954	O	16.963216782	4.539786339	1.282147646	O	16.872783661	4.572052956	1.307599306
O	17.045576096	0.947672844	4.640304565	O	16.975364685	1.001488209	4.655243874	O	16.944471359	1.079791069	4.698935509
O	13.410434723	7.886195660	1.306054354	O	13.385616302	8.000585556	1.340979576	O	13.315269470	8.044273376	1.415571690
O	9.937259674	4.012400627	7.935465336	O	9.884099960	4.112128258	7.922493935	O	9.855758667	4.123336315	7.991371155
O	0.913532376	0.968937278	17.633481979	O	0.924193144	1.067536473	17.611614227	O	0.849885464	1.093578935	17.658193588
O	-0.584210873	-0.692561269	12.360152245	O	-0.693909943	-0.693805575	12.400412560	O	-0.709584415	-0.589971960	12.438422203
O	7.595897675	1.307610989	11.697031021	O	7.448358059	1.405369282	11.668684959	O	7.406161308	1.394357562	11.736660004
O	2.339636326	-0.542605042	9.580905914	O	2.278977156	-0.430633545	9.560983658	O	2.213914156	-0.403094351	9.620536804
O	0.885843277	7.408193111	11.629288673	O	0.858294666	7.562710285	11.663306236	O	0.787810624	7.576507092	11.685202599
O	-0.671960473	2.179531813	9.536102295	O	-0.715953112	2.282475948	9.523548126	O	-0.769592285	2.256612301	9.598537445
O	5.744229317	6.184335232	10.629367828	O	5.689280987	6.280922890	10.497147560	O	5.626297474	6.293548107	10.615196228
O	7.410614491	7.818862915	15.719335556	O	7.420451641	7.969518661	15.698702812	O	7.334571838	7.943486214	15.736161232
O	5.822724342	-0.373813272	16.322204590	O	5.787353516	-0.333305180	16.284267426	O	5.728130817	-0.320615768	16.377174377
O	7.343338013	4.934621811	18.297861099	O	7.373840332	5.067237854	18.356891632	O	7.300405502	5.098465919	18.444641113
O	-0.509362578	5.746097088	16.305923462	O	-0.587589443	5.811525822	16.317970276	O	-0.603284776	5.845816612	16.329151154
O	4.337922096	7.695494652	18.463169098	O	4.373345852	7.757394791	18.448886871	O	4.258788109	7.736602306	18.506280899
O	0.759823561	5.420092106	18.606054306	O	0.689883709	5.506451607	18.620676041	O	0.627774119	5.530464649	18.653484344
O	-1.355487108	1.140882492	16.215364456	O	17.459892273	1.207442760	16.261611938	O	17.395889282	1.225566983	16.272680283
O	5.966441154	-0.817097783	11.737578392	O	5.921873569	-0.763210475	11.738996506	O	5.870116711	-0.757220984	11.857190132
O	5.438979626	0.941530466	18.620901108	O	5.405439854	1.022692919	18.561637878	O	5.351579666	0.987700939	18.679056168
O	17.399520874	6.087434292	11.874984741	O	17.447086334	6.087576866	11.844410896	O	17.325042725	6.191436768	11.925472260
O	1.344855547	-1.227023125	16.178995132	O	1.295949936	-1.176361322	16.180009842	O	1.245715141	-1.122328520	16.218711853
O	-0.118216574	6.957613945	14.001308441	O	-0.156840026	6.979242325	14.008671761	O	-0.167412698	7.071515083	14.042330742
O	3.369452953	0.030825496	17.285327911	O	3.336335182	0.023814440	17.279457092	O	3.280046701	0.073527813	17.344034195
O	6.817413807	3.614832640	10.703052521	O	6.798448563	3.732399464	10.682869911	O	6.669404507	3.738255978	10.853295326
O	6.988671303	0.136649370	14.000511169	O	6.893187523	0.256072760	13.979290009	O	6.817190647	0.277759671	14.075658798
O	3.307140589	7.105019093	10.772324562	O	3.247372866	7.228456497	10.713969231	O	3.198037386	7.303215981	10.816645622
O	-0.244130015	3.303847075	17.363334656	O	-0.263090491	3.382122517	17.344635010	O	-0.320405841	3.414161682	17.353082657
O	10.356501579	0.913667202	17.619085312	O	10.316830635	1.014188290	17.585195541	O	10.277032852	1.043317080	17.686218262
O	7.917643547	8.359603882	12.249501228	O	8.585182190	-0.893161416	12.272686958	O	8.539665222	-0.882549167	12.405735016
O	16.774677277	1.353295207	11.643237114	O	16.829408646	1.461779475	11.693914413	O	16.646997452	1.440385580	11.686064720
O	11.747230530	-0.559561491	9.510721207	O	11.573685646	-0.496045798	9.497941017	O	11.654499054	-0.462568700	9.577327728
O	10.293557167	7.424653530	11.626147270	O	10.181094170	7.443055153	11.591135979	O	10.199099541	7.582247734	11.711410522
O	8.758049011	2.152911186	9.488181114	O	8.749062538	2.251445055	9.505089760	O	8.602210045	2.310912132	9.546306610
O	15.006035805	6.092514992	10.306919098	O	14.936695099	6.195285797	10.568103790	O	14.898887634	6.189970493	10.391324043
O	16.885913849	7.907900333	15.707562447	O	16.837207794	7.980228424	15.691810608	O	16.787488937	8.008264542	15.710268021

O	15.256529808	-0.367226422	16.318534851	O	15.224696159	-0.299512625	16.337041855	O	15.166125298	-0.290186167	16.389036179
O	16.936658859	5.095144272	18.468240738	O	16.877307892	5.116288662	18.480230331	O	16.813489914	5.159961700	18.478614807
O	8.829005241	5.618246555	16.224739075	O	8.806771278	5.767440319	16.271938324	O	8.763330460	5.782632828	16.373193741
O	13.815979004	7.645387173	18.461692810	O	13.762033463	7.725532532	18.468414307	O	13.746059418	7.754413605	18.550222397
O	9.979340553	5.453003883	18.639230728	O	10.023446083	5.533821106	18.640571594	O	11.334612846	7.005836010	0.006843377
O	8.092981339	1.072353363	16.226606369	O	8.011022568	1.213652611	16.209611893	O	7.977215767	1.188640714	16.301988602
O	14.969529152	8.338019371	11.737979889	O	15.523065567	-0.848262012	11.799582481	O	14.846246719	8.420268059	11.830726624
O	14.826631546	0.877650976	18.636991501	O	14.852387428	0.957527041	18.647172928	O	14.769083023	0.987646222	18.684555054
O	8.232972145	5.717129230	11.933013916	O	8.037846565	5.842965126	12.039476395	O	8.127897263	5.894142628	11.937687874
O	10.022659302	8.032073021	16.269987106	O	10.733145714	-1.251025677	16.263528824	O	10.627432823	-1.208910227	16.314571381
O	9.296521187	6.939591408	14.010238647	O	9.293193817	7.066978455	14.017755508	O	9.238160133	7.006675720	14.086493492
O	12.789289474	-0.085510731	17.272493362	O	12.769395828	0.052772999	17.311174393	O	12.697771072	0.008558393	17.382535934
O	16.267196655	3.734606266	10.641847610	O	16.224592209	3.787338734	10.692223549	O	16.186210632	3.833310843	10.693791389
O	16.355922699	0.183637381	13.995963097	O	16.323432922	0.332170129	14.036497116	O	16.226511002	0.307165265	14.057685852
O	12.726423264	7.208786964	10.745511055	O	12.650730133	7.415544987	10.797549248	O	12.619251251	7.279543400	10.802154541
O	9.190919876	3.248044014	17.330644608	O	9.154541016	3.354747534	17.344013214	O	9.068220139	3.363795280	17.429208755
O	2.762300253	3.050902367	15.277255058	O	3.935424805	2.482598305	15.227622032	O	3.940233946	2.361652374	15.043639183
O	3.689851522	5.032099724	14.178536415	O	4.921525002	4.370735645	14.008051872	O	4.723342419	3.776982784	13.005355835
O	5.556471348	2.724098682	13.621799469	O	14.122994423	4.472702980	12.189701080	O	6.823273659	4.702785969	14.265510559
Cu	3.199106455	3.205993176	13.452075005	Cu	4.118711948	2.644380569	13.378298759	Cu	3.958709240	2.109960079	13.269933701
Cu	3.817239046	4.328857899	15.896875381	Cu	4.598860741	4.016903400	15.810597420	Cu	4.602974415	3.807036638	15.869738579
H	15.090462685	6.094345570	0.885904253	H	15.132670403	6.261464119	0.498807132	H	14.965644836	6.205939293	0.963269889
H	2.444053650	0.958270550	14.174231529	H	3.558326006	0.363485217	14.159429550	H	3.606397629	0.229768395	14.686579704
H	1.796063423	1.060629964	12.655645370	H	2.712539196	0.509001017	12.746617317	H	2.591593266	-0.075102448	13.386919022
H	3.390590429	0.683466434	12.852293968	H	4.326807499	0.151540637	12.705062866	H	4.226916313	-0.343845725	13.224289894
H	3.440306664	4.684008598	11.337359428	H	3.582125664	4.157156944	11.418978691	H	3.137438536	2.845487595	11.032375336
H	4.600331306	3.531725645	11.313643456	H	5.050349236	3.470825911	11.152721405	H	4.437749863	1.883064985	10.740454674
H	3.073653460	3.172752380	10.810076714	H	3.664718151	2.637654543	10.790822029	H	2.961150169	1.201132298	11.040536880
H	14.361149788	5.363027573	10.222968102	H	14.451279640	5.543965340	11.265501976	H	14.251131058	5.462954044	10.309195518
H	3.874884367	4.195872307	18.420349121	H	4.105485439	4.252712727	18.291488647	H	3.712652683	4.128706455	18.314435959
H	2.584885120	3.339938641	17.707017899	H	2.971632481	3.297492981	17.454072952	H	2.648135185	3.157898903	17.456205368
H	4.105425358	2.693275452	17.724534988	H	4.452437401	2.675266743	17.851213455	H	4.077467442	2.551209927	18.022827148
H	5.568838596	6.111466408	15.695003510	H	5.807618141	6.204169273	15.648227692	H	5.661714554	6.114385605	15.700786591
H	4.744658470	6.348995209	17.100671768	H	4.781228542	6.283143520	16.933639526	H	4.588815689	6.119227886	16.948915482
H	5.923445702	5.212584972	17.033252716	H	6.193370819	5.458120346	17.095184326	H	6.043640137	5.405604839	17.142763138
H	7.849261284	2.732096672	13.169968605	H	14.872467041	3.895345926	11.875534058	H	5.347434044	3.766865015	12.223399162
H	4.587482452	5.263033867	13.865083694	H	5.872323990	4.458509445	13.788037300	N	3.518222094	0.259043574	13.664505005
H	8.210878372	4.090783119	14.305945396	H	14.291515350	4.674596786	13.126662254	N	3.584753990	1.968860388	11.316025734
N	2.629192829	1.264721274	13.214188576	N	3.610548496	0.707121134	13.195777893	N	3.633492947	3.380960941	17.612493515
N	3.601553440	3.686742783	11.520287514	N	4.081966877	3.264866829	11.482285500	N	5.272955418	5.538446426	16.453737259
N	3.580940247	3.571893215	17.645036697	N	3.963152409	3.533827305	17.554357529	N	6.139170170	3.771714211	14.411035538
N	5.143352985	5.624601841	16.486274719	N	5.418367863	5.660557747	16.421958923				
N	6.319797039	3.535132170	14.202993393	N	12.826230049	3.283381462	16.692832947				
N	7.577123165	3.402415037	13.904778481	N	13.019951820	3.747014999	17.685016632				

Structure L ₃				Structure M ₃			Structure N ₃				
Si	0.104605019	2.550107956	8.192484856	Si	0.108420491	2.546256065	8.214594841	Si	0.104440629	2.460304260	8.217523575
Si	7.913595200	0.754342437	3.136844397	Si	7.924632549	0.740783334	3.156725407	Si	7.922233582	0.681206644	3.138204575
Si	2.389058352	8.248433113	0.917341530	Si	2.397218704	8.249074936	0.925772071	Si	2.384022474	8.159785271	0.906214118
Si	5.507019997	8.377182007	1.175634623	Si	5.524250507	8.374043465	1.165462136	Si	5.543776512	8.312687874	1.152588487
Si	7.882280827	0.705327570	6.255676746	Si	7.891015053	0.701138854	6.276968956	Si	7.873079300	0.635094881	6.256413460
Si	0.079226911	5.717811584	8.340195656	Si	0.062484920	5.718540668	8.350122452	Si	0.077938378	5.629657745	8.367630005
Si	0.126328915	8.003076553	6.219720840	Si	0.119958401	7.996495724	6.227274418	Si	0.173287690	7.929144859	6.254443645
Si	5.565639019	0.483194649	8.402321815	Si	5.567082405	0.472697973	8.436543465	Si	5.577905655	0.422677875	8.415410042
Si	2.428722382	0.426032603	8.200306892	Si	2.430171013	0.421072900	8.204385757	Si	2.448785782	0.352359116	8.219318390
Si	0.118788183	8.099061012	3.129924774	Si	0.125249296	8.108123779	3.136173248	Si	0.145603150	7.990460396	3.149033546
Si	7.925429821	3.041956186	0.978280365	Si	7.932518959	3.034456015	1.007634521	Si	7.917084694	2.986909151	0.969985068
Si	9.557567596	2.544542074	8.168691635	Si	9.534523964	2.525597095	8.187381744	Si	9.546789169	2.470632076	8.175827980
Si	17.368330002	0.788565993	3.126799345	Si	17.384098053	0.792169273	3.135389805	Si	17.421115875	0.698693395	3.135467052
Si	11.765331268	8.219261169	0.982942760	Si	11.780287743	8.257873535	1.007609606	Si	11.781583786	8.186350822	0.989115357
Si	14.874201775	8.449486732	1.190702915	Si	14.888698578	8.457781792	1.189872384	Si	14.899641037	8.376477242	1.191596150
Si	17.304447174	0.706853628	6.236420155	Si	17.297409058	0.699894905	6.250226021	Si	17.334671021	0.611620724	6.264529228
Si	9.473125458	5.655033112	8.370860100	Si	9.469104767	5.676301003	8.429161072	Si	9.492481232	5.626323223	8.384479523
Si	9.510458946	7.978103638	6.256465912	Si	9.505035400	7.968449593	6.294152260	Si	9.518699646	7.919062614	6.251110077
Si	14.971335411	0.527348101	8.340258598	Si	14.979101181	0.503591418	8.356349945	Si	14.990642548	0.422044575	8.353934288
Si	11.842427254	0.396802306	8.200941086	Si	11.834770203	0.406474352	8.229012489	Si	11.845814705	0.340462804	8.188694000
Si	9.522578239	8.038713455	3.153303146	Si	9.536838531	8.028582573	3.189637661	Si	9.526733398	7.999070168	3.159416199
Si	17.317737579	3.070329666	0.933319747	Si	17.326133728	3.081279516	0.943937242	Si	17.351345062	2.985052824	0.973769009
Si	-0.594515622	1.807162285	17.541292191	Si	-0.585830510	1.817362309	17.554096222	Si	-0.587541223	1.724331737	17.570232391
Si	7.251903534	-0.037094593	12.488663673	Si	7.243990421	-0.008111835	12.493218422	Si	7.225028992	-0.052745521	12.489949226
Si	1.700660229	7.519880772	10.307333946	Si	1.699034691	7.523653030	10.316901207	Si	1.696116924	7.431211472	10.327787399
Si	4.826109886	7.611827850	10.553157806	Si	4.827298164	7.626379490	10.584914207	Si	4.816706657	7.576155186	10.581331253
Si	7.220339298	-0.100099564	15.626826286	Si	7.209914207	-0.048882484	15.640021324	Si	7.198326111	-0.097235203	15.625202179
Si	-0.597193301	4.970397949	17.713695526	Si	-0.591538787	4.974315166	17.719554901	Si	-0.590886414	4.888847351	17.731275558
Si	-0.562357664	7.273183346	15.579898834	Si	-0.554331303	7.281013012	15.587851524	Si	-0.575070381	7.196400166	15.593852997
Si	4.865783215	-0.224966168	17.737857819	Si	4.871921062	-0.229857326	17.756513596	Si	4.882214069	-0.287253380	17.746923447
Si	1.734798074	-0.306398153	17.525167465	Si	1.738076448	-0.308034301	17.534646988	Si	1.707108736	-0.399741411	17.548276901
Si	-0.583455443	7.353531361	12.490766525	Si	-0.582549512	7.347455978	12.493947983	Si	-0.581718802	7.268752098	12.501933098
Si	7.275879383	2.265630484	10.353027344	Si	7.245332718	2.276344299	10.364582062	Si	7.292398930	2.219392538	10.342371941
Si	8.856800079	1.743094683	17.598983765	Si	8.842913628	1.781840801	17.602264404	Si	8.842717171	1.725054860	17.585966110
Si	16.677549362	0.042428374	12.485106468	Si	16.681400299	0.043585181	12.498675346	Si	16.673486710	-0.027536690	12.509426117
Si	11.084682465	7.488904476	10.331197739	Si	11.082380295	7.496092796	10.347782135	Si	11.074320793	7.439417839	10.310041428
Si	14.185690880	7.707428455	10.534853935	Si	14.181012154	7.703799248	10.567331314	Si	14.176484108	7.639008522	10.559414864
Si	16.605258942	-0.037469983	15.595721245	Si	16.611005783	-0.024494648	15.609790802	Si	16.600374222	-0.121887207	15.622589111
Si	8.772472382	4.906795025	17.752283096	Si	8.787469864	4.938913345	17.771356583	Si	8.796518326	4.887957573	17.769227982
Si	8.846202850	7.199742317	15.618199348	Si	8.840339661	7.236356258	15.650095940	Si	8.851045609	7.196942329	15.635123253
Si	14.286140442	-0.222467303	17.716499329	Si	14.289334297	-0.203349829	17.721082687	Si	14.299715996	-0.306562066	17.743892670
Si	11.156394005	-0.351910830	17.572351456	Si	11.159038544	-0.328486562	17.610992432	Si	11.156642914	-0.380030870	17.599130630
Si	8.863281250	7.186823845	12.507374763	Si	8.849188805	7.194577694	12.535230637	Si	8.830671310	7.143714905	12.528343201

Si	16.626203537	2.327907801	10.300045013	Si	16.649007797	2.319614887	10.313819885	Si	16.638065338	2.236875534	10.321966171
Al	7.832811832	6.229660034	1.170204043	Al	7.841658115	6.213871479	1.217088580	Al	7.822649002	6.171882153	1.196959615
Al	17.379974365	6.207611561	1.183429480	Al	17.379098892	6.214328289	1.188275695	Al	17.394701004	6.125330925	1.214663744
Al	7.161326885	5.439193249	10.549353600	Al	7.164894581	5.433416367	10.638277054	Al	7.173069954	5.400161266	10.575254440
Al	16.670982361	5.465791702	10.524189949	Al	16.653373718	5.460571289	10.526735306	Al	16.665897369	5.386452198	10.518906593
O	1.556502342	1.799502611	8.318222046	O	1.562913179	1.799366951	8.317140579	O	1.551064730	1.708770037	8.327721596
O	0.004258037	0.131827980	3.053004742	O	0.026464656	0.150402889	3.053274155	O	0.052533299	0.034876361	3.026734591
O	7.988092422	2.159753799	2.337602615	O	8.028878212	2.150762320	2.362409592	O	7.967956543	2.071455240	2.306997538
O	2.887496948	0.273084581	0.121497631	O	2.880355358	0.268398643	0.125603467	O	2.760312319	0.168641016	0.119893327
O	1.469494820	8.262639999	2.240931749	O	1.482632399	8.259615898	2.251443386	O	1.501649499	8.092655182	2.256060362
O	-0.064047918	3.006782532	0.173552796	O	-0.052442245	3.025467157	0.187669516	O	-0.032338545	2.921561480	0.216429263
O	6.260962009	6.984851837	0.975455344	O	6.273659229	6.972917557	0.980976701	O	6.233247280	6.881287098	0.952649355
O	8.057126999	8.725201607	6.390228748	O	8.045767784	8.707512856	6.411940575	O	8.063973427	8.660130501	6.377676964
O	6.473610878	0.519394934	7.063548088	O	6.496109009	0.542055309	7.111553192	O	6.465663433	0.415138721	7.057045937
O	8.044283867	5.679707050	9.080323219	O	8.083146095	5.808285713	9.201841354	O	8.114309311	5.790783882	9.176298141
O	0.075650811	6.545553207	6.932901382	O	0.071519673	6.537075043	6.936318874	O	0.133655310	6.474000931	6.972834587
O	5.002554417	8.437759399	9.143288612	O	5.002683163	8.412690163	9.154613495	O	5.001929283	8.375309944	9.165478706
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O	6.742644787	-0.145618170	2.433882713	O	6.761792660	-0.144131839	2.417004824	O	6.100933552	9.116958618	2.454290628
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O	1.948610783	-0.459324270	6.934636593	O	1.936941862	-0.466316193	6.946629524	O	2.013900280	-0.528778553	6.930071354
O	0.558443785	7.823086739	4.673055649	O	0.551360786	7.816398144	4.678312302	O	0.570111036	7.742836475	4.699841499
O	4.003221512	0.810995936	8.041636467	O	4.006233692	0.770783663	8.035219193	O	4.016839504	0.753515720	8.067214012
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O	7.519492149	1.015696883	4.700204372	O	7.503565788	0.977180362	4.713793755	O	7.520479679	0.956842899	4.698615074
O	3.922164917	8.085800171	1.395276666	O	3.936230659	8.094313622	1.387394428	O	3.940210342	8.109057426	1.323400736
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Cu	3.721604109	2.379789591	13.263833046	Cu	3.571627378	2.063477516	13.319851875	Cu	4.278452396	3.713743210	16.170829773
Cu	3.776339769	3.803254366	16.328441620	Cu	3.857652426	3.701711655	16.350690842	H	15.010210037	6.109336853	0.957379341
H	15.003441811	6.197297096	0.910215497	H	15.036555290	6.247824192	0.671629071	H	3.408908367	0.248468757	14.166921616
H	3.983262062	0.268902183	14.670001984	H	4.100024223	-0.020720601	14.622474670	H	2.703947544	0.469679117	12.684691429
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H	4.387077332	2.079644918	10.745651245	H	4.366197109	1.996659756	10.875340462	H	3.699684620	3.068273783	11.135834694
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H	5.833703041	5.183265209	17.052177429	H	5.991107941	4.999567032	17.127098083	H	7.365206242	3.569932938	14.246615410
H	6.125610828	3.626958847	12.205091476	H	11.612767220	3.795893669	16.090856552	H	7.280697346	4.806294918	13.301043510
N	3.704923630	0.388148308	13.692158699	H	12.373072624	2.538244963	16.531232834	N	3.552623749	0.640196681	13.230881691
N	3.527677059	2.312307358	11.262356758	H	14.642552376	3.264352083	13.480734825	N	4.203300953	3.479445934	11.926898956
N	3.410953999	3.421866655	18.229587555	H	13.413383484	3.540912867	14.386128426	N	3.563374519	3.426666737	17.974842072
N	4.970417023	5.394895554	16.520320892	N	3.754469395	0.113979459	13.667332649	N	5.393759727	5.293765068	16.316913605
N	6.779417992	3.540104151	14.047323227	N	3.454376698	2.121037483	11.343699455				
				N	3.332720757	3.522769928	18.235044479				
				N	5.201184273	5.161599159	16.470314026				
				N	10.582006454	3.135884047	12.070591927				
				N	10.385725021	2.732090712	13.089303017				
ts4				Structure O ₃				Structure P ₃			
Si	0.060432851	2.415743351	8.171847343	Si	0.056456923	2.422658205	8.162076950	Si	0.114696443	2.468727589	8.182585716

Si	7.884250164	0.645276129	3.117279768	Si	7.886362076	0.627020001	3.091408014	Si	7.931901455	0.723283291	3.105977058
Si	2.344583273	8.135099411	0.919717550	Si	2.355312824	8.143216133	0.892387927	Si	2.424883604	8.196546555	0.904668450
Si	5.433813572	8.262552261	1.198535442	Si	5.459913254	8.248765945	1.115795732	Si	5.511710167	8.326664925	1.136605024
Si	7.822302818	0.572852552	6.234505177	Si	7.826060295	0.585848451	6.213040829	Si	7.860537529	0.653152645	6.223788738
Si	0.003416598	5.586437225	8.306092262	Si	0.011240244	5.594453335	8.306500435	Si	0.061341703	5.640662193	8.305376053
Si	0.057297200	7.890104771	6.206182480	Si	0.074707091	7.884984016	6.193571091	Si	0.139259964	7.947826385	6.201116562
Si	5.505228043	0.325082660	8.369988441	Si	5.523194790	0.351325989	8.387103081	Si	5.574618340	0.393805981	8.387970924
Si	2.382217407	0.305277348	8.218965530	Si	2.374794245	0.307111681	8.198061943	Si	2.438155651	0.357910931	8.215163231
Si	0.045736313	7.981034279	3.125346184	Si	0.072596863	7.984876633	3.110681295	Si	0.126014963	8.040218353	3.109357595
Si	7.875452518	2.922379494	0.941192329	Si	7.879383564	2.934058666	0.942250133	Si	7.943994522	3.006068230	0.945806324
Si	9.478565216	2.407924414	8.171639442	Si	9.477032661	2.396991730	8.140545845	Si	9.526038170	2.488716125	8.148837090
Si	17.320032120	0.676205754	3.101714849	Si	17.335197449	0.675933540	3.095438242	Si	17.375539780	0.734485269	3.097322464
Si	11.717047691	8.132883072	0.933543801	Si	11.725058556	8.130131721	0.941976488	Si	11.781563759	8.195757866	0.932431221
Si	14.832246780	8.347063065	1.153491497	Si	14.844364166	8.340249062	1.142921209	Si	14.892510414	8.398731232	1.142660022
Si	17.262132645	0.594211698	6.206032753	Si	17.259901047	0.584392726	6.201572418	Si	17.321788788	0.638053894	6.207583427
Si	9.406831741	5.552699566	8.360883713	Si	9.419761658	5.575044632	8.373575211	Si	9.464817047	5.631284237	8.350779533
Si	9.456923485	7.840863705	6.229465485	Si	9.444247246	7.845434666	6.222523212	Si	9.520882607	7.928667545	6.211384773
Si	14.918535233	0.413708210	8.333111763	Si	14.925933838	0.397922814	8.317739487	Si	14.973586082	0.450791597	8.309293747
Si	11.779383659	0.277192116	8.173234940	Si	11.780943871	0.282468557	8.148110390	Si	11.843508720	0.356768787	8.142406464
Si	9.461328506	7.910248756	3.134811163	Si	9.475198746	7.917067528	3.120090485	Si	9.534432411	8.011036873	3.116848946
Si	17.261270523	2.960905552	0.915168941	Si	17.284286499	2.959381580	0.912021995	Si	17.329238892	3.017307997	0.910140991
Si	-0.638187110	1.701717734	17.520933151	Si	-0.630230606	1.705249786	17.508430481	Si	-0.578164220	1.754514694	17.517448425
Si	7.124336243	-0.148986042	12.455276489	Si	7.173717499	-0.109658778	12.445099831	Si	7.196374416	-0.059327960	12.441770554
Si	1.642653227	7.352695942	10.285087585	Si	1.640527725	7.380122185	10.268939018	Si	1.707958460	7.404892445	10.279767990
Si	4.745771885	7.485199928	10.535189629	Si	4.771814823	7.497869492	10.530916214	Si	4.817097187	7.567820549	10.553808212
Si	7.115782261	-0.168567061	15.607431412	Si	7.149573326	-0.148848534	15.577924728	Si	7.211692810	-0.110671163	15.586790085
Si	-0.633976102	4.867275715	17.713714600	Si	-0.637968063	4.868686676	17.694004059	Si	-0.565994442	4.917221069	17.699090958
Si	-0.611984253	7.162070274	15.575865746	Si	-0.606755435	7.164260387	15.561021805	Si	-0.538036227	7.210618973	15.566229820
Si	4.795227051	-0.336690903	17.719005585	Si	4.808629990	-0.317031026	17.698280334	Si	4.865252495	-0.260298967	17.703891754
Si	1.686710954	-0.420340121	17.534198761	Si	1.694700599	-0.404607117	17.509309769	Si	1.765698671	-0.356092691	17.503477097
Si	-0.635494053	7.218931198	12.487739563	Si	-0.628118753	7.219987392	12.472551346	Si	-0.576834559	7.261595726	12.462653160
Si	7.202253342	2.137586594	10.329034805	Si	7.215275764	2.151639462	10.307511330	Si	7.276339531	2.217948437	10.329031944
Si	8.774484634	1.646911860	17.549007416	Si	8.804509163	1.667422891	17.537841797	Si	8.851483345	1.720941424	17.540714264
Si	16.639169693	-0.079843879	12.467604637	Si	16.651809692	-0.078067601	12.456474304	Si	16.697975159	-0.031781077	12.451489449
Si	11.007096291	7.389875889	10.292992592	Si	11.025103569	7.383913517	10.272503853	Si	11.071802139	7.456654549	10.278009415
Si	14.124774933	7.602404594	10.515194893	Si	14.135132790	7.598755360	10.512988091	Si	14.173239708	7.646264553	10.498358727
Si	16.572460175	-0.132703424	15.578323364	Si	16.578815460	-0.134714484	15.568006516	Si	16.634458542	-0.093799710	15.575478554
Si	8.734817505	4.828693390	17.718685150	Si	8.739280701	4.821926117	17.696577072	Si	8.799714088	4.887957096	17.692884445
Si	8.776823997	7.113711357	15.590837479	Si	8.791230202	7.136032581	15.586936951	Si	8.855919838	7.189713478	15.574999809
Si	14.236572266	-0.321446776	17.701091766	Si	14.254420280	-0.325893402	17.697057724	Si	14.303132057	-0.276811004	17.685922623
Si	11.095934868	-0.455874503	17.560045242	Si	11.112008095	-0.442377210	17.569158554	Si	11.168274879	-0.382471561	17.538850784
Si	8.755808830	7.055777073	12.474450111	Si	8.771236420	7.101490498	12.480373383	Si	8.825441360	7.139856339	12.460900307
Si	16.566062927	2.201146126	10.289052963	Si	16.582695007	2.199765921	10.276689529	Si	16.632085800	2.247522593	10.286477089
Al	7.770233631	6.125752926	1.176232696	Al	7.770205975	6.111782551	1.132576823	Al	7.846866131	6.197506905	1.130818963

Al	17.322479248	6.100397587	1.190766096	Al	17.338298798	6.102617264	1.168218136	Al	17.398155212	6.155226707	1.164327502
Al	7.114832401	5.298393250	10.566184044	Al	7.126336098	5.342444897	10.572247505	Al	7.188706875	5.377821445	10.574520111
Al	16.604524612	5.348878860	10.514826775	Al	16.609722137	5.344579697	10.513302803	Al	16.655279160	5.397583008	10.492576599
O	1.526228666	1.697259545	8.389514923	O	1.514812350	1.691114783	8.313226700	O	1.566168070	1.733154178	8.360699654
O	-0.040521920	0.027692944	3.049264908	O	-0.026185587	0.025675625	3.041207314	O	0.004150152	0.066412777	3.026890278
O	7.944998741	2.047008276	2.309312105	O	7.960084438	2.031101227	2.287105083	O	8.006422043	2.137528896	2.315480471
O	2.852322102	0.173962340	0.146355808	O	2.883988380	0.188341662	0.118811488	O	2.985732794	0.234895229	0.114628874
O	1.369285941	8.106257439	2.200750828	O	1.403420568	8.130640030	2.191478491	O	1.452788830	8.218683243	2.188366890
O	-0.140771970	2.884323120	0.124467649	O	-0.117764764	2.879526615	0.120043211	O	-0.057783622	2.955021620	0.139510453
O	6.194093704	6.875941753	0.944950223	O	6.201444626	6.857357025	0.846812844	O	6.283632278	6.953882694	0.875516653
O	8.014250755	8.602771759	6.357339859	O	7.998130798	8.602878571	6.352338791	O	8.083238602	8.700817108	6.336760044
O	6.406862736	0.332421243	7.023615360	O	6.426379204	0.407257438	7.040381908	O	6.452578068	0.410494328	7.020626545
O	8.009549141	5.660178661	9.121436119	O	8.053178787	5.781726837	9.170750618	O	8.073603630	5.751581669	9.121137619
O	0.005877316	6.422742367	6.904376030	O	0.006010652	6.422590733	6.898268223	O	0.086392105	6.483488560	6.906248093
O	4.868610382	8.266396523	9.096608162	O	4.982348919	8.290083885	9.108405113	O	4.966655731	8.328737259	9.107241631
O	1.228167772	6.159253597	9.255329132	O	1.242413044	6.175769329	9.246335030	O	1.273977518	6.202771664	9.272516251
O	18.144184113	1.815003633	6.855122089	O	18.091651917	1.826158166	6.869642735	O	18.156185150	1.875526071	6.883062363
O	6.030362129	9.112558365	2.448195457	O	6.062185287	9.094255447	2.366465807	O	6.107033730	9.204864502	2.364674568
O	6.012073517	1.459161520	9.419534683	O	5.960464954	1.505625486	9.451997757	O	6.096674919	1.524346471	9.425649643
O	17.908905029	6.811195850	2.633745909	O	17.951547623	6.813039780	2.596955776	O	18.033031464	6.845671654	2.592648983
O	1.153594971	8.833570480	6.962415695	O	1.182590723	8.822651863	6.937002659	O	1.935750961	-0.495717824	6.931857586
O	0.522668540	7.727223873	4.666073799	O	0.533627033	7.710960388	4.649693012	O	0.581637681	7.777438641	4.652047157
O	3.946555853	0.694603682	8.009434700	O	3.953542233	0.652603209	8.025375366	O	4.006785393	0.740577161	8.050650597
O	7.495687962	4.427791119	1.239234090	O	7.479961872	4.421781540	1.288856506	O	7.546439171	4.505185604	1.249356866
O	7.490576267	0.913877964	4.679879189	O	7.467308998	0.883960605	4.649542332	O	7.499138355	0.964308143	4.662193775
O	3.853025913	7.972688198	1.476089358	O	3.881009579	7.979300976	1.395610690	O	3.940304279	8.010297775	1.431583166
O	0.341307223	4.008543491	7.992137432	O	0.330050707	4.016051292	7.986467838	O	0.374874771	4.061719418	7.985930443
O	10.925427437	1.653888226	8.270130157	O	10.941232681	1.671289444	8.253750801	O	10.970426559	1.721852779	8.242994308
O	9.346396446	-0.057934999	3.035084963	O	9.357308388	-0.054604009	3.034183264	O	9.399049759	0.031415284	3.046617508
O	17.349046707	2.056601524	2.267055988	O	17.367292404	2.062977076	2.269153595	O	17.402240753	2.123583555	2.270291805
O	12.286470413	0.204445243	0.224599719	O	12.294147491	0.193583772	0.216232508	O	12.363956451	0.244234398	0.179282755
O	10.853552818	8.101222038	2.286211014	O	10.891271591	8.129821777	2.313640356	O	10.942443848	8.241622925	2.300563574
O	9.312660217	2.763355017	0.158965498	O	9.307550430	2.812849283	0.131760702	O	9.379707336	2.857728720	0.151828945
O	15.579858780	6.815563679	0.974776268	O	15.592704773	6.811458588	0.977530837	O	15.659901619	6.879224300	0.969923913
O	17.428817749	8.605247498	6.308817863	O	17.453025818	8.612054825	6.295840740	O	17.508419037	8.660363197	6.304626942
O	15.859388351	0.401502728	7.011254787	O	15.849783897	0.348109424	6.985448837	O	15.906649590	0.408516586	6.983171463
O	17.443359375	5.759047508	9.067779541	O	17.452306747	5.772789001	9.074013710	O	17.486829758	5.816699505	9.047403336
O	9.380275726	6.395167828	6.960081577	O	9.390508652	6.405792236	6.965584755	O	9.449193954	6.493185043	6.958920002
O	14.411249161	8.372868538	9.122914314	O	14.405826569	8.361515999	9.116104126	O	14.423955917	8.401376724	9.093179703
O	10.648139000	6.170660496	9.279005051	O	10.706084251	6.151242256	9.259723663	O	10.711914063	6.222177029	9.283413887
O	8.635808945	1.830582261	6.892446041	O	8.678930283	1.842821121	6.821223736	O	8.667437553	1.922430992	6.872034550
O	15.510389328	9.061029434	2.427924395	O	15.525691032	9.066573143	2.406813860	O	15.564512253	9.125949860	2.411043406
O	15.386486053	1.597647071	9.333582878	O	15.424670219	1.585230470	9.300942421	O	15.484915733	1.612857103	9.316273689
O	8.591520309	6.695613861	2.584901333	O	8.621331215	6.727897644	2.497876167	O	8.688081741	6.812399864	2.501472950

O	10.611953735	8.762558937	6.926082134	O	10.602714539	8.789999962	6.884348869	O	11.382432938	-0.541455686	6.877219200
O	9.894976616	7.651544571	4.685318947	O	9.857841492	7.623263836	4.675285816	O	9.939681053	7.706472874	4.663827896
O	13.362166405	0.634377420	7.946093082	O	13.367151260	0.630342603	7.940965652	O	13.424689293	0.729801476	7.927635193
O	16.859542847	4.455237865	1.305483341	O	16.880525589	4.456053734	1.291361690	O	16.909696579	4.515202045	1.272196412
O	16.897970200	0.943537474	4.655752659	O	16.906843185	0.933042884	4.645393372	O	16.965522766	0.993028104	4.652854443
O	13.294656754	7.935318470	1.372078061	O	13.307537079	7.911609650	1.347172379	O	13.358862877	7.966012955	1.354302883
O	9.783634186	3.992861271	8.011530876	O	9.724275589	3.997715473	8.032629967	O	9.827634811	4.074377537	7.970126629
O	0.810066342	0.952212095	17.651876450	O	0.827556372	0.968042970	17.632617950	O	0.866781712	0.995148778	17.632263184
O	-0.711227834	-0.724901378	12.415486336	O	-0.699906468	-0.722076714	12.401910782	O	-0.656563044	-0.686474562	12.380579948
O	7.342491150	1.282014370	11.718286514	O	7.352704048	1.316140890	11.707660675	O	7.442986012	1.367920399	11.718592644
O	2.203326941	-0.548637748	9.611662865	O	2.143246651	-0.527224898	9.594472885	O	2.212682724	-0.512181461	9.591215134
O	0.741941512	7.367209435	11.630773544	O	0.749839842	7.361413956	11.621377945	O	0.816964209	7.403994560	11.638901711
O	-0.831277907	2.110542297	9.504861832	O	-0.802518725	2.118034601	9.520457268	O	-0.744140506	2.168951511	9.546491623
O	5.592424393	6.147576332	10.560254097	O	5.543178558	6.105813026	10.578597069	O	5.672448635	6.239252567	10.636471748
O	7.318877220	7.851090908	15.706518173	O	7.304990768	7.848406792	15.705597878	O	7.365422249	7.885042191	15.721282005
O	5.741089821	-0.535775125	16.408096313	O	5.707883358	-0.356886208	16.332588196	O	5.776291370	-0.327557683	16.351528168
O	7.321183681	5.037045479	18.452648163	O	7.289215088	4.943050861	18.372087479	O	7.352088928	5.044281960	18.366882324
O	-0.666710675	5.720576286	16.316476822	O	-0.650626600	5.722381115	16.298563004	O	-0.563282132	5.762127399	16.296079636
O	4.140603065	7.634379387	18.518339157	O	4.187954903	7.634123802	18.433570862	O	4.197830677	7.689682007	18.439998627
O	0.634232402	5.418023109	18.615385056	O	0.620579481	5.420672894	18.607891083	O	0.684044600	5.475796223	18.616199493
O	17.401916504	1.132567167	16.205204010	O	17.405906677	1.127280831	16.201873779	O	17.446550369	1.178145528	16.214523315
O	5.802379608	-0.857911706	11.764789581	O	5.881178856	-0.887692809	11.784152031	O	5.860245705	-0.764092684	11.783612251
O	5.307625771	0.852268577	18.686365128	O	5.311091900	0.874706030	18.666641235	O	5.379929543	0.920568824	18.677902222
O	17.259963989	6.059489727	11.929390907	O	17.260025024	6.059248924	11.929529190	O	17.331909180	6.084905148	11.913471222
O	1.222737670	-1.269162059	16.223823547	O	1.230057478	-1.264400959	16.210802078	O	1.310934901	-1.217753649	16.197172165
O	-0.191487610	6.930256844	14.026192665	O	-0.181253076	6.943004608	14.014412880	O	-0.148787200	6.970149994	14.010246277
O	3.244439602	-0.007334709	17.316617966	O	3.262324572	0.025682569	17.259180069	O	3.323363304	0.101579309	17.254081726
O	6.673647881	3.605246544	10.679992676	O	6.804643631	3.642501831	10.653809547	O	6.764170647	3.686147690	10.692111015
O	6.780474663	0.119462013	14.031231880	O	6.800506115	0.167033672	14.019064903	O	6.871466637	0.199048162	14.028709412
O	3.167745113	7.079854488	10.761169434	O	3.177081108	7.208210945	10.739593506	O	3.236226797	7.175576210	10.755702019
O	-0.320675492	3.293426037	17.341909409	O	-0.322193861	3.295685291	17.330974579	O	-0.262143016	3.343894958	17.319955826
O	10.240576744	0.923329711	17.632242203	O	10.261680603	0.938909769	17.657905579	O	10.308284760	0.990114927	17.641839981
O	7.761339664	8.350182533	12.275595665	O	8.549594879	-0.937496901	12.318415642	O	8.518899918	-0.965467215	12.280551910
O	16.677017212	1.311469793	11.650850296	O	16.675846100	1.313239336	11.642230988	O	16.722507477	1.385152102	11.674829483
O	11.588171005	-0.548648715	9.569190025	O	11.582198143	-0.564082980	9.533192635	O	11.674490929	-0.493665278	9.528038025
O	10.125638008	7.389471531	11.640557289	O	10.128712654	7.359192848	11.610332489	O	10.182744026	7.493932247	11.619027138
O	8.628482819	2.093504906	9.537218094	O	8.605074883	1.993655086	9.463785172	O	8.700824738	2.181438684	9.525165558
O	14.862092018	6.063212395	10.351489067	O	14.862165451	6.055031776	10.353156090	O	14.911359787	6.105518341	10.337171555
O	16.776390076	7.902202606	15.683999062	O	16.779159546	7.897576809	15.683443069	O	16.852792740	7.950242043	15.703355789
O	15.171203613	-0.365995765	16.373151779	O	15.174537659	-0.364054620	16.361003876	O	15.222979546	-0.333030522	16.348392487
O	16.818500519	5.031179428	18.497228622	O	16.804620743	5.036982536	18.459165573	O	16.875644684	5.086067200	18.458887100
O	8.680950165	5.644766808	16.290277481	O	8.716888428	5.671530247	16.289670944	O	8.816860199	5.725186825	16.279806137
O	13.729829788	7.645489693	18.500848770	O	13.735284805	7.634764671	18.486038208	O	13.776153564	7.688759327	18.481904984
O	9.974691391	5.441533089	18.624095917	O	9.929809570	5.433812141	18.659301758	O	9.992299080	5.487160683	18.663579941

O	7.954588413	1.074171782	16.244750977	O	7.986166954	1.088836789	16.229314804	O	8.035202026	1.140875816	16.232826233
O	14.844837189	8.308145523	11.772842407	O	14.863169670	8.301686287	11.766222000	O	14.912327766	8.360655785	11.741642952
O	14.707201004	0.881779671	18.673620224	O	14.733917236	0.870447874	18.672334671	O	14.799607277	0.914684176	18.656394958
O	8.034336090	5.716273308	11.993743896	O	7.960092545	5.802184105	12.040023804	O	8.125614166	5.787240505	11.996047974
O	9.915321350	8.016128540	16.321289063	O	9.898324966	8.071419716	16.315021515	O	10.663652420	-1.254596949	16.271190643
O	9.197731972	6.960834503	14.040771484	O	9.227614403	6.982439518	14.044602394	O	9.270566940	7.043817520	14.028850555
O	12.675722122	-0.106651187	17.314386368	O	12.689680099	-0.102046490	17.323322296	O	12.745710373	-0.033121705	17.306339264
O	16.168767929	3.699553490	10.667320251	O	16.168794632	3.694339275	10.660126686	O	16.218091965	3.747488499	10.648452759
O	16.212511063	0.178857446	14.016225815	O	16.224143982	0.179205060	14.006851196	O	16.285932541	0.200313449	14.009300232
O	12.585489273	7.216307163	10.759181023	O	12.592749596	7.231880665	10.771408081	O	12.639867783	7.260784149	10.777069092
O	9.037921906	3.249699831	17.396579742	O	9.091163635	3.258283854	17.346923828	O	9.118256569	3.315485001	17.354490280
O	4.935378075	2.087282658	15.658835411	O	3.401657104	2.382769108	14.883758545	O	3.236436844	2.464396954	15.107323647
O	4.992076397	3.837267637	13.470701218	O	4.463362694	4.368745327	13.817072868	O	4.198298931	4.516227245	13.975444794
Cu	4.096916676	2.880493879	12.222102165	Cu	3.839551449	2.719207287	13.025749207	Cu	3.460776091	2.856710672	13.183977127
Cu	4.732263088	3.782649517	16.236270905	Cu	4.259233475	3.914526939	15.703495026	Cu	4.166997910	3.989632130	15.842043877
H	14.937890053	6.088729858	0.882433653	H	14.949589729	6.080693245	0.895816088	H	15.022108078	6.142329216	0.894624949
H	2.981339931	0.900717616	13.358393669	H	2.771411896	0.392296553	13.147363663	H	2.616444111	0.761920750	11.810546875
H	2.501547813	0.830692768	11.782577515	H	2.821843147	0.777031422	11.557017326	H	4.109550476	0.410040021	12.401116371
H	4.009976864	0.321455836	12.214399338	H	4.183479309	0.249135911	12.309806824	H	2.796611071	0.364787698	13.387845993
H	3.484708309	4.582085609	10.489152908	H	4.306477547	4.393861771	11.117052078	H	3.606268644	4.501890182	11.254742622
H	4.506810665	3.436055660	9.910650253	H	4.423761368	2.888189316	10.492930412	H	4.900244236	3.516510248	11.086779594
H	2.867468596	3.152631998	9.892360687	H	2.934997082	3.556777239	10.743192673	H	3.415076971	3.030907631	10.546779633
H	14.213610649	5.339594841	10.242522240	H	14.212802887	5.332653522	10.248245239	H	14.260477066	5.381643295	10.251948357
H	3.748594761	4.061339378	18.590539932	H	3.881175280	4.136321068	18.294340134	H	3.925057650	4.206830978	18.448453903
H	2.570475101	3.348947048	17.629095078	H	2.625880241	3.305372953	17.579292297	H	2.667843342	3.325773716	17.792539597
H	3.871529818	2.462732792	18.150243759	H	4.052051544	2.553430557	17.904470444	H	4.136450291	2.629800081	18.050743103
H	5.346165180	6.203875065	15.739320755	H	5.699968338	6.045803547	15.610302925	H	5.676753044	6.060548782	15.636673927
H	4.570439339	6.155234337	17.188188553	H	4.667010784	6.160320282	16.875463486	H	4.714769363	6.235137939	16.949254990
H	6.098522663	5.613551617	17.098091125	H	6.016099930	5.258918762	17.028242111	H	6.046881199	5.305201054	17.058759689
H	4.997715950	2.210980415	14.689270973	H	3.509763241	1.521183014	15.323629379	H	5.053049088	4.795104980	13.603997231
H	5.938148022	3.908281803	13.229413986	H	5.321907520	4.684052467	13.482421875	H	3.443289995	1.610990763	15.527559280
N	3.297243118	1.046548367	12.393026352	N	3.349660635	0.843855739	12.433996201	H	1.338249207	4.671142578	13.308171272
N	3.631365776	3.566826105	10.435484886	N	3.871925831	3.459002018	11.144886017	H	0.548673451	3.459720135	12.535553932
N	3.573371172	3.389788389	17.826452255	N	3.642157078	3.435093880	17.572927475	H	0.940171003	3.313606739	14.122540474
N	5.204092979	5.631227016	16.573331833	N	5.261220932	5.503036976	16.357151031	N	3.226744175	0.890626550	12.623148918
								N	3.887317181	3.518095255	11.312276840
								N	3.676158667	3.494407654	17.742296219
								N	5.265789509	5.549440861	16.420173645
								N	1.282889128	3.652948856	13.220192909
Structure Q₃				ts5				Structure A			
Si	0.111344039	2.443337202	8.249779701	Si	0.092674077	2.443238974	8.288076401	Si	0.062787652	2.488001347	8.345581055
Si	7.950971127	0.683286905	3.169215918	Si	7.922149658	0.706389308	3.207546711	Si	7.904357910	0.665149331	3.259986162
Si	2.419319868	8.218028069	0.950245500	Si	2.398022175	8.198570251	0.980299294	Si	2.393449068	8.193976402	1.060106397
Si	5.530155659	8.295038223	1.184905887	Si	5.523376942	8.325926781	1.238930583	Si	5.480361462	8.289840698	1.301761866

Si	7.855834484	0.619890094	6.277751446	Si	7.859600544	0.657290280	6.327646732	Si	7.845445633	0.622872889	6.378610611
Si	0.053642452	5.616729259	8.341883659	Si	0.051336288	5.605600834	8.400504112	Si	0.008716166	5.645285606	8.477866173
Si	0.121147633	7.915413857	6.251277924	Si	0.127619952	7.916281223	6.278968811	Si	0.099183977	7.963845730	6.343591690
Si	5.570557117	0.380983055	8.431371689	Si	5.550834179	0.418547869	8.472402573	Si	5.519732475	0.438694954	8.529117584
Si	2.441074848	0.338625968	8.260749817	Si	2.421811104	0.339958906	8.248893738	Si	2.402659893	0.385964811	8.302776337
Si	0.144371107	8.038809776	3.164861679	Si	0.123156190	8.017143250	3.199718237	Si	0.090992168	8.029586792	3.257080078
Si	7.979905128	2.983993053	1.012683153	Si	7.927308559	3.013962269	1.049927354	Si	7.942065239	2.954846859	1.130996823
Si	9.509654999	2.456408739	8.222276688	Si	9.515876770	2.487674952	8.274030685	Si	9.493626595	2.459733963	8.312067986
Si	17.384641647	0.728411436	3.171834707	Si	17.397975922	0.736850381	3.216431856	Si	17.347429276	0.731312215	3.280567169
Si	11.794302940	8.182131767	1.018428922	Si	11.790156364	8.216218948	1.062097073	Si	11.755349159	8.166297913	1.134072661
Si	14.904443741	8.378021240	1.225553393	Si	14.891875267	8.404489517	1.267266154	Si	14.869935036	8.384332657	1.336425543
Si	17.301963806	0.598798394	6.278441429	Si	17.289239883	0.583748043	6.321117401	Si	17.260391235	0.630059958	6.387560844
Si	9.464082718	5.594532967	8.434246063	Si	9.473568916	5.630197525	8.485372543	Si	9.481692314	5.572020531	8.533293724
Si	9.499467850	7.880397797	6.286867619	Si	9.496741295	7.926910877	6.347669601	Si	9.475055695	7.891253471	6.418738842
Si	14.960297585	0.427137554	8.378615379	Si	14.958713531	0.428103566	8.423170090	Si	14.938700676	0.439409137	8.513181686
Si	11.816622734	0.316723406	8.227049828	Si	11.819630623	0.348475933	8.304536819	Si	11.788895607	0.310288310	8.387834549
Si	9.537428856	7.987633228	3.196099758	Si	9.511537552	7.992911339	3.257338762	Si	9.501029015	7.912405968	3.323530436
Si	17.374763489	2.993640184	0.978765190	Si	17.345785141	3.007602692	1.033086896	Si	17.318237305	3.007810831	1.083491921
Si	-0.566888571	1.748795152	17.583673477	Si	-0.583715439	1.749697804	17.629241943	Si	-0.598461330	1.759216070	17.685394287
Si	7.191082954	-0.096291304	12.518802643	Si	7.176504135	-0.070585191	12.553318977	Si	7.214650631	-0.120704710	12.618648529
Si	1.708262205	7.390047073	10.323700905	Si	1.674832702	7.380191803	10.356374741	Si	1.670297146	7.440359116	10.426955223
Si	4.817150593	7.545325756	10.612080574	Si	4.788566589	7.567880630	10.639564514	Si	4.795577526	7.525369167	10.652233124
Si	7.234954834	-0.113325000	15.661707878	Si	7.201005936	-0.044030190	15.702010155	Si	7.185035706	-0.129016280	15.755331039
Si	-0.570926368	4.919941902	17.752683640	Si	-0.596585631	4.913640499	17.780757904	Si	-0.609851599	4.920304775	17.840480804
Si	-0.516364336	7.205481529	15.613725662	Si	-0.549003541	7.207660675	15.656666756	Si	-0.558626115	7.222426891	15.729928017
Si	4.891149521	-0.270316720	17.775306702	Si	4.864687920	-0.235906124	17.832666397	Si	4.849269867	-0.309078574	17.889318466
Si	1.780503750	-0.361819386	17.540512085	Si	1.741668463	-0.363812804	17.600294113	Si	1.752624273	-0.353188992	17.674568176
Si	-0.576385856	7.251837730	12.508466721	Si	-0.597113013	7.273500919	12.559950829	Si	-0.579921186	7.315291405	12.626973152
Si	7.250479221	2.196605206	10.394701004	Si	7.230921268	2.224476814	10.429654121	Si	7.205162525	2.209357262	10.513438225
Si	8.892760277	1.709705114	17.628629684	Si	8.851428986	1.755967259	17.649139404	Si	8.839946747	1.696177721	17.711147308
Si	16.694967270	-0.035761654	12.516998291	Si	16.676624298	-0.024270773	12.575532913	Si	16.642980576	-0.008229971	12.652489662
Si	11.056739807	7.421366692	10.340324402	Si	11.058732986	7.430991650	10.407912254	Si	11.051852226	7.387017250	10.464423180
Si	14.161502838	7.642454147	10.581047058	Si	14.151811600	7.642010689	10.648439407	Si	14.143799782	7.648802757	10.716362000
Si	16.643014908	-0.093538642	15.642925262	Si	16.618064880	-0.101257205	15.690223694	Si	16.598596573	-0.086684227	15.758796692
Si	8.798598289	4.885544777	17.779745102	Si	8.840837479	4.912421227	17.858530045	Si	8.792438507	4.852350235	17.933084488
Si	8.880965233	7.178039074	15.660260201	Si	8.866517067	7.217937469	15.718034744	Si	8.846116066	7.150432110	15.771381378
Si	14.335027695	-0.314149022	17.757045746	Si	14.305416107	-0.287519336	17.803174973	Si	14.290580750	-0.305965662	17.875734329
Si	11.199228287	-0.391416550	17.636827469	Si	11.179194450	-0.361166954	17.665798187	Si	11.148553848	-0.418692946	17.727550507
Si	8.814754486	7.094375134	12.560658455	Si	8.780017853	7.116415501	12.607361794	Si	8.792591095	7.094665527	12.677877426
Si	16.628005981	2.239156961	10.342350006	Si	16.627431870	2.247542858	10.384926796	Si	16.598367691	2.267534971	10.469292641
Al	7.830529213	6.183343410	1.186918378	Al	7.825393677	6.190150738	1.313519478	Al	7.805449963	6.130055904	1.372509956
Al	17.416494370	6.143757820	1.218324065	Al	17.378383636	6.148199558	1.250198960	Al	17.366275787	6.145402431	1.301281929
Al	7.177722454	5.336668491	10.689601898	Al	7.145319462	5.375916481	10.709496498	Al	7.109139442	5.334207058	10.743041992
Al	16.650865555	5.388442039	10.533980370	Al	16.639408112	5.396875381	10.581495285	Al	16.632236481	5.403980732	10.649191856

O	1.571112871	1.715153933	8.412319183	O	1.548555732	1.709197998	8.443209648	O	1.526297569	1.756560564	8.498025894
O	0.009797081	0.058641851	3.094059706	O	0.022259444	0.060182452	3.159711838	O	-0.022920027	0.065180689	3.220705032
O	8.027534485	2.083492756	2.357418299	O	8.022150993	2.096992970	2.383929014	O	8.085476875	2.076284647	2.490386248
O	2.940117359	0.248394042	0.157881171	O	2.875792980	0.232911557	0.208103240	O	2.951462030	0.241259620	0.288322270
O	1.478057623	8.234743118	2.260495186	O	1.461586595	8.173759460	2.297864914	O	1.425024271	8.209568024	2.355160236
O	-0.000372691	2.913976908	0.232115313	O	-0.045027770	2.937642097	0.264880657	O	-0.068736151	2.951708555	0.319545776
O	6.246261120	6.890712738	0.931225598	O	6.294666290	6.956929684	0.998962283	O	6.288613796	6.936541557	1.121107578
O	8.065317154	8.659618378	6.393823147	O	8.053229332	8.688079834	6.463784695	O	8.026374817	8.646127701	6.524394989
O	6.446435928	0.375112176	7.067065239	O	6.450486660	0.424440503	7.125575066	O	6.439948082	0.438724279	7.198836803
O	8.111882210	5.708634377	9.273675919	O	8.123291969	5.765722275	9.327317238	O	8.135063171	5.639910221	9.381814957
O	0.075323403	6.438859463	6.931295395	O	0.113125503	6.469089508	7.019404411	O	0.094209015	6.535067558	7.119327068
O	4.982490540	8.331982613	9.182977676	O	4.947702408	8.369419098	9.220874786	O	4.888851166	8.384223938	9.260931969
O	1.269386292	6.206485748	9.293549538	O	1.264496088	6.130641460	9.394938469	O	1.176007867	6.171448708	9.530690193
O	18.136438370	1.821001410	6.978196621	O	18.093221664	1.817175865	7.035623074	O	18.073680878	1.874083519	7.080766201
O	6.150236607	9.130885124	2.438373327	O	6.079005241	9.178920746	2.515785456	O	6.716623783	-0.173386633	2.527254581
O	6.086316109	1.528536797	9.455801964	O	6.047424793	1.564057708	9.509658813	O	5.993186474	1.568361878	9.605660439
O	18.056882858	6.841137886	2.643147230	O	18.000165939	6.851620674	2.676028013	O	17.990669250	6.849648952	2.725703001
O	1.904849768	-0.540866435	7.014984131	O	1.925085068	-0.483704388	6.950272560	O	1.903815389	-0.434426606	7.001310825
O	0.593652487	7.775584221	4.710914135	O	0.563502073	7.710106850	4.738864899	O	0.521065950	7.728816032	4.803347111
O	4.007366657	0.717038929	8.061719894	O	3.988112211	0.742031336	8.097841263	O	3.965786934	0.799546599	8.145747185
O	7.608590126	4.482977390	1.334174514	O	7.556887627	4.499518394	1.416295409	O	7.528587818	4.437982082	1.466683865
O	7.506724358	0.948945045	4.720660210	O	7.517448902	0.981969833	4.769423485	O	7.485420227	0.919118583	4.822362423
O	3.942911863	8.059656143	1.455104709	O	3.931730986	8.056652069	1.459013224	O	3.902847052	7.988768101	1.588823557
O	0.372811615	4.034074783	8.038392067	O	0.353059411	4.030331135	8.053055763	O	0.356957793	4.077155113	8.133161545
O	10.954042435	1.689931393	8.303243637	O	10.958853722	1.722231627	8.410418510	O	10.916325569	1.674154520	8.491912842
O	9.436300278	0.026391357	3.156548262	O	9.394384384	0.019198090	3.168912649	O	9.337552071	-0.092976391	3.211038351
O	17.413085938	2.122594595	2.355656385	O	17.426761627	2.141820908	2.414849281	O	17.375583649	2.119210720	2.452460766
O	12.387689590	0.240091801	0.278317690	O	12.366312027	0.262654841	0.302325428	O	12.299944878	0.204812974	0.360675693
O	10.948354721	8.209370613	2.381399870	O	10.894424438	8.205072403	2.389812708	O	10.896884918	8.162428856	2.487365484
O	9.427452087	2.835175514	0.233569905	O	9.366935730	2.892827988	0.239784583	O	9.380914688	2.847896576	0.319146454
O	15.665854454	6.853440762	1.081079364	O	15.631031036	6.871645927	1.106727481	O	15.618841171	6.860562325	1.150111198
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O	15.877760887	0.368932843	7.041743279	O	15.866005898	0.324849188	7.080271244	O	15.849179268	0.381774664	7.170710564
O	17.477827072	5.795647144	9.081356049	O	17.467826843	5.792974472	9.123995781	O	17.401119232	5.785383224	9.156559944
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O	15.487759590	1.597960234	9.367609024	O	15.511801720	1.610540390	9.381879807	O	15.466710091	1.625966311	9.481356621
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O	10.667411804	8.792171478	6.978607178	O	11.339835167	-0.543356419	7.044828415	O	10.626194000	8.806616783	7.132326126
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O	13.400886536	0.685023606	8.024623871	O	13.400747299	0.712988913	8.077539444	O	13.370738983	0.683208466	8.179618835

O	16.951194763	4.495398998	1.317321301	O	16.899425507	4.505011559	1.363749623	O	16.885728836	4.503923416	1.440737009
O	16.965694427	0.977756202	4.727652073	O	16.960317612	0.969771147	4.770473957	O	16.913040161	0.993800640	4.834878922
O	13.369242668	7.951583385	1.445741057	O	13.353630066	8.017324448	1.529229403	O	13.330970764	7.984356403	1.571419835
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O	0.879034877	0.991691828	17.626968384	O	0.860886574	1.000380158	17.711269379	O	0.839610457	0.991482258	17.777023315
O	-0.664616406	-0.699464440	12.423409462	O	-0.677088797	-0.670958638	12.501336098	O	-0.720451593	-0.674926400	12.571162224
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Cu	4.452998638	3.974565983	15.557523727	Cu	4.926688194	4.315089226	15.435473442	Cu	5.137386799	4.044002533	15.082732201
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H	2.636858940	0.885026574	11.504433632	H	2.574284077	0.778698683	11.265543938	H	2.727821827	0.218674779	12.253082275
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H	7.319896698	3.232964516	15.338768005	H	7.426541328	3.611109257	15.114291191	H	7.786073685	4.170490265	15.212389946
N	3.148751497	1.041355848	12.378187180	N	3.036504745	0.873185396	12.172863007	N	3.423493862	0.967912376	12.250971794
N	3.706025600	3.692235231	11.090278625	N	3.702230215	3.594930172	11.129523277	N	3.385302544	3.487119436	10.605302811
N	3.922951698	3.427805424	17.480314255	N	3.624996185	3.524674892	16.753118515	N	3.529016972	3.216273308	16.014595032
N	5.253067017	5.674314976	16.285655975	N	5.563373089	5.749633789	16.630516052	N	5.430476189	5.452748299	16.496908188
N	1.098042965	3.502712727	13.247474670	N	0.997485638	3.221643448	13.081256866	N	1.557324409	4.531137466	12.686299324
N	6.562563419	3.442371845	14.683748245	N	6.672725677	3.852992535	14.463729858	N	7.095664501	3.967529297	14.483567238

Table S8. Cartesian coordinates of RC, TS, IM, and PC for NH₂NO self-decomposition.

Structure A				ts1			Structure B				
Si	0.126935542	2.470517159	8.013442993	Si	0.138879597	2.468534231	8.029371262	Si	0.157806396	2.441827536	8.039543152
Si	7.941133976	0.656771064	2.979287386	Si	7.951760292	0.659534574	2.988707781	Si	7.937094212	0.646656811	2.965903759
Si	2.419070959	8.161301613	0.770132005	Si	2.433354139	8.151018143	0.790373385	Si	2.427414417	8.143082619	0.779767036
Si	5.530753613	8.303808212	1.043948054	Si	5.538378716	8.300268173	1.055379391	Si	5.546506405	8.292058945	1.027628422
Si	7.907699108	0.623101890	6.127501488	Si	7.911434650	0.617500544	6.132910728	Si	7.935659409	0.624884844	6.111620903
Si	0.126905441	5.637632847	8.203438759	Si	0.157463610	5.629832745	8.224172592	Si	0.116442800	5.597784996	8.182619095
Si	0.165856242	7.925550461	6.089161396	Si	0.165098608	7.926204681	6.103682518	Si	0.185785055	7.914692402	6.060341835
Si	5.584330559	0.443310916	8.258350372	Si	5.586672306	0.441832840	8.268195152	Si	5.604557991	0.436297715	8.240238190
Si	2.453398705	0.346597552	8.077112198	Si	2.457583666	0.345366955	8.091948509	Si	2.477406025	0.329836071	8.020161629
Si	0.138834447	7.969607830	2.998301983	Si	0.143393964	7.973560810	3.010839224	Si	0.176876247	7.997797966	2.965690613
Si	7.992717266	2.961902857	0.841234863	Si	7.996555328	2.962633133	0.845899522	Si	8.001610756	2.951149702	0.821922719
Si	9.571305275	2.447799206	8.073434830	Si	9.572208405	2.447048664	8.077211380	Si	9.589894295	2.447503567	8.060656548
Si	17.432695389	0.682505965	2.957473040	Si	17.432018280	0.674420834	2.966144800	Si	17.437511444	0.692706347	2.972810268
Si	11.827690125	8.182919502	0.811910748	Si	11.832344055	8.182271004	0.812220812	Si	11.839271545	8.184258461	0.815125227
Si	14.938962936	8.371100426	0.983908892	Si	14.943937302	8.372905731	0.989289403	Si	14.939740181	8.371117592	1.010962009
Si	17.350503922	0.641116202	6.069227695	Si	17.356464386	0.639873862	6.079277992	Si	17.360460281	0.602955222	6.082739830
Si	9.508690834	5.615464211	8.249505997	Si	9.513582230	5.617397785	8.249847412	Si	9.533607483	5.618827343	8.246213913
Si	9.566113472	7.918040752	6.115636826	Si	9.576276779	7.917614460	6.114504814	Si	9.592088699	7.922560692	6.111238480
Si	15.021571159	0.469612598	8.189949989	Si	15.022076607	0.479873598	8.196501732	Si	15.042913437	0.450642347	8.192255020
Si	11.894538879	0.345166445	8.050383568	Si	11.895628929	0.347680271	8.052680016	Si	11.918170929	0.348839343	8.049495697
Si	9.586473465	7.932694435	2.995976210	Si	9.593101501	7.936102390	3.000852346	Si	9.589980125	7.924915791	2.994081020
Si	17.363594055	2.980098963	0.794838011	Si	17.358579636	2.984412193	0.806001365	Si	17.391239166	2.981016874	0.800932646
Al	7.879945278	6.142812729	1.059864044	Al	7.885631561	6.147762299	1.062261701	Al	7.904506683	6.135784149	1.055712104
Al	17.416284561	6.122964382	1.067595720	Al	17.425434113	6.120252609	1.079874873	Al	17.411306381	6.113170147	0.977054954
O	1.566879511	1.709035635	8.127206802	O	1.577804685	1.711820602	8.173930168	O	1.601015806	1.693101764	8.155688286
O	0.067421436	0.023036644	2.893033028	O	0.070867509	0.028061479	2.896027565	O	0.068210483	0.033898219	2.896762371
O	8.099688530	2.087661743	2.225244045	O	8.101483345	2.091684580	2.232642412	O	8.100541115	2.073588848	2.204078197
O	2.901975632	0.240611061	0.082779318	O	2.913581610	0.222412750	0.088209353	O	2.243631840	-0.575160265	9.353986740
O	1.470549107	8.049260139	2.076700211	O	1.475148559	8.053355217	2.088991642	O	1.561984777	8.183934212	2.143370867
O	-0.737507105	2.151098967	9.364195824	O	-0.055804770	2.906006813	0.006002630	O	0.005672225	2.910543442	0.050675865
O	6.358653545	6.952512741	0.934837162	O	6.358903885	6.945148945	0.934372783	O	6.386152267	6.948669910	0.926625967
O	8.095752716	8.638974190	6.258270741	O	8.103934288	8.635663033	6.254264832	O	8.120523453	8.640084267	6.245589733
O	6.478126526	0.383199692	6.879975319	O	6.488170624	0.371219873	6.895222187	O	6.513370514	0.382483661	6.873000622
O	8.072438240	5.776332855	8.945816040	O	8.080658913	5.787683487	8.950876236	O	8.102489471	5.784601688	8.950144768
O	0.036206931	6.446918011	6.770830154	O	0.071415722	6.469557762	6.820154667	O	0.176549911	6.483758450	6.819378376
O	5.023779392	8.397234917	8.997346878	O	5.022277355	8.397690773	9.011048317	O	5.048354149	8.396036148	8.989375114
O	1.404322863	6.239305496	9.048853874	O	1.433398008	6.206975937	9.087704659	O	1.278284788	6.144743919	9.204080582
O	18.169275284	1.906079531	6.697469234	O	-0.654279470	1.896128178	6.711250305	O	18.166957855	1.847347021	6.760874271
O	6.715849876	-0.175461993	2.318532228	O	6.737072468	-0.182518750	2.324992418	O	6.015926361	9.209247589	2.313709259
O	6.145794392	1.619054317	9.219106674	O	6.147006512	1.621877313	9.225711823	O	6.146474838	1.619139433	9.203675270
O	17.972429276	6.800117493	2.545430183	O	17.975955963	6.812071323	2.546607018	O	18.092029572	6.840918541	2.358734846
O	1.323984146	8.815741539	6.809443951	O	1.312402487	8.837953568	6.816760540	O	2.020726681	-0.505071402	6.700081825
O	0.604815960	7.722319126	4.542370796	O	0.604031861	7.728477001	4.555879116	O	0.566211581	7.666056156	4.508767605

O	4.027335644	0.749269962	7.887135029	O	4.031988144	0.746250808	7.888798714	O	4.052884579	0.724615812	7.844204426
O	7.630990982	4.446711540	1.257792830	O	7.644697189	4.451211452	1.253907204	O	7.655046940	4.439563751	1.233206272
O	7.618141651	0.958100796	4.559325218	O	7.616742611	0.960550308	4.566933155	O	7.630741596	0.959042609	4.546670914
O	3.949957609	8.002552032	1.266844749	O	3.960889101	8.003795624	1.299000382	O	3.971233845	7.952697754	1.215057135
O	0.412394464	4.063307762	7.845664978	O	0.428753376	4.057851791	7.847480297	O	0.428340852	4.030095100	7.823309422
O	11.026223183	1.715997458	8.145128250	O	11.028745651	1.718807697	8.152885437	O	11.044091225	1.715225935	8.148387909
O	9.360898972	-0.118361488	2.857178211	O	9.378967285	-0.105804212	2.875470161	O	9.350661278	-0.138152361	2.845643520
O	17.455890656	2.087053061	2.160650253	O	17.435096741	2.071316719	2.156544924	O	17.447805405	2.096476793	2.171770096
O	12.374855995	0.228898749	0.059458748	O	12.374840736	0.228451893	0.060040612	O	12.412466049	0.227851763	0.057342853
O	10.974785805	8.209445953	2.181499243	O	10.979504585	8.205480576	2.181756020	O	10.969478607	8.216557503	2.172023296
O	9.443437576	2.850818872	0.068852648	O	9.445884705	2.848083973	0.072582372	O	9.451586723	2.840482235	0.047905721
O	15.693021774	6.850145340	0.779273093	O	15.704594612	6.857272148	0.767846227	O	15.675181389	6.838248730	0.810034394
O	17.559341431	8.677410126	6.190413475	O	17.548196793	8.666954041	6.204757690	O	17.562194824	8.636681557	6.194310665
O	15.941639900	0.411448658	6.858187199	O	15.938150406	0.431801856	6.862532616	O	15.939501762	0.363365531	6.848457813
O	17.625194550	5.838859081	9.051444054	O	17.638351440	5.805521965	9.055191040	O	17.481517792	5.733781815	8.832759857
O	9.514721870	6.460584164	6.839659691	O	9.526032448	6.460041046	6.839109898	O	9.543368340	6.465188026	6.836608410
O	14.468857765	8.413906097	8.958873749	O	14.472334862	8.427134514	8.969371796	O	14.473377228	8.403478622	8.980337143
O	10.726576805	6.198410034	9.197575569	O	10.733800888	6.198064804	9.196885109	O	10.750959396	6.201631069	9.195898056
O	8.721488953	1.886244535	6.779830456	O	8.729336739	1.879153013	6.782584190	O	8.764936447	1.888434410	6.748145580
O	15.644446373	9.064334869	2.249205828	O	15.643486977	9.048814774	2.266807556	O	15.643808365	9.074608803	2.271161318
O	15.487000465	1.630141497	9.214716911	O	15.483202934	1.648086548	9.214509964	O	15.551877022	1.619257092	9.183280945
O	8.821343422	6.630678177	2.460521460	O	8.815583229	6.639554024	2.469620943	O	8.834758759	6.612542629	2.468714237
O	10.712491035	8.849228859	6.785948753	O	10.721726418	8.853996277	6.783050537	O	11.427621841	-0.535873890	6.778100967
O	9.967661858	7.699473381	4.566506863	O	9.984505653	7.697478294	4.567312241	O	9.989575386	7.704086781	4.561293125
O	13.459653854	0.705104947	7.810840130	O	13.460250854	0.714760900	7.818581581	O	13.483819962	0.715881288	7.824341297
O	16.970901489	4.472067833	1.224502444	O	16.970729828	4.471760273	1.263546944	O	16.962467194	4.471221924	1.200428963
O	16.996006012	0.935711443	4.504466057	O	17.002798080	0.941503882	4.513795376	O	17.012950897	0.944360495	4.523605347
O	13.397678375	7.976629734	1.239893079	O	13.402600288	7.976381779	1.239773393	O	13.400905609	7.969891548	1.271152973
O	9.821663857	4.047234058	7.868485928	O	9.818742752	4.046938419	7.869526386	O	9.838899612	4.048985958	7.866086960
O	15.823335648	4.252222538	6.804040909	O	15.926388741	4.468186855	6.659683704	O	15.494462967	4.521686554	6.858179569
Cu	7.049530029	5.221220493	5.580275059	Cu	7.036978245	5.203368187	5.581730366	Cu	7.050464153	5.208781719	5.587510109
H	16.804151535	4.583230495	3.910636902	H	16.708358765	4.464487076	3.760565996	H	16.692638397	4.424362659	4.040039539
H	17.560503006	5.125081539	5.442513466	H	16.992128372	5.004187107	6.012016296	H	16.238607407	5.138779640	7.101232052
H	8.630745888	5.171634197	3.728346109	H	8.609537125	5.171698093	3.722792625	H	8.623712540	5.164091587	3.727591515
H	9.103852272	4.108008385	4.921339035	H	9.089888573	4.097905636	4.901883602	H	9.092434883	4.084958076	4.909114361
H	7.957864285	3.671090841	3.821200371	H	7.938338280	3.670175791	3.805145502	H	7.938032150	3.668230772	3.811486244
H	6.511597157	6.146176815	7.724359035	H	6.518161297	6.124371529	7.731588840	H	6.531744480	6.133857727	7.738275051
H	5.664360046	7.015983105	6.611741066	H	5.655606270	6.991206646	6.629389286	H	5.669158936	6.997664452	6.633256435
H	5.089844704	5.562793255	7.120862007	H	5.092393398	5.535385132	7.143519878	H	5.108528614	5.540690422	7.147967339
H	15.139421463	6.200834751	0.301500797	H	15.162424088	6.223252773	0.257893860	H	15.038071632	6.133983612	0.579489231
N	16.801214218	4.663911819	4.924749851	N	16.665988922	4.616103649	4.779331207	N	16.642160416	4.748623371	5.021446228
N	8.297533035	4.451363087	4.393292427	N	8.280399323	4.445323467	4.382223129	N	8.286981583	4.440881252	4.388131142
N	5.943668365	6.064353466	6.864560604	N	5.940941811	6.040823460	6.878687859	N	5.956626892	6.047870159	6.883669853
N	15.770525932	4.145297050	5.564402580	N	15.679675102	4.125051498	5.412330627	N	15.662405014	4.178724766	5.524281025

ts2				Structure C			ts3				
Si	0.168374002	2.402345181	8.031788826	Si	0.190472782	2.444307327	8.028848648	Si	0.181770802	2.474535227	8.007736206
Si	7.935918331	0.601473391	2.953161955	Si	7.982959270	0.617918968	2.892224073	Si	8.019325256	0.651422381	2.890310287
Si	2.434888363	8.115037918	0.759940684	Si	2.460730791	8.170310974	0.753511548	Si	2.488044500	8.189077377	0.741437852
Si	5.545648098	8.243094444	1.022151589	Si	5.578165531	8.257079124	0.947872043	Si	5.596183300	8.297393799	0.936983347
Si	7.943816662	0.597264707	6.095199108	Si	7.967853069	0.602577865	6.037125111	Si	7.965263844	0.625985384	6.031363487
Si	0.125625014	5.550514698	8.162701607	Si	0.115061879	5.599976540	8.154818535	Si	0.159243643	5.646033764	8.167537689
Si	0.174207687	7.863266945	6.042842865	Si	0.190731883	7.902678013	6.039014339	Si	0.214845002	7.923916817	6.045255184
Si	5.610607624	0.390034080	8.217127800	Si	5.631471634	0.423758328	8.160960197	Si	5.632996082	0.478646278	8.159354210
Si	2.492611885	0.283524096	8.000331879	Si	2.517814636	0.332079649	7.984329700	Si	2.521605492	0.361373365	8.008525848
Si	0.164539695	7.978577614	2.951073885	Si	0.213426813	8.038393021	2.943812847	Si	0.209956586	8.023915291	2.951223612
Si	8.008263588	2.902582407	0.795666575	Si	8.030354500	2.929350853	0.747551560	Si	8.041307449	2.973354340	0.751108885
Si	9.584588051	2.411349297	8.031188011	Si	9.615063667	2.421452522	7.986705780	Si	9.619457245	2.447998524	7.979132175
Si	17.433885574	0.642202377	2.965333462	Si	17.455974579	0.685547829	2.969568491	Si	17.470561981	0.681140661	2.936841249
Si	11.858945847	8.158569336	0.808328629	Si	11.891692162	8.148386002	0.730471373	Si	11.899724007	8.168163300	0.722385883
Si	14.959157944	8.339015961	1.019738674	Si	14.996375084	8.376551628	1.031921506	Si	15.011734009	8.365806580	0.988540769
Si	17.353599548	0.575118601	6.071344376	Si	17.385835648	0.622678101	6.073889256	Si	17.396949768	0.641897559	6.051933765
Si	9.542312622	5.580128193	8.237094879	Si	9.593330383	5.595978737	8.171554565	Si	9.593715668	5.614470482	8.159903526
Si	9.612000465	7.868711948	6.097997189	Si	9.635155678	7.896781921	6.034387589	Si	9.628475189	7.914379597	6.029689312
Si	15.039655685	0.482063770	8.182971954	Si	15.068399429	0.497737527	8.187798500	Si	15.072713852	0.495719314	8.168642998
Si	11.926463127	0.306363404	8.026685715	Si	11.944062233	0.321495295	7.984143734	Si	11.943553925	0.340313375	7.982534409
Si	9.594010353	7.883826733	2.977270126	Si	9.595408440	7.887478352	2.926759005	Si	9.612731934	7.929827690	2.924851656
Si	17.400995255	2.963425159	0.779137671	Si	17.419382095	2.992715836	0.778141499	Si	17.419019699	3.000469923	0.762819707
Al	7.908448219	6.089458466	1.037814140	Al	7.931120872	6.114896297	1.002512813	Al	7.928422451	6.152360916	0.987111092
Al	17.369375229	6.098573208	0.978336990	Al	17.408576965	6.138612270	0.978539467	Al	17.433841705	6.158417702	1.014812469
O	1.609318018	1.645136833	8.100023270	O	1.636194229	1.692463636	8.101346970	O	1.618585825	1.711431980	8.079963684
O	0.093312949	0.035893351	2.926010132	O	0.113836378	0.079471081	2.905730724	O	0.132098898	0.080597505	2.871226311
O	8.096722603	2.019539118	2.176141024	O	8.115650177	2.045330763	2.126913786	O	8.128766060	2.074751616	2.118871927
O	2.286223412	-0.586199641	9.360891342	O	2.340706825	-0.530606866	9.351696968	O	3.036257505	0.264240921	0.028548786
O	1.542349935	8.130819321	2.105209112	O	1.604149580	8.230828285	2.123637199	O	1.571081519	8.149083138	2.071829319
O	0.029130103	2.868087053	0.045800794	O	0.040210381	2.879863739	0.030912928	O	-0.660963416	2.141835213	9.365659714
O	6.385728836	6.898511887	0.920616686	O	6.416929722	6.915673256	0.776365101	O	6.413455009	6.949171543	0.707865655
O	8.173738480	8.644079208	6.253097534	O	8.173095703	8.631718636	6.171492577	O	8.164676666	8.651037216	6.163838387
O	6.528791428	0.310408652	6.856235504	O	6.551740646	0.335633337	6.802139759	O	6.539273739	0.381726146	6.790826321
O	8.102723122	5.738420963	8.930315018	O	8.222144127	5.793229103	8.963757515	O	8.224180222	5.798080921	8.952496529
O	0.102303565	6.405782223	6.765598297	O	0.127969950	6.442780495	6.752165318	O	0.126737118	6.458519459	6.742815018
O	5.039799690	8.359675407	8.989385605	O	5.058025360	8.392974854	8.929006577	O	5.050686836	8.448689461	8.926253319
O	1.300806522	6.152602196	9.129972458	O	1.270853996	6.218945980	9.140833855	O	1.397485018	6.249199867	9.067656517
O	18.144407272	1.822469234	6.763364315	O	-0.652946353	1.878078580	6.740853786	O	18.160652161	1.936902046	6.708699703
O	6.016771793	9.158370018	2.307652712	O	6.090481758	9.137479782	2.242887020	O	6.155224800	9.142333984	2.231523752
O	6.153647900	1.583867788	9.166982651	O	6.184304237	1.609126091	9.114844322	O	6.196172237	1.661760569	9.108738899
O	18.036214828	6.857794285	2.353431702	O	18.126588821	6.896204948	2.325562716	O	18.067474365	6.870973587	2.438671589
O	1.332884550	8.791238785	6.717233181	O	1.345947981	8.832589149	6.715647221	O	1.360124111	8.839441299	6.753946781
O	0.567814887	7.634854317	4.493632317	O	0.591825843	7.690777302	4.488921165	O	0.644979775	7.736139297	4.497372627

O	4.063502312	0.685549200	7.795789242	O	4.088763714	0.727135360	7.742873669	O	4.084233761	0.782413900	7.759366989
O	7.663778305	4.390130043	1.215296388	O	7.681297302	4.418070793	1.155288219	O	7.690364361	4.456354618	1.184416413
O	7.620083809	0.915918648	4.531592369	O	7.659996986	0.933236837	4.470738411	O	7.664896965	0.957419515	4.463540554
O	3.969461441	7.903384686	1.214720249	O	4.006335258	7.920526981	1.168130279	O	4.026179790	7.989297867	1.210855603
O	0.469038010	3.988392830	7.812793255	O	0.483640790	4.034273148	7.838739872	O	0.463664711	4.065790176	7.830379009
O	11.027349472	1.655491829	8.077721596	O	11.064380646	1.685785770	8.059506416	O	11.066200256	1.704577565	8.056975365
O	9.353263855	-0.176641315	2.852028847	O	9.421549797	-0.128693342	2.785837173	O	9.475082397	-0.063125387	2.804123402
O	17.391344070	1.991855264	2.085922480	O	17.413675308	2.039828777	2.100398779	O	17.422962189	2.050382614	2.087840319
O	12.434617043	0.207788542	0.046253357	O	11.709333420	-0.554181933	9.345199585	O	11.728981018	-0.521319628	9.355500221
O	10.969560623	8.184842110	2.155663013	O	10.943705559	8.076004028	2.026831865	O	10.970183372	8.098168373	2.033958435
O	9.456790924	2.777081251	0.018085524	O	8.790438652	2.072515011	9.340681076	O	8.798984528	2.113280773	9.340669632
O	15.733139038	6.902833462	0.588618636	O	15.747470856	6.914118767	0.691499054	O	15.755776405	6.895598412	0.680427253
O	17.557899475	8.606846809	6.183768272	O	17.581897736	8.651265144	6.183617115	O	17.608379364	8.685503960	6.175643444
O	15.929288864	0.301271081	6.832178593	O	15.967567444	0.368592918	6.844529152	O	15.972026825	0.403296649	6.818326950
O	17.499814987	5.657260418	8.829685211	O	17.479473114	5.700349808	8.800971031	O	17.600305557	5.806970596	8.928599358
O	9.533651352	6.406103611	6.812039852	O	9.550034523	6.433681965	6.756799698	O	9.547908783	6.451455116	6.745824814
O	14.445440292	8.488903999	9.043579102	O	14.501693726	8.504281998	9.047675133	O	14.533470154	8.490626335	9.002022743
O	10.744704247	6.189965248	9.181668282	O	10.904408455	6.164607048	9.036579132	O	10.893873215	6.197284698	9.028559685
O	8.733964920	1.894155979	6.714758873	O	8.772161484	1.881499052	6.677892208	O	8.773307800	1.896988630	6.678020954
O	15.659341812	8.968232155	2.324886799	O	15.659797668	9.022278786	2.344393730	O	15.680737495	9.019163132	2.300536871
O	15.564316750	1.709876418	9.084351540	O	15.565986633	1.728884220	9.105701447	O	15.559000015	1.725631237	9.100730896
O	8.834965706	6.574293137	2.449702024	O	8.750947952	6.598697186	2.479812622	O	8.729549408	6.675940514	2.457541466
O	10.801164627	8.755214691	6.772217274	O	10.783926964	8.816518784	6.714639187	O	10.771512032	8.834872246	6.720445633
O	9.995794296	7.650667191	4.544695854	O	10.042820930	7.690560818	4.484611511	O	10.049867630	7.704726696	4.482432365
O	13.481466293	0.714772105	7.783279896	O	13.505128860	0.715110242	7.788664818	O	13.510492325	0.716699302	7.769095898
O	17.027513504	4.443625927	1.218990922	O	17.064287186	4.481468678	1.204391122	O	17.073398590	4.493103504	1.181320548
O	17.013298035	0.934428394	4.515789032	O	17.042835236	0.967581689	4.518643379	O	17.055212021	0.966080904	4.489369392
O	13.412046432	7.960786343	1.280194521	O	13.433817863	7.995767117	1.234431028	O	13.449706078	7.998991013	1.205349445
O	9.856220245	4.009046555	7.869981289	O	9.886066437	4.023061275	7.802782536	O	9.879451752	4.045365334	7.771589279
O	13.279326439	5.947945118	6.777529716	O	13.014503479	5.392724037	7.207323551	O	12.953665733	5.234370232	7.189832687
Cu	7.046068668	5.198792458	5.562437534	Cu	7.038140297	5.206898212	5.588770866	Cu	6.970284939	5.261574268	5.627555847
H	16.370399475	5.781750679	7.051568985	H	16.066749573	5.523016930	7.233423710	H	15.844541550	4.040448189	6.643177032
H	13.082613945	6.900518894	6.649930954	H	12.444426537	5.556655884	8.002082825	H	12.431976318	5.617511749	7.939706802
H	8.617009163	5.119817257	3.703916073	H	8.570302010	5.133856773	3.706386089	H	8.519603729	5.209117413	3.743611336
H	9.055594444	4.021009922	4.879082203	H	9.055851936	4.046994686	4.875054359	H	9.019112587	4.146453857	4.926005840
H	7.892532349	3.643347740	3.777735472	H	7.873687744	3.642796993	3.805826664	H	7.846967220	3.710021019	3.855887175
H	6.556847095	6.116991997	7.718933582	H	6.473894596	6.195099354	7.731469154	H	6.194498062	6.122641563	7.797723770
H	5.721722126	7.023611546	6.626430511	H	5.674988270	7.032716751	6.570734978	H	5.623379230	7.084181786	6.607049942
H	5.113716125	5.579798222	7.122509480	H	5.077589035	5.598738670	7.105160713	H	4.874637127	5.660081863	6.937499046
H	14.804610252	5.970863819	8.953639984	H	14.681674957	5.827237606	9.126919746	H	14.660260201	5.686310768	9.191666603
N	15.477814674	5.839491844	6.506990433	N	15.145230293	5.403745174	6.761434078	N	15.108471870	4.478053093	7.167517662
N	8.259782791	4.402721882	4.360794067	N	8.242325783	4.412308216	4.373589993	N	8.200290680	4.491052628	4.417783260
N	5.978504181	6.060927868	6.862732410	N	5.941951275	6.086089611	6.855756760	N	5.792864323	6.103239059	6.849458694
N	14.599524498	5.913491249	7.353131771	N	14.311171532	5.512100220	7.661753654	N	14.300909042	5.032354832	7.826302052

Structure D				ts4			Structure E				
Si	0.217433929	2.497099161	7.961150646	Si	0.210461318	2.488007069	8.031271935	Si	0.187783301	2.520504951	8.012378693
Si	8.051229477	0.666672349	2.875082254	Si	8.022221565	0.650236130	2.933099985	Si	7.997866631	0.669117689	2.960429430
Si	2.519199371	8.185693741	0.709915698	Si	2.501028061	8.207905769	0.758399606	Si	2.480383873	8.215117455	0.773313046
Si	5.618176460	8.304167747	0.918034434	Si	5.606214046	8.298088074	0.969378233	Si	5.586489201	8.324158669	1.006800175
Si	7.985315800	0.637491047	6.010896206	Si	7.987269878	0.614884257	6.071797848	Si	7.973647118	0.643197656	6.103453636
Si	0.218814015	5.659934044	8.142557144	Si	0.161151886	5.665972710	8.176906586	Si	0.143721819	5.669899464	8.191959381
Si	0.235352069	7.942980289	6.024589062	Si	0.227701604	7.942997932	6.054837227	Si	0.218969643	7.962962627	6.066633701
Si	5.648386478	0.495740116	8.148024559	Si	5.647205353	0.482682347	8.193521500	Si	5.629246712	0.513934016	8.221574783
Si	2.537827730	0.379845440	8.002240181	Si	2.542454243	0.381890774	8.016627312	Si	2.522598982	0.395129144	8.026855469
Si	0.233034208	8.016542435	2.939099550	Si	0.229972482	8.029778481	2.957910299	Si	0.224261001	8.020706177	2.990155220
Si	8.056916237	2.992385387	0.735467613	Si	8.048038483	2.976878881	0.791721523	Si	8.031228065	2.998372555	0.817418694
Si	9.647084236	2.464456081	7.960407257	Si	9.649979591	2.440815687	8.030846596	Si	9.632745743	2.462357521	8.060940742
Si	17.520627975	0.717715979	2.901440144	Si	17.484487534	0.731463432	2.972016811	Si	17.472257614	0.723709166	2.985749245
Si	11.936301231	8.171083450	0.698049009	Si	11.888889313	8.150632858	0.776855528	Si	11.874523163	8.187870026	0.799998343
Si	15.046541214	8.386273384	0.938651145	Si	15.004543304	8.389693260	1.030168056	Si	14.985887527	8.390729904	1.040957928
Si	17.426395416	0.656921387	6.011607647	Si	17.413846970	0.648100972	6.082946777	Si	17.389009476	0.674209118	6.078578472
Si	9.619057655	5.632106781	8.137067795	Si	9.625789642	5.595931053	8.207746506	Si	9.587006569	5.627211571	8.232506752
Si	9.652782440	7.940610886	6.005903721	Si	9.638533592	7.904744148	6.077290058	Si	9.620638847	7.928853512	6.104977131
Si	15.101652145	0.492400765	8.129987717	Si	15.108866692	0.437439919	8.208290100	Si	15.089777946	0.453642964	8.213000298
Si	11.972494125	0.364739656	7.967883587	Si	11.949782372	0.319837570	8.045054436	Si	11.944403648	0.348603308	8.060221672
Si	9.636370659	7.946766853	2.908709526	Si	9.616367340	7.931073189	2.969854593	Si	9.612455368	7.952216148	2.995395184
Si	17.456752777	3.016247034	0.729477942	Si	17.453096390	2.997943163	0.788541198	Si	17.439586639	3.005118370	0.794417262
Al	7.947388649	6.171770096	0.971789479	Al	7.940319061	6.148182869	1.003327370	Al	7.930839539	6.171724796	1.039499521
Al	17.487670898	6.163243294	1.020079970	Al	17.465974808	6.158441067	1.001563549	Al	17.446636200	6.143467426	1.037316918
O	1.662311196	1.744636297	8.075259209	O	1.655890703	1.740697265	8.119358063	O	1.613840818	1.741348743	8.110321999
O	0.164092690	0.076293930	2.849226713	O	0.108932644	0.060492590	2.873875618	O	0.093459040	0.044908062	2.962733746
O	8.141913414	2.089300632	2.099806309	O	8.120750427	2.068557262	2.153395414	O	8.096725464	2.087449074	2.178856134
O	3.057818651	0.272504777	0.019142192	O	3.058700085	0.271978825	0.027460519	O	3.032214403	0.275333822	0.032198008
O	1.569992185	8.109115601	2.016140938	O	1.591596723	8.209356308	2.093218565	O	1.575693607	8.223031998	2.113397121
O	-0.640459836	2.169765234	9.309514046	O	0.058470901	2.902114868	0.030716604	O	0.035903517	2.976997614	0.018035902
O	6.428472042	6.952643871	0.645556927	O	6.426528931	6.953868389	0.718462408	O	6.421176434	6.985498905	0.787785232
O	8.179662704	8.656859398	6.124728680	O	8.166261673	8.625847816	6.192867279	O	8.149193764	8.651831627	6.227669716
O	6.566732407	0.407308221	6.784524918	O	6.566802502	0.365113258	6.837879658	O	6.548654079	0.393680513	6.862158298
O	8.279413223	5.819869041	8.966114998	O	8.227469444	5.754572868	8.958311081	O	8.180110931	5.785096169	8.968873024
O	0.143388510	6.484231472	6.728579521	O	0.164594680	6.482435226	6.760214806	O	0.122291386	6.521775246	6.800759792
O	5.064178467	8.461432457	8.911114693	O	5.050018311	8.454045296	8.962829590	O	5.033727169	8.494092941	9.007944107
O	1.503027201	6.259958744	8.994525909	O	1.385111332	6.266077995	9.100552559	O	1.361447692	6.266260147	9.124720573
O	-0.607139468	1.915063500	6.664950371	O	-0.627986550	1.910263777	6.743782043	O	-0.673862576	1.949610472	6.736963272
O	6.211942673	9.128679276	2.210578680	O	6.161269188	9.135019302	2.272297144	O	6.116609573	9.168627739	2.316022635
O	6.210756302	1.676499844	9.099254608	O	6.211027622	1.665428162	9.138326645	O	6.187611580	1.709841847	9.157431602
O	18.067548752	6.861480713	2.474776268	O	18.145391464	6.845503807	2.414340734	O	18.131246567	6.847026348	2.435935974
O	2.061698437	-0.532718062	6.746969700	O	2.059159994	-0.517266750	6.751269341	O	2.057045460	-0.500945807	6.753338337
O	0.699995995	7.763405800	4.481958866	O	0.652248740	7.746792793	4.505742550	O	0.662660539	7.724503040	4.529438496

O	4.103806496	0.798430800	7.749285221	O	4.107445240	0.796725690	7.774224281	O	4.086333275	0.823124230	7.798398972
O	7.706450462	4.476044178	1.166632175	O	7.688459873	4.455615997	1.232235670	O	7.689071655	4.478253365	1.267583609
O	7.675509930	0.975265384	4.445273876	O	7.670335293	0.962103426	4.508414745	O	7.670587540	0.985030293	4.538949966
O	4.052798271	8.003011703	1.218028903	O	4.035157204	7.985741138	1.230423808	O	4.014177799	7.991253853	1.239727974
O	0.510844529	4.085508347	7.776773453	O	0.469856679	4.082996845	7.864680290	O	0.477437794	4.106831074	7.816635609
O	11.101695061	1.734806418	8.067724228	O	11.103733063	1.705191612	8.129355431	O	11.087015152	1.726063967	8.146411896
O	9.521117210	-0.028233618	2.808215857	O	9.482461929	-0.057405114	2.850252151	O	9.446888924	-0.058155999	2.865357637
O	17.532806396	2.102827072	2.078868866	O	17.501451492	2.142305136	2.178403139	O	17.543769836	2.099025965	2.143607616
O	11.757001877	-0.521164894	9.327880859	O	12.380915642	0.198524401	0.040604208	O	12.409552574	0.242268682	0.069898061
O	10.989281654	8.082668304	1.998818398	O	10.997378349	8.104761124	2.118693590	O	10.989258766	8.149844170	2.144478321
O	8.812366486	2.145339966	9.315839767	O	9.504030228	2.874456167	0.025332425	O	9.483895302	2.878165722	0.047415093
O	15.804312706	6.911600590	0.687088907	O	15.715028763	6.850358009	0.915311575	O	15.704328537	6.851776123	0.912142634
O	17.618921280	8.687235832	6.131564140	O	17.610742569	8.680275917	6.183958054	O	17.610860825	8.723927498	6.156254292
O	15.997484207	0.426257730	6.779075623	O	15.987320900	0.401419342	6.845972538	O	15.975998878	0.397943795	6.855058670
O	-1.130292416	5.841711998	8.983869553	O	17.584777832	5.843256474	8.912328720	O	17.569679260	5.789514542	8.941937447
O	9.574169159	6.479675293	6.730218410	O	9.592948914	6.445432186	6.797443867	O	9.557532310	6.467160225	6.818571568
O	14.516696930	8.447351456	8.906348228	O	14.604199409	8.395678520	8.992025375	O	14.563155174	8.416637421	9.008847237
O	10.949302673	6.196003914	8.988832474	O	10.878519058	6.173306942	9.121474266	O	10.832086563	6.224644184	9.139014244
O	8.819372177	1.893424153	6.656772137	O	8.818798065	1.867000103	6.726785660	O	8.801697731	1.900019169	6.753436565
O	15.718302727	9.100180626	2.210693359	O	15.649207115	9.154531479	2.291731834	O	15.651859283	9.132059097	2.304519176
O	15.590007782	1.668022275	9.119731903	O	15.596344948	1.634131789	9.184406281	O	15.590152740	1.648554325	9.182342529
O	8.721412659	6.706598282	2.459572792	O	8.733710289	6.686749458	2.477824450	O	8.769434929	6.684899807	2.495882988
O	11.472939491	-0.514645338	6.695171356	O	10.767202377	8.854678154	6.757842541	O	11.451826096	-0.533547401	6.787964344
O	10.092956543	7.716342449	4.462944508	O	10.044342995	7.687459946	4.527758121	O	10.027655602	7.716838837	4.556620121
O	13.534292221	0.750925958	7.742216110	O	13.531807899	0.657436609	7.867838860	O	13.521096230	0.699471712	7.860853672
O	17.074567795	4.504882813	1.134461761	O	17.047357559	4.497175694	1.171607375	O	16.997556686	4.486200809	1.233277917
O	17.071905136	0.973660946	4.448791027	O	17.072622299	0.991589308	4.524864674	O	17.021186829	1.038277149	4.524634838
O	13.485023499	8.006024361	1.181943655	O	13.449866295	8.028665543	1.260080099	O	13.435004234	8.019673347	1.269998074
O	9.906068802	4.065062046	7.731846333	O	9.931180000	4.030937672	7.799894333	O	9.906424522	4.057570457	7.858517170
O	12.926121712	5.026712894	7.378968239	O	15.097039223	4.685214996	3.449674845	O	15.387317657	3.982143879	3.688597918
Cu	6.830528259	5.313475132	5.690702915	Cu	6.902884483	5.328591347	5.682960510	Cu	6.959117413	5.335102558	5.656283855
H	14.615408897	4.000460148	6.325499058	H	13.764179230	3.984696865	3.459408998	H	15.792695999	3.315536499	4.269782543
H	12.370560646	5.467656136	8.079738617	H	15.963011742	4.294444084	3.186268806	H	16.068632126	4.146505356	3.005607128
H	8.401000023	5.298352242	3.799010277	H	8.455587387	5.252382278	3.792441607	H	8.520109177	5.243476868	3.782545090
H	8.914601326	4.253890514	4.986768723	H	8.958975792	4.215375423	4.994051933	H	9.003913879	4.192556858	4.981138706
H	7.750853062	3.790672779	3.920975447	H	7.786687851	3.754894495	3.934319735	H	7.833869934	3.752683163	3.909866571
H	5.801379681	5.998413086	7.871363163	H	5.933494568	6.053617954	7.855593681	H	6.121509552	6.135415077	7.825867176
H	5.528392792	7.118651390	6.720337391	H	5.699078560	7.199049473	6.719179630	H	5.710181713	7.206131935	6.662159920
H	4.621588707	5.751051426	6.752371311	H	4.718770981	5.881954193	6.758713245	H	4.821143150	5.837865829	6.860110760
H	14.694447517	5.652044296	9.253850937	H	15.065307617	6.138150692	1.158015370	H	15.033919334	6.122939110	0.949446678
N	15.039764404	4.342842102	7.214553356	N	13.090501785	4.282232285	2.523748398	N	12.847098351	4.094433784	1.437478304
N	8.088483810	4.581725597	4.478813648	N	8.137540817	4.547341824	4.481581688	N	8.190233231	4.537186623	4.464936256
N	5.574830532	6.105615616	6.869933605	N	5.691126347	6.183743000	6.862196445	N	5.777231693	6.202198029	6.857490063
N	14.210970879	4.928646564	7.905856133	N	13.937557220	4.936612129	2.049806833	N	13.667315483	4.802893162	1.190759301

Table S9. Cartesian coordinates of RC, TS, IM, and PC for NH₂NO decomposition with the assistance of Brønsted acid sites.

Structure A				ts1			Structure B				
Si	0.160183311	2.459873438	8.102834702	Si	0.152831256	2.529242039	8.082130432	Si	0.170706570	2.516541481	8.059185982
Si	7.958600044	0.656858087	2.995927095	Si	7.925916672	0.718780220	2.980329752	Si	7.942526817	0.713177562	2.974157810
Si	2.437233686	8.180811882	0.834352136	Si	2.390634537	8.346739769	0.889121056	Si	2.423170567	8.311454773	0.853213847
Si	5.557077408	8.298173904	1.057399750	Si	5.523611069	8.365924835	1.038394809	Si	5.550347328	8.363961220	1.027109981
Si	7.942067146	0.622989178	6.144258499	Si	7.936041832	0.700304866	6.129358292	Si	7.954247475	0.701770306	6.122926235
Si	0.111371100	5.631557465	8.245349884	Si	0.111141145	5.724718571	8.249239922	Si	0.126526952	5.706346035	8.217498779
Si	0.182209790	7.942637444	6.121929646	Si	0.164221644	8.035890579	6.130816460	Si	0.189184457	8.020388603	6.112422943
Si	5.617974281	0.429268718	8.274503708	Si	5.617934227	0.489958346	8.256987572	Si	5.636477947	0.489980042	8.248501778
Si	2.489506721	0.363001108	8.094238281	Si	2.502044678	0.454986155	8.052180290	Si	2.518544197	0.439209223	8.039777756
Si	0.174843445	8.040697098	3.031516790	Si	0.179593012	8.018647194	3.007619619	Si	0.216610879	8.015606880	2.988704205
Si	8.015264511	2.955967903	0.861509323	Si	8.009037018	3.020003319	0.850732148	Si	8.027328491	3.018377781	0.847831249
Si	9.591788292	2.452687263	8.086732864	Si	9.583762169	2.530046225	8.067675591	Si	9.602391243	2.532946587	8.063075066
Si	17.415323257	0.688131630	3.026631594	Si	17.322301865	0.770170391	3.017211676	Si	17.372596741	0.750061393	2.990566015
Si	11.851039886	8.182811737	0.845091999	Si	11.829589844	8.250696182	0.838794291	Si	11.853863716	8.259818077	0.839123547
Si	14.971879005	8.367745399	1.077989101	Si	14.940285683	8.419998169	1.117092490	Si	14.970600128	8.386533737	1.070024610
Si	17.351556778	0.636901736	6.137812138	Si	17.334308624	0.732314408	6.157375336	Si	17.355506897	0.708647013	6.133346081
Si	9.543966293	5.618071556	8.278383255	Si	9.506243706	5.695071220	8.264662743	Si	9.517935753	5.697594643	8.260555267
Si	9.605732918	7.922245979	6.141662121	Si	9.604790688	8.000375748	6.138319016	Si	9.617040634	7.998691082	6.134507179
Si	15.041143417	0.513297319	8.259846687	Si	15.039841652	0.470408082	8.301383972	Si	15.054573059	0.480532646	8.266901970
Si	11.910799980	0.347422004	8.082747459	Si	11.909809113	0.419189095	8.090253830	Si	11.929062843	0.423908055	8.086389542
Si	9.604084969	7.923064232	3.021165609	Si	9.576679230	7.976875305	3.012215376	Si	9.601968765	7.978724003	3.010390759
Si	17.392757416	3.003703594	0.840447366	Si	17.461214066	2.997460604	0.886465609	Si	17.479934692	2.993346453	0.863775671
Al	7.911925316	6.139078617	1.081330419	Al	7.879733562	6.203012943	1.082101941	Al	7.911091805	6.195873260	1.081671953
Al	17.370822906	6.164399147	1.082214594	Al	17.266986847	6.181432247	1.224665880	Al	17.317718506	6.180175781	1.160421848
O	1.615281463	1.731515408	8.195265770	O	1.624311686	1.830570221	8.082026482	O	1.642183542	1.812767982	8.073183060
O	0.076118395	0.082025081	2.983098269	O	-0.196559995	-0.153923661	2.884144068	O	-0.110288978	-0.115880735	2.854564190
O	8.129929543	2.093839169	2.253792524	O	8.131532669	2.159136057	2.245702982	O	8.150661469	2.149475336	2.235371828
O	2.944242001	0.223386854	0.075277634	O	2.940604687	0.348480225	0.055435099	O	2.965362787	0.324955612	0.038837504
O	1.546536446	8.201780319	2.181642056	O	1.557429671	8.491935730	2.265718222	O	1.605896354	8.430149078	2.239266634
O	0.012926400	2.877164841	0.097045608	O	0.054861877	2.892637491	0.081292719	O	0.074089028	2.882450581	0.061986387
O	6.389746666	6.950065136	0.971225858	O	6.351252079	7.012831211	0.970757425	O	6.399525166	7.025336266	0.962795377
O	8.135327339	8.645092964	6.286737442	O	8.148321152	8.743767738	6.285681248	O	8.161844254	8.741309166	6.273969173
O	6.513010025	0.383962214	6.899889469	O	6.512830734	0.457898617	6.890021801	O	6.531635284	0.467095435	6.880685806
O	8.101469040	5.779178143	8.968291283	O	8.059341431	5.821664810	8.956583977	O	8.066909790	5.799500942	8.939388275
O	0.094965041	6.484816074	6.845701218	O	0.076435328	6.570071697	6.872695923	O	0.109019995	6.552160740	6.838047981
O	5.042672157	8.373373032	8.998358727	O	5.008143902	8.426735878	8.971812248	O	5.034313679	8.429029465	8.963482857
O	1.300371289	6.208006859	9.211437225	O	1.110353470	6.351747513	9.347153664	O	1.157383919	6.327579975	9.297929764
O	-0.669529676	1.871363401	6.814227581	O	18.130104065	2.020589113	6.789862156	O	18.147150040	1.992617011	6.771275043
O	6.724857330	-0.150779352	2.316544056	O	6.680765629	-0.068101972	2.290723801	O	6.694536209	-0.069318727	2.286030531

O	6.165316582	1.591126680	9.258309364	O	6.160854340	1.636053085	9.259911537	O	6.183466434	1.640442371	9.247837067
O	18.065008163	6.885778904	2.467624664	O	-0.367778122	6.673655510	2.337722063	O	-0.389092416	6.687825680	2.340203524
O	2.005053759	-0.506918073	6.803250790	O	2.049700260	-0.472630024	6.789123058	O	2.069776773	-0.479733407	6.770761013
O	0.592061281	7.718061447	4.576841831	O	0.526841760	7.775649071	4.585071564	O	0.558497667	7.780611992	4.565650463
O	4.062708378	0.737552524	7.887363911	O	4.071344376	0.846398711	7.867222309	O	4.088681221	0.837574899	7.863572121
O	7.649961948	4.444038868	1.257529616	O	7.610692501	4.505495548	1.229176044	O	7.633139133	4.499897480	1.248567462
O	7.640289783	0.951270401	4.577136993	O	7.608339787	1.009842396	4.562434673	O	7.639029503	1.017093897	4.555965900
O	3.976541519	7.973978519	1.272240758	O	3.934118509	8.040840149	1.239839673	O	3.968547583	8.015020370	1.211448193
O	0.403408527	4.059659004	7.895993233	O	0.382669687	4.155201912	7.977745533	O	0.406407595	4.136812687	7.930706024
O	11.039404869	1.713931203	8.176548958	O	11.038040161	1.796603680	8.138045311	O	11.062552452	1.808134913	8.130410194
O	9.365972519	-0.137152404	2.878583670	O	9.313011169	-0.102374800	2.857993364	O	9.330018044	-0.107632868	2.854456902
O	17.374872208	2.043215513	2.156571627	O	17.625719070	2.185626268	2.286898613	O	17.621025085	2.174612761	2.263912678
O	12.372527122	0.218797714	0.076039262	O	12.338192940	0.293422878	0.074908838	O	12.375961304	0.309457600	0.082365304
O	10.984843254	8.215826988	2.207276344	O	10.942225456	8.280352592	2.188450098	O	10.970695496	8.291804314	2.193386316
O	9.452117920	2.843678951	0.071682528	O	9.447685242	2.918214798	0.058528159	O	9.468711853	2.928158522	0.055006392
O	15.722858429	6.905910015	0.744748652	O	15.848555565	7.120409966	1.176574230	O	15.852082253	7.063097954	1.038543940
O	17.536109924	8.642738342	6.236169338	O	17.572763443	8.788318634	6.336035252	O	17.592164993	8.765688896	6.317298412
O	15.932994843	0.379665613	6.902739048	O	15.926754951	0.479952931	6.936434269	O	15.936981201	0.445792437	6.896914005
O	17.490116119	5.802765846	8.929548264	O	17.365081787	5.864014149	8.881206512	O	17.411680222	5.852954865	8.855212212
O	9.552709579	6.466539383	6.869081497	O	9.512966156	6.539171696	6.852797985	O	9.532026291	6.536381721	6.847465038
O	14.523860931	8.518379211	9.109425545	O	14.458896637	8.375736237	8.980686188	O	14.464992523	8.379727364	8.946659088
O	10.746548653	6.193825722	9.241403580	O	10.700839996	6.282007217	9.217013359	O	10.697104454	6.293128490	9.226899147
O	8.757870674	1.892138243	6.781162739	O	8.739679337	1.985238314	6.759288788	O	8.757102966	1.986570954	6.757209301
O	15.635057449	9.012673378	2.404854059	O	16.026222229	0.088052735	2.298291206	O	16.115585327	0.004799500	2.266485929
O	15.547681808	1.761307240	9.153789520	O	15.599130630	1.585950375	9.325709343	O	15.622424126	1.576990128	9.299669266
O	8.845544815	6.614457607	2.490176916	O	8.822992325	6.657905102	2.489894867	O	8.855936050	6.656811714	2.486294746
O	11.446196556	-0.528995097	6.793340683	O	11.460979462	-0.469827950	6.799190044	O	11.461856842	-0.468272001	6.806375027
O	9.990576744	7.693392754	4.590002537	O	9.970967293	7.767920017	4.581995010	O	9.995138168	7.764296055	4.581007957
O	13.479640961	0.725840151	7.879725456	O	13.487632751	0.818169653	7.935537338	O	13.500107765	0.820943534	7.908930302
O	17.074718475	4.495594501	1.280555725	O	17.046178818	4.502439976	1.160495877	O	17.077230453	4.498150349	1.147186995
O	17.009822845	0.978680730	4.581532955	O	17.008358002	1.026174545	4.597716331	O	17.031415939	0.984775245	4.569762707
O	13.413461685	8.016431808	1.288697600	O	13.371683121	8.045029640	1.273541331	O	13.396807671	8.039238930	1.270365119
O	9.842775345	4.050228119	7.882953167	O	9.833292007	4.130016804	7.875001431	O	9.870418549	4.133402824	7.867260933
O	13.967533112	5.369893551	8.001434326	O	14.813053131	6.630053520	6.588755131	O	15.407213211	6.306245327	7.306835651
Cu	7.103865147	5.177635193	5.595642567	Cu	7.124876976	4.960496902	5.625604630	Cu	7.089223385	4.896021843	5.639706135
H	15.897221565	6.653743267	5.982426643	H	14.156823158	3.860179901	7.728405476	H	12.868422508	4.570551395	7.550298691
H	16.254821777	6.201496124	7.680752277	H	16.670726776	5.975039482	8.197978020	H	16.664846420	6.028316498	8.166253090
H	8.676738739	5.162128448	3.738530397	H	8.669833183	5.230818272	3.735329866	H	8.650325775	5.242339134	3.757562399
H	9.175695419	4.109137058	4.931268692	H	9.297744751	4.205423832	4.885456085	H	9.277386665	4.203422546	4.894243717
H	8.035775185	3.645745754	3.834589481	H	8.196023941	3.649809837	3.789757252	H	8.191461563	3.657071590	3.778836489
H	6.583521366	6.092728615	7.742734909	H	6.547413826	5.826943398	7.771841526	H	6.475105286	5.741663933	7.787374496
H	5.688462734	6.940856934	6.647857189	H	5.345957756	6.327809811	6.745625019	H	5.230315685	6.143696785	6.769610882
H	5.164037228	5.472119331	7.167458057	H	5.323001862	4.799356461	7.352931499	H	5.325593948	4.623212814	7.389177322
H	14.609338760	5.737421036	9.186134338	H	14.677618027	6.997031212	7.510556221	H	14.888231277	7.056614399	7.732011795

N	15.590676308	6.264759541	6.871031761	N	14.389701843	4.865049362	7.789649010	N	13.413006783	5.451230049	7.577827454
N	8.361199379	4.434011459	4.404187679	N	8.443061829	4.451881886	4.380259514	N	8.424150467	4.450773716	4.386880875
N	5.998093605	5.997264862	6.894500256	N	5.938416481	5.530269623	6.986841679	N	5.882984161	5.394744873	7.012276649
N	14.379214287	5.817793369	6.886761189	N	14.512404442	5.276017666	6.623797417	N	14.569083214	5.149558544	7.285079002
ts2				Structure C				Structure D			
Si	0.198152065	2.544766188	8.063773155	Si	0.206987262	2.563946962	8.064236641	Si	0.277174115	2.621788979	7.955389977
Si	7.981889248	0.730561912	2.964904070	Si	8.020603180	0.734459579	2.958995581	Si	8.127430916	0.813555717	2.881073475
Si	2.460330963	8.279524803	0.826373637	Si	2.507586002	8.268680573	0.803070843	Si	2.589646578	8.335442543	0.697221816
Si	5.585120678	8.378352165	1.011365771	Si	5.632154942	8.378590584	0.996671140	Si	5.709174156	8.461961746	0.916021168
Si	7.974022865	0.720225692	6.103300571	Si	7.986511230	0.724952161	6.095559597	Si	8.068949699	0.780252874	6.011088848
Si	0.132626772	5.693756580	8.209666252	Si	0.162741899	5.712175369	8.205272675	Si	0.265741289	5.791659355	8.128959656
Si	0.211816996	8.011909485	6.093989849	Si	0.231747001	8.029921532	6.095313549	Si	0.328359276	8.084248543	6.002123356
Si	5.643553257	0.544975340	8.226464272	Si	5.659498215	0.584768653	8.220151901	Si	5.737448215	0.653481185	8.145628929
Si	2.528601885	0.434188485	8.034015656	Si	2.541075706	0.446031809	8.053334236	Si	2.620009184	0.518920541	7.960531235
Si	0.221528530	8.080747604	2.976316929	Si	0.248873278	8.141043663	2.993441343	Si	0.314985573	8.175361633	2.908334970
Si	8.031527519	3.055151224	0.827583611	Si	8.035725594	3.084537029	0.816745341	Si	8.124950409	3.150070906	0.739597917
Si	9.629334450	2.550506592	8.053750992	Si	9.636920929	2.561296940	8.044329643	Si	9.724646568	2.615150928	7.970620632
Si	17.428703308	0.779791296	2.998237371	Si	17.497880936	0.786496639	2.995326281	Si	17.563993454	0.830649078	2.896117687
Si	11.897054672	8.265922546	0.824647367	Si	11.920153618	8.269283295	0.812833190	Si	11.997967720	8.320791245	0.723235965
Si	14.996592522	8.421982765	1.061541796	Si	15.010615349	8.483884811	1.050176501	Si	15.109002113	8.493603706	0.951693177
Si	17.391819000	0.722160280	6.124728680	Si	17.409980774	0.741761088	6.111527920	Si	17.493232727	0.784944415	6.008142948
Si	9.583531380	5.707601547	8.251289368	Si	9.642801285	5.707667828	8.238979340	Si	9.704817772	5.782746792	8.157345772
Si	9.626136780	8.008649826	6.121425629	Si	9.642230988	8.005978584	6.116526127	Si	9.692986488	8.068239212	6.025008678
Si	15.068855286	0.556181848	8.239917755	Si	15.079991341	0.609006822	8.216075897	Si	15.169500351	0.625086129	8.129958153
Si	11.957409859	0.439229012	8.072654724	Si	11.958528519	0.434745669	8.075094223	Si	12.035569191	0.488919318	8.001450539
Si	9.614832878	8.009832382	3.011116505	Si	9.628935814	8.040942192	3.009233713	Si	9.706260681	8.098409653	2.932572365
Si	17.448534012	3.075883389	0.838246524	Si	17.437387466	3.101461887	0.822572887	Si	17.512926102	3.142270565	0.713017642
Al	7.939420700	6.221716404	1.082437277	Al	7.967360497	6.245951176	1.068492293	Al	8.036385536	6.332859993	0.992290676
Al	17.341861725	6.241801739	1.020661712	Al	17.442842484	6.235403538	1.046674728	Al	17.531299591	6.305142879	0.973022342
O	1.644452810	1.793112993	8.128831863	O	1.641700745	1.796336889	8.157923698	O	1.731418252	1.879180431	8.044693947
O	0.032419190	0.062144399	2.901096821	O	0.161650419	0.188983351	2.928203344	O	0.224281862	0.224114820	2.843884706
O	8.134234428	2.151713371	2.189610481	O	8.094174385	2.143126726	2.152949810	O	8.203627586	2.224133253	2.082095146
O	3.024389029	0.305846512	0.028852491	O	3.039571285	0.315528512	0.047508717	O	2.427641153	-0.346548438	9.325774193
O	1.630814314	8.380265236	2.207575321	O	1.638786197	8.298220634	2.165166140	O	1.679253340	8.314958572	2.030394554
O	0.057017628	2.976313353	0.063399374	O	0.053260799	3.014327049	0.064078748	O	-0.570690393	2.281581879	9.306988716
O	6.430824280	7.037532330	0.855677009	O	6.443456650	7.026919842	0.747212112	O	6.495364666	7.090046406	0.677100122
O	8.166070938	8.744517326	6.239154816	O	8.188160896	8.756896973	6.229977608	O	8.216634750	8.777137756	6.121576786
O	6.551644325	0.514967859	6.862687111	O	6.560193062	0.513913512	6.855597496	O	6.651388168	0.617457926	6.789097309
O	8.172031403	5.793672085	8.987295151	O	8.263331413	5.809751987	9.028668404	O	8.337409019	5.921410561	8.957350731
O	0.168217659	6.556550980	6.824943066	O	0.155219018	6.573261261	6.815864086	O	0.260495394	6.626996517	6.718108177
O	5.070632458	8.517048836	8.993576050	O	5.102545738	8.588596344	9.031861305	O	5.192255974	8.643621445	8.931097984
O	1.226335883	6.308060169	9.257302284	O	1.332471967	6.310194969	9.186502457	O	1.510029554	6.371003628	9.046285629
O	-0.657840014	1.996582866	6.775482655	O	-0.641401410	2.009303570	6.774807453	O	-0.561688244	2.059975863	6.659774303
O	6.765296459	-0.123053737	2.309694529	O	6.170053959	9.183423996	2.326502800	O	6.969223976	-0.116886973	2.225619316

O	6.194505692	1.741864443	9.178161621	O	6.187078953	1.828647494	9.131832123	O	6.256065845	1.887424707	9.080600739
O	-0.565521121	6.860606194	2.320236444	O	-0.695264995	6.997481346	2.396595716	O	-0.648946226	7.012099266	2.385943413
O	2.078881741	-0.458419383	6.749409676	O	2.088189840	-0.449908257	6.773933411	O	2.174724579	-0.384862304	6.686929703
O	0.571461916	7.767410755	4.540888786	O	0.629277945	7.809546471	4.544193745	O	0.749858081	7.887719154	4.453462601
O	4.096185684	0.866659880	7.836305141	O	4.102464676	0.881919384	7.834728718	O	4.187743664	0.954303145	7.746555805
O	7.652418613	4.528299332	1.269838572	O	7.669871807	4.553580284	1.286098480	O	7.773530960	4.633193493	1.169357061
O	7.665175438	1.061398864	4.539659500	O	7.677464008	1.067005396	4.529272079	O	7.774378777	1.152090192	4.449788094
O	4.014477730	8.014122963	1.208488464	O	4.056741714	8.038015366	1.213000894	O	4.133981705	8.158354759	1.160708785
O	0.514678299	4.136515617	7.886485100	O	0.525547981	4.150135517	7.861542702	O	0.563615739	4.214033604	7.773339272
O	11.104672432	1.840016007	8.135881424	O	11.088819504	1.812517405	8.131901741	O	11.228792191	1.930651188	8.092838287
O	9.415184975	-0.022549748	2.874572039	O	9.489605904	0.050429478	2.880309343	O	9.598818779	0.128686219	2.826095819
O	17.517621994	2.177744389	2.193710089	O	17.450218201	2.152516127	2.143907785	O	17.536130905	2.196710348	2.039397717
O	12.427440643	0.319929510	0.069759794	O	12.464581490	0.341226339	0.094070360	O	12.500491142	0.398320317	0.014895709
O	10.969965935	8.250259399	2.146303415	O	10.991454124	8.218334198	2.130703926	O	11.053151131	8.239945412	2.027282000
O	9.482969284	2.975650549	0.042011846	O	9.487867355	2.999027252	0.039129350	O	8.884020805	2.285380602	9.318045616
O	15.800354004	7.062081814	0.763034463	O	15.792350769	7.035030842	0.692980766	O	15.872784615	7.048357964	0.636104107
O	17.608251572	8.763822556	6.276056767	O	17.624706268	8.781875610	6.241664410	O	-1.127416492	8.831627846	6.137289524
O	15.965378761	0.476438522	6.885869503	O	15.983283997	0.490489244	6.870559692	O	16.075738907	0.525528610	6.784882545
O	17.456888199	5.771722794	8.796620369	O	17.535531998	5.797520161	8.873482704	O	-1.142319202	5.953440666	8.879157066
O	9.550390244	6.542901039	6.833237648	O	9.555691719	6.540382385	6.820651531	O	9.644050598	6.598570347	6.726428032
O	14.422038078	8.527623177	9.021472931	O	14.484483719	8.604942322	9.056165695	O	14.594184875	8.616393089	8.954030037
O	10.809735298	6.307007790	9.164855003	O	10.888610840	6.330706596	9.122040749	O	10.970552444	6.388502598	9.018733978
O	8.806971550	1.990845919	6.742437363	O	8.802325249	1.998421192	6.740755558	O	8.946763039	2.011582851	6.662444592
O	16.246665955	-0.144622743	2.342516899	O	15.722284317	9.121493340	2.347381830	O	15.781626701	9.174889565	2.249779701
O	15.596803665	1.736913443	9.203800201	O	15.595270157	1.817967296	9.153392792	O	15.645940781	1.851318359	9.066160202
O	8.790450096	6.718514919	2.531288862	O	8.725851059	6.797902584	2.548117876	O	8.773675919	6.871232986	2.488553286
O	11.455842018	-0.447910547	6.805872917	O	11.477535248	-0.472977519	6.822156906	O	11.471529007	-0.361713290	6.748876572
O	10.041555405	7.788012981	4.574130535	O	10.065354347	7.807471752	4.567863941	O	10.160307884	7.875486374	4.488481998
O	13.507941246	0.883166611	7.842622757	O	13.513587952	0.879975319	7.829192162	O	13.595071793	0.855892003	7.738145828
O	17.045267105	4.563046455	1.205115914	O	17.069299698	4.582175732	1.271963835	O	17.167085648	4.635916710	1.127590060
O	17.057458878	1.043211460	4.567274570	O	17.083980560	1.064762354	4.547545910	O	17.135972977	1.104809761	4.448553562
O	13.425627708	8.076015472	1.312159181	O	13.465635300	8.116388321	1.325129509	O	13.542687416	8.165054321	1.214992523
O	9.952599525	4.143547058	7.849739075	O	9.952943802	4.143954754	7.815067291	O	9.996965408	4.205597401	7.746135235
O	15.342250824	6.078748226	7.451148510	O	15.025916100	5.566695213	7.602026939	O	13.073612213	3.974918365	8.582180023
Cu	6.923854351	4.798650742	5.821442127	Cu	6.754578114	4.740663052	6.030673504	Cu	6.662055016	4.756911755	6.107245922
H	12.739331245	3.844075203	7.615467072	H	13.002231598	3.243169069	7.461779594	H	15.191547394	5.387197018	6.938361168
H	16.319009781	5.865119457	7.788935661	H	16.009380341	5.480869770	7.526939869	H	12.466523170	3.244235039	8.282522202
H	8.409904480	5.349794388	3.877413034	H	8.162272453	5.458378315	4.036388397	H	8.003465652	5.524698257	4.076505661
H	9.125578880	4.320281982	4.954820156	H	8.961823463	4.468761444	5.079090118	H	8.885999680	4.639580727	5.134725571
H	8.036359787	3.747553110	3.860918045	H	7.881157398	3.842918873	4.006576538	H	7.846677780	3.892194510	4.101709366
H	6.060423851	5.653736115	7.948472500	H	5.612602711	5.475767136	8.137686729	H	5.495502472	5.418462276	8.226880074
H	4.792288303	5.514559746	6.908653736	H	4.502216816	4.854831219	7.088506699	H	4.415659428	4.722596645	7.189613342
H	5.380139351	4.187588692	7.672442913	H	5.475438118	3.855210304	7.950922012	H	5.466886044	3.790869713	8.037618637
H	14.978052139	6.387830734	8.342035294	H	14.888567924	5.997650146	9.092006683	H	14.856721878	5.833009720	9.067449570

N	13.394959450	4.655258656	7.631378651	N	13.336083412	4.206154823	7.651016712	N	14.624504089	5.188515663	7.771426201
N	8.239776611	4.532526016	4.489461899	N	8.048655510	4.629957676	4.643511295	N	7.956277370	4.711905003	4.709321499
N	5.656794071	5.060095310	7.211503506	N	5.461233616	4.740139961	7.428294182	N	5.384932995	4.673982620	7.516667843
N	14.507811546	4.472316742	7.326241970	N	14.515735626	4.225820541	7.331204891	N	13.822146416	4.270140171	7.499811172
Structure E				ts3				Structure F			
Si	0.172541738	2.571025848	8.099317551	Si	0.138341367	2.565256119	8.180542946	Si	0.262173235	2.582887888	8.012261391
Si	7.926970482	0.786540270	2.994313478	Si	7.922501087	0.739109516	3.011922359	Si	8.085783958	0.756032169	2.913924932
Si	2.413125277	8.366179466	0.878796518	Si	2.384423494	8.382792473	0.964749753	Si	2.553509951	8.292328835	0.735153794
Si	5.543644428	8.426668167	1.049297094	Si	5.510991096	8.383059502	1.067969680	Si	5.686986446	8.402722359	0.944441974
Si	7.964329243	0.784331918	6.144320011	Si	7.914378643	0.707924247	6.169897556	Si	8.043608665	0.748435855	6.042726517
Si	0.107007504	5.748501778	8.242328644	Si	0.077879429	5.762641907	8.328749657	Si	0.233085334	5.749583244	8.157538414
Si	0.186166346	8.063088417	6.131817818	Si	0.157569319	8.065587044	6.203590870	Si	0.287129462	8.051746368	6.024105549
Si	5.635250568	0.573423147	8.268280029	Si	5.598029137	0.520814896	8.294345856	Si	5.713432312	0.593590200	8.173827171
Si	2.517735004	0.491564870	8.066352844	Si	2.493623495	0.500029206	8.128432274	Si	2.580855608	0.476472080	7.984027863
Si	0.207890064	8.078804016	3.013657570	Si	0.187273324	8.113335609	3.096437693	Si	0.292639315	8.162723541	2.935586691
Si	8.028824806	3.093052626	0.857196748	Si	8.004442215	3.048166275	0.897837698	Si	8.068015099	3.103096008	0.770738780
Si	9.609560013	2.609491110	8.086401939	Si	9.576763153	2.543688059	8.109848976	Si	9.690179825	2.563809872	8.001165390
Si	17.367956161	0.821023464	3.028681993	Si	17.300029755	0.809429407	3.130282402	Si	17.541763306	0.815933049	2.950696945
Si	11.868312836	8.322420120	0.861914456	Si	11.816610336	8.262627602	0.871974707	Si	11.947730064	8.257954597	0.769655466
Si	14.945223808	8.452613831	1.103379488	Si	14.948542595	8.458325386	1.211815357	Si	15.054125786	8.492850304	1.033896208
Si	17.352664948	0.752067983	6.166584015	Si	17.332029343	0.764774919	6.250147820	Si	17.457801819	0.741522372	6.058928013
Si	9.545181274	5.780014992	8.277112961	Si	9.529320717	5.700850487	8.302250862	Si	9.685848236	5.713576317	8.208402634
Si	9.633063316	8.082188606	6.154328346	Si	9.582894325	8.018106461	6.174703121	Si	9.685657501	8.018352509	6.074880600
Si	15.053037643	0.517839074	8.308101654	Si	15.038000107	0.532299042	8.396897316	Si	15.140157700	0.588838339	8.183403015
Si	11.947086334	0.503117025	8.109277725	Si	11.882766724	0.415758967	8.132209778	Si	11.998794556	0.432085693	8.039729118
Si	9.579311371	8.058999062	3.031657934	Si	9.555419922	7.997898579	3.045641899	Si	9.657997131	8.038360596	2.979705572
Si	17.469995499	3.060573339	0.910374820	Si	17.414011002	3.058629274	0.947696507	Si	17.490247726	3.116242647	0.750471950
Al	7.923274517	6.282850266	1.101977348	Al	7.875666142	6.219026089	1.113835931	Al	7.993385792	6.264278889	1.036343098
Al	17.297842026	6.244069099	1.168539524	Al	17.252120972	6.255793571	1.285546184	Al	17.506942749	6.269855499	0.984091401
O	1.641851187	1.863033056	8.128362656	O	1.612266064	1.869478345	8.198852539	O	1.723363638	1.857171059	8.103461266
O	-0.110296041	-0.041461900	2.906490803	O	-0.152546674	-0.022022635	3.044506073	O	0.204710409	0.214140594	2.888907671
O	8.113994598	2.220289469	2.244254112	O	8.117333412	2.186578512	2.292976856	O	8.152657509	2.162628889	2.104649067
O	2.981389046	0.386700302	0.072445929	O	2.975780010	0.387291849	0.130699426	O	2.347600698	-0.420004934	9.323136330
O	1.600483298	8.493765831	2.268620968	O	1.574490070	8.559225082	2.352868080	O	1.670948267	8.305059433	2.088136196
O	0.065171249	2.978663206	0.106837891	O	0.022766337	2.917536974	0.166737378	O	0.115128167	3.014205694	0.013586532
O	6.396160603	7.089159489	0.961161435	O	6.362821579	7.048124790	0.960209787	O	6.461187840	7.028200150	0.692097902
O	8.180240631	8.828406334	6.301564693	O	8.112055779	8.737347603	6.330884457	O	8.227532387	8.768355370	6.172447681
O	6.546061516	0.551547408	6.909440994	O	6.483822823	0.469908178	6.919692039	O	6.627102852	0.560963154	6.822104454
O	8.117367744	5.928136826	8.993850708	O	8.096016884	5.830784798	9.013619423	O	8.325551987	5.838916779	9.024304390
O	0.120031416	6.602744102	6.865500927	O	0.091371834	6.601416588	6.946084499	O	0.261946529	6.605569839	6.765341759
O	5.034891129	8.522772789	9.004169464	O	4.963456154	8.453818321	9.004529953	O	5.184351921	8.592618942	8.970997810
O	1.121048689	6.390186787	9.330508232	O	1.740000844	7.143352032	0.079219215	O	1.436232567	6.303503990	9.129075050
O	-0.689898252	2.023207664	6.818211555	O	18.139186859	2.053533554	6.870136738	O	-0.578326762	1.987349510	6.734212399
O	6.686204433	-0.028355926	2.326306581	O	6.682443619	-0.059179746	2.321966171	O	6.240896225	9.204402924	2.269108057

O	6.172533512	1.746612072	9.249217033	O	6.176925659	1.648739100	9.292869568	O	6.201934814	1.843610406	9.101570129
O	-0.416481376	6.767138481	2.350340366	O	-0.410045922	6.812956333	2.391423464	O	-0.663759351	7.019105911	2.359043837
O	2.051385164	-0.426610500	6.803095818	O	2.016475677	-0.420807183	6.871433735	O	2.103883266	-0.367438138	6.680536747
O	0.563209057	7.820106030	4.585615635	O	0.539700150	7.808619022	4.662499428	O	0.699197769	7.829227448	4.477678776
O	4.086380005	0.891284168	7.863956451	O	4.056444168	0.894308269	7.905417442	O	4.154842854	0.861205757	7.775478363
O	7.667146683	4.582715988	1.247370601	O	7.588618279	4.526313782	1.283698797	O	7.687510967	4.571575165	1.232869387
O	7.638513565	1.099482298	4.577826977	O	7.606917858	1.018225789	4.597877502	O	7.719113350	1.093890905	4.479432106
O	3.963181496	8.063783646	1.219987869	O	3.928095102	8.034172058	1.287090421	O	4.102007866	8.121743202	1.167904258
O	0.425933897	4.184519291	7.939521790	O	0.356043100	4.190898895	8.061432838	O	0.533378005	4.176718712	7.808482170
O	11.066490173	1.872835636	8.160521507	O	11.025728226	1.801909208	8.181121826	O	11.127624512	1.802381277	8.126818657
O	9.325076103	-0.015122503	2.874382257	O	9.322306633	-0.060274288	2.875820875	O	9.562142372	0.076235637	2.860806227
O	17.623167038	2.255942345	2.319942236	O	17.509878159	2.198398113	2.325335741	O	17.486291885	2.177368164	2.084403276
O	12.452037811	0.383478284	0.105318941	O	12.244297028	0.286741555	0.101545699	O	12.463535309	0.317241997	0.045986436
O	10.921993256	8.349451065	2.169183969	O	10.930256844	8.253972054	2.223181486	O	11.012741089	8.169951439	2.079496622
O	9.475449562	2.986815929	0.074545868	O	9.451796532	2.979079485	0.117835514	O	8.818666458	2.272037506	9.345139503
O	15.831811905	7.133131981	1.053776860	O	15.777694702	7.102295876	1.232885718	O	15.783989906	6.982421398	0.766570270
O	17.578855515	8.796604156	6.312510490	O	17.551698685	8.805748940	6.371949673	O	17.652807236	8.763727188	6.156607628
O	15.937860489	0.492027998	6.941958904	O	15.927508354	0.519768894	7.026286602	O	16.041547775	0.452259541	6.831931591
O	17.385906219	5.841293335	8.850481987	O	17.327692032	5.906620979	8.930621147	O	17.625242233	5.918793201	8.854914665
O	9.543564796	6.615817547	6.857397079	O	9.521800041	6.557206631	6.895432949	O	9.602449417	6.560773373	6.799405575
O	14.319461823	8.433148384	8.977222443	O	14.565072060	8.520112038	9.176849365	O	14.610878944	8.608248711	9.055979729
O	10.757162094	6.375017166	9.206089973	O	10.744422913	6.271299362	9.245371819	O	10.962305069	6.301841736	9.079893112
O	8.781852722	2.063514948	6.770709515	O	8.710193634	1.984369516	6.820734978	O	8.869615555	2.013935089	6.683605671
O	16.117910385	0.078454360	2.290329218	O	16.034248352	0.001820013	2.503532648	O	15.768912315	9.131720543	2.326536655
O	15.638772964	1.586998940	9.357843399	O	15.536099434	1.754603148	9.338899612	O	15.649874687	1.833790660	9.078246117
O	8.808294296	6.734378338	2.549854040	O	8.778800964	6.687310219	2.540890217	O	8.711094856	6.821919918	2.534414530
O	11.496882439	-0.406218946	6.835261345	O	11.435203552	-0.439604133	6.816825867	O	11.518382072	-0.453165442	6.768445015
O	10.012187004	7.877846718	4.596704006	O	9.942749977	7.791434288	4.617094517	O	10.118607521	7.797104359	4.529821873
O	13.512598991	0.991320312	7.903982639	O	13.468461037	0.749452233	8.017435074	O	13.569361687	0.808660746	7.820879459
O	17.028013229	4.558478355	1.184555650	O	17.082069397	4.568600178	1.287487388	O	17.124603271	4.613459110	1.150181413
O	17.011116028	1.051392913	4.607500553	O	16.977067947	1.130908966	4.705440998	O	17.118930817	1.091950655	4.502421856
O	13.381267548	8.083183289	1.374727130	O	13.362369537	8.131148338	1.305229783	O	13.501619339	8.136517525	1.277848125
O	9.860275269	4.208618641	7.891143322	O	9.844824791	4.139489174	7.883361340	O	9.990005493	4.152224541	7.778058052
O	13.680101395	3.842813492	7.252874851	O	14.731277466	3.604287148	6.287239552	O	15.509853363	6.295983791	6.943514824
Cu	7.033030987	5.002543926	5.738934040	Cu	7.098617554	5.196922302	5.660603046	Cu	6.718375683	4.669599056	6.103753567
H	16.588079453	5.682204247	8.150058746	H	16.631614685	5.822062492	8.235380173	H	16.327007294	6.236563206	7.484332085
H	13.595416069	2.860224724	7.389683247	H	15.498949051	3.228089333	5.805252075	H	15.577535629	7.164471149	6.512213707
H	8.566448212	5.329890251	3.825814009	H	8.652596474	5.242705822	3.786848783	H	8.064057350	5.460773468	4.085179329
H	9.201965332	4.287885666	4.954925537	H	9.205690384	4.218263626	4.981419086	H	8.934551239	4.541306019	5.130758286
H	8.093734741	3.749285221	3.859844685	H	8.077343941	3.698911190	3.896261454	H	7.885331154	3.829983234	4.081802368
H	6.367588520	6.001807213	7.827770710	H	6.567103386	6.117180347	7.800505161	H	5.520497322	5.349065304	8.201860428
H	5.078719139	6.159590721	6.799347401	H	5.590911388	6.888619423	6.716207027	H	4.469935417	4.596444130	7.174531460
H	5.358051300	4.733413219	7.566504002	H	5.181744099	5.395420074	7.269769669	H	5.539917469	3.716874599	8.053628922
H	14.467451096	5.941126823	7.336335659	H	13.482322693	4.992126465	7.549225807	H	15.242643356	6.397528172	0.173173860

N	15.280801773	5.309307575	7.477699757	N	14.454825401	5.366388321	7.616165161	N	13.641235352	4.550784588	8.329545975
N	8.342117310	4.542489529	4.461843014	N	8.374250412	4.503939152	4.458147049	N	8.007751465	4.636926174	4.703814983
N	5.818503857	5.520070553	7.099030495	N	5.970324039	5.972254753	6.967372417	N	5.437171936	4.584940910	7.510222435
N	15.005925179	4.098842621	7.482233524	N	15.276358604	4.713755131	6.978034019	N	13.251307487	4.016170025	7.436425209

Table S10. Cartesian coordinates of RC, TS, IM, and PC for NH₂NO decomposition with the assistance of Brønsted acid site and Cu-OH site.

Structure A				ts1			Structure B				
Si	0.227257073	2.294058084	8.164631844	Si	0.358432531	2.193869829	8.110644341	Si	0.353486896	2.199212074	8.111852646
Si	8.050048828	0.632081985	3.010885954	Si	8.177125931	0.513422370	2.938331127	Si	8.170155525	0.522795200	2.944167852
Si	2.538851976	8.063424110	0.862558365	Si	2.659265518	7.930266857	0.791991174	Si	2.661112070	7.929744244	0.793447554
Si	5.670812607	8.235909462	1.013125539	Si	5.789811611	8.115088463	0.955236256	Si	5.788879871	8.124427795	0.962128818
Si	7.953561306	0.620756507	6.146855831	Si	8.081191063	0.520889759	6.078951359	Si	8.077397346	0.527296185	6.082658291
Si	0.236192048	5.426086426	8.356278419	Si	0.381454349	5.340296745	8.225779533	Si	0.373480260	5.342239857	8.235597610
Si	7.926482201	6.060536861	0.947603941	Si	8.050441742	5.937436581	0.910084188	Si	8.051071167	5.943294525	0.912703931
Si	5.667494774	0.418629289	8.281398773	Si	5.799781322	0.297217071	8.220025063	Si	5.792418003	0.306757808	8.224687576
Si	2.557655811	0.220767319	8.035395622	Si	2.684196711	0.116837740	7.983008862	Si	2.682100773	0.119396746	7.985501766
Si	0.218531087	7.966677189	2.916809797	Si	0.348185420	7.853383541	2.849850893	Si	0.344173908	7.852036953	2.852821827
Si	8.056827545	2.928675413	0.869846106	Si	8.197367668	2.807255030	0.802252829	Si	8.188187599	2.812397718	0.802674770
Si	9.623308182	2.359350681	8.081162453	Si	9.753595352	2.259800673	8.011541367	Si	9.749891281	2.262351990	8.013829231
Si	17.446676254	0.674285054	3.016959429	Si	17.546672821	0.542350411	2.956962109	Si	17.542842865	0.544257522	2.958476067
Si	11.956520081	8.097508430	0.829038680	Si	12.086098671	7.998184681	0.760539174	Si	12.080851555	8.002239227	0.760276318
Si	15.098855019	8.289270401	1.026125550	Si	15.219178200	8.159207344	0.965657711	Si	15.214564323	8.162044525	0.969475210
Si	17.379453659	0.546898127	6.201852798	Si	17.523714066	0.416702807	6.137464523	Si	17.514707565	0.425537258	6.137411594
Si	9.573420525	5.477488041	8.255918503	Si	9.679754257	5.384588718	8.179306984	Si	9.682138443	5.387062073	8.178577423
Si	17.408227921	6.165337086	0.910412610	Si	17.556119919	6.043167591	0.836526334	Si	17.544345856	6.039829254	0.849900484
Si	15.102430344	0.513203859	8.318581581	Si	15.231083870	0.404116213	8.253157616	Si	15.225428581	0.405813873	8.256232262
Si	12.015844345	0.266504943	8.091084480	Si	12.152998924	0.163119793	8.056662560	Si	12.145242691	0.163595021	8.056585312
Si	9.627223015	7.847440720	2.924789190	Si	9.750452042	7.728420258	2.861964703	Si	9.746871948	7.737641335	2.864406109
Si	17.475738525	2.994451284	0.913157105	Si	17.596092224	2.883593082	0.847451270	Si	17.588706970	2.886657715	0.850387692
Al	0.173007190	7.893449783	6.081608772	Al	0.338545978	7.697438240	6.046408176	Al	0.328612715	7.699970722	6.050357819
Al	9.700253487	7.930838585	6.153018951	Al	9.829637527	7.812713146	6.112696648	Al	9.816388130	7.810729980	6.116774082
O	1.657904863	1.552659035	8.291149139	O	1.794722080	1.452568650	8.253247261	O	1.786713123	1.450989604	8.254079819
O	0.046466976	-0.038024753	2.757538080	O	0.149643704	-0.166317552	2.702274323	O	0.145475462	-0.168018430	2.710951805
O	8.156408310	2.074197292	2.255585670	O	8.298171997	1.957553625	2.189124346	O	8.291091919	1.964511871	2.190582037
O	2.367978573	-0.731123447	9.351092339	O	1.830835581	8.541586876	9.284795761	O	1.830916405	8.541452408	9.285025597
O	1.675999999	8.214233398	2.215590477	O	1.803623796	8.115427971	2.149059772	O	1.795654535	8.115386009	2.145582914
O	0.080375291	2.803994179	0.183523342	O	0.206596315	2.690832376	0.126287013	O	0.198124409	2.701688766	0.126158789
O	6.510218143	6.842235088	0.823796988	O	6.640243530	6.723623753	0.794496655	O	6.645863533	6.737578392	0.800668240
O	8.158751488	8.693346024	6.314647198	O	8.297857285	8.605323792	6.248439789	O	8.289792061	8.609890938	6.249400616
O	6.514820576	0.417684257	6.889702797	O	6.647455692	0.301752925	6.827737808	O	6.647036076	0.316632748	6.837191582
O	8.084836006	5.545006752	8.935137749	O	8.212579727	5.445683479	8.909685135	O	8.218471527	5.447893620	8.915131569
O	0.480536699	6.241081238	6.903306484	O	0.653240025	6.141984463	6.844208717	O	0.615742028	6.159775734	6.864288330

O	5.210544586	8.349315643	8.998816490	O	5.349683762	8.228373528	8.940940857	O	5.343198299	8.244868279	8.953746796
O	2.030052185	6.740242004	0.038615812	O	1.468405247	5.866790295	9.345348358	O	1.467593312	5.866689205	9.348877907
O	-0.627572298	1.805666447	6.867869377	O	-0.479454219	1.663251162	6.815466881	O	-0.482379526	1.666306376	6.815432072
O	6.233915329	9.083916664	2.299170494	O	6.355170727	8.970995903	2.232524872	O	6.346308708	8.977488518	2.246251822
O	6.198744774	1.588407159	9.286903381	O	6.343571186	1.468256950	9.216649055	O	6.322223663	1.480568886	9.227262497
O	-0.558680952	6.766777992	2.122364044	O	-0.408964783	6.650726795	2.048518658	O	-0.424282551	6.648334980	2.064866543
O	1.474328041	8.855856895	6.692327499	O	1.586001754	8.777927399	6.627741814	O	1.577425957	8.781333923	6.629970551
O	0.415422648	7.520269871	4.429128170	O	0.572664320	7.416801453	4.361466408	O	0.572246015	7.421533585	4.366281033
O	4.120625496	0.707977057	7.973961353	O	4.256443024	0.590200782	7.914608955	O	4.249186993	0.600068033	7.907339096
O	7.696641445	4.478153706	1.233705640	O	7.818723202	4.352129459	1.170033693	O	7.819492340	4.358003616	1.173467278
O	7.664455414	0.951305866	4.561915398	O	7.791391373	0.821095765	4.489778519	O	7.786057949	0.841769993	4.495050907
O	4.119088650	7.860156536	1.249626875	O	4.245059490	7.732983589	1.184890151	O	4.244263649	7.735557556	1.190880179
O	0.555222750	3.886096001	8.008335114	O	0.682502568	3.772812843	7.930066586	O	0.678878903	3.776743889	7.930361748
O	11.009987831	1.548654795	8.147159576	O	11.135901451	1.441153288	8.064588547	O	11.132097244	1.443429112	8.066995621
O	9.496931076	-0.139277816	2.938732862	O	8.930928230	9.136628151	2.840809107	O	8.924143791	9.142672539	2.846527815
O	17.452304840	2.153099775	2.310051680	O	17.546060562	2.006560564	2.223308325	O	17.546127319	2.006530762	2.223322392
O	12.434763908	0.137170687	0.096085422	O	12.594492912	0.078077197	0.095405057	O	12.588556290	0.082916677	0.098219395
O	11.064959526	8.066085815	2.208922386	O	11.182263374	7.922086716	2.135322809	O	11.175832748	7.926358700	2.132694006
O	9.491877556	2.848165035	0.104350172	O	9.635562897	2.740864992	0.043370917	O	9.625172615	2.738240957	0.040629402
O	15.968988419	6.925753117	0.815624118	O	16.116897583	6.817737103	0.745718837	O	16.104957581	6.814519405	0.753893971
O	17.456411362	8.549657822	6.454295635	O	17.617612839	8.423964500	6.352758884	O	17.608648300	8.432126999	6.353194714
O	15.900121689	0.510649085	6.909981251	O	16.050033569	0.361911356	6.857570171	O	16.043027878	0.369604588	6.858988762
O	17.549043655	5.652291298	8.863080025	O	17.690099716	5.500042439	8.795925140	O	17.685760498	5.490153313	8.815680504
O	9.485551834	6.265483856	6.811612606	O	9.529349327	6.151991844	6.733143806	O	9.529666901	6.150214195	6.732881069
O	14.579623222	8.456897736	9.052949905	O	14.663953781	8.357578278	9.009475708	O	14.670336723	8.360752106	9.013946533
O	10.690613747	6.166866302	9.212605476	O	10.803259850	6.119830132	9.093510628	O	10.808428764	6.120001316	9.092341423
O	8.710075378	1.936625719	6.788389683	O	8.826095581	1.844088316	6.721119881	O	8.825622559	1.851098657	6.720291615
O	15.580098152	9.128843307	2.343852758	O	15.675204277	8.986372948	2.300881147	O	15.670586586	8.990910530	2.303718805
O	15.612881660	1.704266548	9.297034264	O	15.739989281	1.612733603	9.208456993	O	15.735080719	1.615797997	9.209116936
O	8.775244713	6.663435936	2.201028109	O	8.882637024	6.507760048	2.198030472	O	8.880204201	6.511341095	2.206304789
O	11.038781166	8.767324448	6.780556202	O	11.166163445	8.603392601	6.792027950	O	11.154524803	8.604510307	6.793636799
O	9.780260086	7.277913094	4.470247269	O	9.884423256	7.192348957	4.417579651	O	9.897419930	7.204660892	4.417647362
O	13.531151772	0.817929268	8.046260834	O	13.662281036	0.723142803	7.963223457	O	13.657155991	0.719369590	7.963121414
O	17.181844711	4.576070309	1.174639463	O	17.302650452	4.460021496	1.140713215	O	17.287763596	4.458554745	1.156829238
O	17.158042908	0.866856813	4.605229855	O	17.268196106	0.751126170	4.548962116	O	17.260667801	0.758121967	4.548888206
O	13.519651413	7.851439953	1.196734905	O	13.639419556	7.705054283	1.122867346	O	13.634443283	7.715346336	1.127022862
O	9.972995758	3.943682194	7.935479641	O	10.093250275	3.847917795	7.876543045	O	10.093306541	3.848860979	7.877691746
O	7.235155582	4.726358414	4.969709873	O	6.927012444	4.968927860	5.112761497	O	6.976682663	4.889905930	5.028701782
O	2.837491751	5.586835861	6.136281013	O	3.221128464	5.492689610	6.003156185	O	3.236525536	5.487166405	5.999509335
Cu	8.681898117	5.738032341	5.092019081	Cu	8.578801155	5.807212353	4.989091873	Cu	8.634617805	5.781675339	4.941147327
H	7.371697903	3.771540880	4.818645477	H	6.877213001	4.002008915	5.009030819	H	6.918980598	3.917780638	5.008216381
H	1.434112787	5.935556412	6.531146526	H	2.262074709	5.712466240	6.292675495	H	2.292459965	5.709177017	6.286563873
H	5.493740559	6.684515953	7.181126595	H	5.712522030	6.686931133	7.260571003	H	5.720037460	6.676789761	7.258647442
H	5.242884636	5.478058815	5.880572796	H	5.995756149	5.415295601	5.770622253	H	6.179055691	5.291274548	5.624044895

N	4.874226093	6.121158123	6.600222111	N	5.219201088	6.083424091	6.587530136	N	5.235007763	6.068652153	6.580865383
N	3.611482382	6.279901028	6.850924969	N	3.986316681	6.219857216	6.807664871	N	4.011894703	6.223193169	6.813156128
Structure C				ts2				Structure D			
Si	0.271372199	2.263347149	8.084304810	Si	0.306181192	2.231101274	8.083886147	Si	0.190293133	2.254880905	8.088196754
Si	8.089137077	0.558627844	2.917463064	Si	8.130288124	0.575033247	2.918923855	Si	7.993357658	0.577717781	2.999191046
Si	2.600762367	7.974951744	0.766693115	Si	2.632713079	7.965239048	0.760139763	Si	2.548017740	8.045430183	0.824557900
Si	5.717781544	8.172402382	0.917065382	Si	5.753679276	8.186406136	0.918476045	Si	5.666957378	8.188989639	1.006712198
Si	7.994875431	0.588842988	6.056016445	Si	8.033202171	0.615554452	6.061374187	Si	7.939002991	0.510988951	6.122809887
Si	0.273694098	5.394132137	8.213074684	Si	0.310141563	5.372972965	8.210253716	Si	0.163251102	5.358098507	8.320899963
Si	8.002494812	5.999255180	0.892300487	Si	8.033378601	6.001741886	0.904486120	Si	7.950582027	6.037925720	0.919635832
Si	5.702856541	0.375768125	8.197259903	Si	5.742079258	0.377876580	8.209044456	Si	5.646907330	0.440927327	8.280582428
Si	2.608120918	0.171133161	7.974035263	Si	2.643981218	0.158521354	7.957502365	Si	2.570823908	0.160508037	8.080407143
Si	0.293543160	7.891979694	2.850593090	Si	0.323106706	7.883405209	2.825366020	Si	0.224285647	7.819238663	2.932998419
Si	8.094725609	2.86611279	0.776597261	Si	8.135442734	2.872432470	0.789399147	Si	7.994785309	2.921765327	0.864441872
Si	9.668260574	2.318382025	7.975821495	Si	9.702101707	2.334753513	7.974720955	Si	9.638217926	2.275795221	8.119881630
Si	17.505685806	0.602797627	2.946865797	Si	17.528379440	0.584748805	2.934960842	Si	17.457256317	0.558265209	2.995025635
Si	12.024972916	8.056153297	0.762621939	Si	12.052605629	8.055949211	0.771981895	Si	11.946909904	7.974728107	0.809585273
Si	15.163311958	8.225243568	0.949702322	Si	15.187088013	8.207188606	0.945884347	Si	15.088007927	8.185092926	1.003541946
Si	17.427293777	0.498987913	6.117338181	Si	17.457387924	0.449886888	6.114904404	Si	17.338376999	0.531504929	6.149899960
Si	9.667288780	5.439402103	8.193424225	Si	9.682588577	5.447596550	8.195762634	Si	9.614931107	5.401461124	8.244976044
Si	17.463716507	6.074891567	0.879513681	Si	17.502553940	6.070206165	0.838352978	Si	17.351900101	6.019563675	0.984524965
Si	15.150936127	0.455607116	8.245883942	Si	15.181611061	0.436052322	8.235512733	Si	15.081583977	0.393731296	8.290100098
Si	12.073808670	0.202940762	8.005154610	Si	12.100564003	0.204963148	8.026082993	Si	11.969279289	0.204477131	8.054902077
Si	9.685140610	7.794012547	2.856215000	Si	9.716934204	7.787644386	2.866927385	Si	9.630016327	7.865817070	2.894259453
Si	17.528347015	2.935675144	0.854219079	Si	17.570646286	2.916856527	0.840855837	Si	17.463712692	2.887426615	0.881282508
Al	0.244753480	7.748501778	6.037213326	Al	0.282659411	7.740865231	6.019427776	Al	0.187581211	7.846695423	6.065891266
Al	9.757614136	7.878358841	6.095009327	Al	9.775730133	7.881366730	6.108455181	Al	9.660665512	7.824479103	6.121272087
O	1.688351393	1.486733556	8.228976250	O	1.739717960	1.484706640	8.219155312	O	1.595471859	1.464730263	8.144721985
O	0.101899341	-0.123804249	2.713287354	O	0.122258723	-0.138182402	2.675789118	O	0.069233730	-0.173029765	2.839313269
O	8.212471962	1.989614487	2.144623756	O	8.291161537	2.012831688	2.163735151	O	8.007260323	1.975682497	2.179348946
O	1.800996423	8.611076355	9.291895866	O	1.819273949	8.587945938	9.266568184	O	3.124959707	0.116697900	0.146888629
O	1.740121484	8.135698318	2.124505043	O	1.777440190	8.138591766	2.119912624	O	1.654390097	8.017709732	2.168805122
O	0.125531346	2.780974388	0.104113825	O	0.178331330	2.742280483	0.114385277	O	0.068329237	2.805437565	0.121321052
O	6.610438824	6.808557987	0.714257658	O	6.643241405	6.817225456	0.765781760	O	6.536375046	6.830019951	0.765772343
O	8.265489578	8.728549004	6.290737152	O	8.294583321	8.749819756	6.299938202	O	8.019188881	8.481101990	6.205332756
O	6.576491833	0.400954545	6.822480202	O	6.617307663	0.440734446	6.836389065	O	6.512068748	0.401498854	6.905199051
O	8.186217308	5.490274906	8.898783684	O	8.201532364	5.488073349	8.901523590	O	8.107933044	5.459431171	8.907864571
O	0.407833517	6.216575623	6.850459576	O	0.530914545	6.189311504	6.833820820	O	0.056408107	6.103056431	6.785833359
O	5.243330956	8.321090698	8.928771973	O	5.287528992	8.310165405	8.915562630	O	5.146671295	8.414431572	9.067959785
O	1.393286467	5.940534592	9.291788101	O	1.418869972	5.917397499	9.299202919	O	1.295780897	6.146055698	9.151462555
O	-0.580385745	1.748281479	6.791074753	O	-0.558578610	1.695829391	6.808360100	O	18.124853134	1.831173182	6.804898262
O	6.283269405	8.996604919	2.217368126	O	6.303840160	9.050837517	2.199976683	O	6.178204536	8.965959549	2.350557566
O	6.225193977	1.558906555	9.195475578	O	6.252386093	1.540749311	9.238375664	O	6.124241352	1.676466227	9.225127220
O	-0.512908459	6.690604210	2.098060608	O	-0.449554265	6.684592724	2.035433292	O	-0.613635719	6.622674942	2.201285362

O	1.516407251	8.789619446	6.640825272	O	1.551306844	8.787289619	6.617938995	O	1.510378838	8.567368507	6.877892971
O	0.545726299	7.469570160	4.361250877	O	0.543508530	7.452206612	4.338886261	O	0.490180016	7.368873596	4.444667339
O	4.165061474	0.675149560	7.866061211	O	4.202102661	0.663358331	7.869575500	O	4.094339848	0.705139041	7.907877922
O	7.756297112	4.417578220	1.158189297	O	7.777685165	4.421076775	1.160447836	O	7.677930355	4.471223354	1.267465115
O	7.702309132	0.868963540	4.469197750	O	7.737752914	0.877269149	4.471048832	O	7.620597363	0.868673563	4.558227539
O	4.182686806	7.752600670	1.158514261	O	4.217447758	7.757623196	1.148728728	O	4.108027935	7.730499268	1.173562884
O	0.613826036	3.834446907	7.899487495	O	0.624971390	3.810557365	7.893076420	O	0.568751216	3.847918510	7.928533554
O	11.025834084	1.463629246	7.995767593	O	11.047566414	1.462035060	8.012727737	O	11.047705650	1.519417048	8.331548691
O	9.542063713	-0.204265520	2.854652643	O	9.568744659	-0.213366002	2.849020243	O	9.464976311	-0.141767129	2.890475035
O	17.541872025	2.074350595	2.236811399	O	17.550848007	2.060207844	2.228119135	O	17.533588409	2.008127213	2.246026039
O	12.484205246	0.096634872	0.027979087	O	12.526183128	0.108407721	0.057563014	O	11.052551270	8.592310905	9.324427605
O	11.116257668	8.007413864	2.134117603	O	11.152372360	7.998375416	2.148466349	O	11.071249008	8.091526985	2.186710835
O	8.827936172	2.052082300	9.347046852	O	8.855365753	2.070293665	9.339844704	O	9.427896500	2.816142559	0.097572371
O	16.030490875	6.860230446	0.767460465	O	16.063386917	6.846543789	0.759131849	O	15.936655045	6.796891689	0.830480278
O	17.543300629	8.522833824	6.328577995	O	17.564908981	8.466631889	6.331856251	O	17.515586853	8.595764160	6.377632618
O	15.949343681	0.440012276	6.835763454	O	15.972901344	0.396991074	6.820958138	O	15.885028839	0.403886974	6.879155159
O	17.610227585	5.508543491	8.855898857	O	17.629604340	5.521596909	8.796794891	O	17.525388718	5.465098381	8.958748817
O	9.553725243	6.236970425	6.772085190	O	9.549742699	6.237431526	6.772210121	O	9.621354103	6.257300854	6.884467602
O	14.609252930	8.392562866	8.969666481	O	14.630414963	8.374213219	8.965866089	O	14.615081787	8.342460632	9.025493622
O	10.789545059	6.107157230	9.152070045	O	10.801976204	6.130747318	9.144427299	O	10.726292610	5.945384979	9.321141243
O	8.712171555	1.985861301	6.651547909	O	8.747943878	2.016322613	6.647472382	O	8.843089104	1.713960648	6.789874554
O	15.638926506	9.074172020	2.258261681	O	15.651233673	9.059581757	2.256892443	O	15.614771843	9.010862350	2.313874245
O	15.670741081	1.631443262	9.234678268	O	15.722135544	1.620542288	9.205314636	O	15.615510941	1.589509010	9.261653900
O	8.833398819	6.567606926	2.180739641	O	8.878728867	6.552537918	2.190000296	O	8.802180290	6.665257454	2.159742594
O	11.130990982	8.675696373	6.709793091	O	11.147059441	8.663782120	6.743343830	O	11.566499710	-0.501845479	6.672058582
O	9.852280617	7.248164654	4.404432297	O	9.858835220	7.250144005	4.418905735	O	9.812074661	7.282129288	4.417486668
O	13.576298714	0.790503085	7.979438782	O	13.607256889	0.786017060	7.981492996	O	13.519707680	0.686409116	8.017417908
O	17.191110611	4.495068550	1.178633094	O	17.255649567	4.487488747	1.140883565	O	17.113853455	4.435619831	1.251507282
O	17.175539017	0.807466269	4.526436806	O	17.222196579	0.773465395	4.521772861	O	17.097152710	0.824659586	4.557985306
O	13.578947067	7.808875561	1.141076326	O	13.605446815	7.784180164	1.137381554	O	13.520933151	7.792426586	1.196286678
O	10.042495728	3.897185564	7.852427959	O	10.087632179	3.910199404	7.865829945	O	9.946628571	3.849693298	7.877831936
O	7.691497803	4.203967094	5.261938095	O	7.572052002	4.245125771	5.239208698	O	9.190328598	3.755364180	4.408706665
O	5.747478008	5.599830627	6.685671329	O	5.422794342	5.508384705	6.535003662	O	7.132204533	6.296447754	4.937313557
Cu	8.915029526	5.615236282	4.923836708	Cu	8.840571404	5.648462296	4.939664364	Cu	8.936812401	5.489708900	4.624297619
H	8.036022186	3.410330057	5.757132053	H	7.905267715	3.475313425	5.770238876	H	9.326648712	3.249498129	5.232645988
H	6.120028019	6.073189259	7.459844589	H	5.921800613	5.905423641	7.280213833	H	7.260403633	7.140138149	5.473428726
H	2.688279390	5.525434017	6.116423130	H	2.199142456	5.805225372	6.445977688	H	0.061014116	5.457931042	6.052116394
H	6.876494408	4.539251804	5.730441570	H	6.692910671	4.537851810	5.606054783	H	6.485240459	5.748807907	5.421349525
N	3.694871902	5.310109615	5.954679489	N	3.197762728	5.526629448	6.151025295	N	3.447720528	5.396259785	6.631088734
N	4.315746784	5.852937222	6.850347042	N	4.012331486	5.889706612	6.950294495	N	4.530936718	5.409510612	6.377859116

Table S11. Cartesian coordinates of RC, TS, IM, and PC for HONO reacting with NH₃ over Brønsted acid sites.

Structure A				Structure B				Structure C			
Si	0.134118378	2.561081409	7.955313206	Si	0.131355524	2.560137749	7.916229725	Si	0.118816733	2.603334188	7.905612469
Si	7.951905727	0.798972607	2.874207020	Si	7.965430737	0.795575202	2.824816465	Si	7.944492817	0.828678250	2.818669796
Si	2.408786297	8.267505646	0.709969342	Si	2.421511173	8.283834457	0.657477498	Si	2.409761429	8.320907593	0.669795036
Si	5.535919666	8.417325974	0.937307298	Si	5.553153992	8.424476624	0.865434766	Si	5.523399830	8.457907677	0.873680472
Si	7.903047085	0.747194767	6.015156746	Si	7.911586285	0.756578386	5.945364952	Si	7.896413803	0.764602542	5.948983669
Si	0.109300375	5.727715015	8.142247200	Si	0.089184582	5.744328499	8.081629753	Si	0.089171290	5.778854370	8.092170715
Si	0.156267613	8.023009300	6.001770020	Si	0.158683479	8.024514198	5.938212872	Si	0.158147961	8.070758820	5.947566986
Si	5.591286182	0.537940025	8.143857002	Si	5.592920780	0.590225935	8.065558434	Si	5.572577477	0.616803765	8.071134567
Si	2.452385426	0.438322127	7.953846455	Si	2.460889816	0.454867482	7.886383057	Si	2.454432964	0.497369230	7.906189919
Si	0.133671060	8.098860741	2.914130926	Si	0.144423619	8.110278130	2.840407372	Si	0.127860606	8.115077019	2.852208853
Si	7.974069595	3.090702295	0.732858837	Si	7.963504314	3.116006851	0.660797536	Si	7.959401131	3.143176079	0.666560531
Si	9.558878899	2.578785658	7.964753151	Si	9.566974640	2.579653025	7.909929276	Si	9.556051254	2.601203442	7.909271717
Si	17.427921295	0.797460079	2.897426844	Si	17.417140961	0.808746338	2.851726294	Si	17.367254257	0.810925066	2.835654497
Si	11.818692207	8.299064636	0.719020724	Si	11.847272873	8.294835091	0.672826588	Si	11.832078934	8.312492371	0.648969293
Si	14.947058678	8.476725578	0.927400291	Si	14.978002548	8.425573349	0.897479951	Si	14.963542938	8.432023048	0.885218620
Si	17.338468552	0.729476869	6.005726337	Si	17.339420319	0.725651264	5.971060753	Si	17.338659286	0.771958888	5.952107906
Si	9.526116371	5.732901573	8.145342827	Si	9.585157394	5.732308388	8.099978447	Si	9.539560318	5.760415554	8.066803932
Si	9.577989578	8.051584244	6.007084846	Si	9.596933365	8.055705070	5.945232391	Si	9.575222015	8.071928024	5.929465294
Si	15.022326469	0.568470478	8.122057915	Si	15.028452873	0.551687300	8.108777046	Si	15.012292862	0.590275466	8.092809677
Si	11.881295204	0.466212690	7.945205212	Si	11.892393112	0.457136691	7.899489880	Si	11.877549171	0.481844068	7.892213345
Si	9.544570923	8.048624992	2.896401405	Si	9.540360451	8.079306602	2.855981827	Si	9.544708252	8.111007690	2.825021982
Si	17.384313583	3.082463264	0.722034931	Si	17.402229309	3.087737560	0.685989201	Si	17.358804703	3.124419689	0.675552905
Al	7.860424995	6.257886887	0.961674213	Al	7.880346298	6.276531219	0.912366033	Al	7.863552570	6.310354233	0.874682844
Al	17.356042862	6.238718510	0.957931757	Al	17.300361633	6.296202183	0.863413632	Al	17.297565460	6.314202309	0.895823240
O	1.604685903	1.833231211	8.059637070	O	1.617508411	1.852402329	7.995191574	O	1.592760324	1.882894278	8.029150009
O	0.073470235	0.159893483	2.859815359	O	0.060270727	0.159452364	2.788832188	O	-0.000200123	0.139328510	2.768383503
O	8.082328796	2.213254213	2.099241257	O	8.013888359	2.180028439	1.990383387	O	8.009801865	2.230473518	2.012171507
O	2.194242477	-0.449140221	9.294494629	O	2.253553867	-0.425360829	9.242017746	O	2.257407665	-0.383314431	9.260423660
O	1.498776674	8.243169785	2.039254904	O	1.538776278	8.293490410	2.002542257	O	1.502785325	8.337084770	1.997307539
O	-0.695561528	2.230155230	9.317316055	O	-0.680976987	2.184336185	9.274267197	O	-0.740991175	2.245692015	9.244107246
O	6.307968140	7.031661987	0.789639413	O	6.324032784	7.039852142	0.592699349	O	6.308738232	7.084731102	0.628083467
O	8.113528252	8.780733109	6.169999123	O	8.131138802	8.794734001	6.068514347	O	8.104114532	8.795661926	6.076663017
O	6.470849991	0.466600597	6.764072895	O	6.484675407	0.458317280	6.698778629	O	6.466969490	0.484164894	6.704319477
O	8.113413811	5.901329041	8.876756668	O	8.186309814	5.890966415	8.862945557	O	8.105722427	5.904100895	8.772727013
O	0.118806750	6.585962772	6.754487038	O	0.158690393	6.575236797	6.673725605	O	0.132280797	6.628772736	6.694990158
O	5.022032261	8.490808487	8.880500793	O	5.029392242	8.575945854	8.861207962	O	4.959789753	8.593370438	8.852659225
O	1.369085550	6.260035038	9.084244728	O	1.350525379	6.279909134	9.035902977	O	1.347184896	6.323596478	9.037898064
O	18.153478622	1.988218427	6.661720276	O	18.155448914	1.994094133	6.616743565	O	-0.673061967	2.030460119	6.594034195
O	6.748931885	-0.071649551	2.195685863	O	6.819802284	-0.171684429	2.168694496	O	6.772389412	-0.099245235	2.160348654
O	6.139074802	1.712344289	9.105365753	O	6.137375355	1.806694746	8.980415344	O	6.139238358	1.810614944	8.996880531
O	17.999334335	6.957597733	2.371873379	O	18.068773270	6.943125248	2.268468380	O	18.090656281	6.897980690	2.318280935
O	2.004136801	-0.415289313	6.650074482	O	1.999133945	-0.406694174	6.596296310	O	1.996591806	-0.367691040	6.616418839
O	0.560343504	7.778146744	4.455171108	O	0.563298285	7.802437782	4.390697956	O	0.576591849	7.858085155	4.403711796

O	4.024669170	0.859844089	7.796533108	O	4.030877590	0.886753798	7.697370529	O	4.014889240	0.955804348	7.710230827
O	7.510536194	4.569797039	1.067865491	O	7.521576881	4.592734814	1.048021317	O	7.517200470	4.624160767	1.025426984
O	7.593931198	1.067791581	4.451297760	O	7.575108528	1.098153830	4.390084267	O	7.570318222	1.106434703	4.392642498
O	3.950289965	8.122706413	1.171354175	O	3.976143837	8.099179268	1.098297119	O	3.951495647	8.125478745	1.135061979
O	0.428185582	4.154460907	7.782344341	O	0.412882566	4.158943176	7.760523796	O	0.413079858	4.198172569	7.746341705
O	11.014599800	1.839357018	8.044166565	O	11.006712914	1.819612265	7.989470005	O	11.020131111	1.869091511	8.001955986
O	9.384794235	0.045707241	2.773640633	O	9.441421509	0.119617313	2.781007051	O	9.406487465	0.129579812	2.734662533
O	17.450513840	2.185099602	2.079757452	O	17.461429596	2.218837261	2.063538313	O	17.411510468	2.206819773	2.014188051
O	11.626618385	-0.434985042	9.285312653	O	11.615348816	-0.446959555	9.230908394	O	11.635787964	-0.395044237	9.242353439
O	10.933187485	8.279993057	2.055707455	O	10.899599075	8.251281738	1.969947696	O	10.923444748	8.314582825	1.977779388
O	8.742293358	2.282764912	9.337866783	O	8.741820335	2.307214022	9.287561417	O	8.737209320	2.322967529	9.287977219
O	15.651627541	6.960226536	0.711839437	O	15.647325516	6.961722374	0.694883704	O	15.682245255	7.007496357	0.679329634
O	17.541114807	8.762537003	6.144835472	O	17.541088104	8.755270004	6.105477810	O	17.539560318	8.805416107	6.079873085
O	15.912351608	0.506722867	6.767188549	O	15.914919853	0.517951608	6.743546009	O	15.925971985	0.564368904	6.748755455
O	17.553510666	5.901756287	8.898265839	O	17.518249512	5.956795692	8.788027763	O	17.525871277	5.948843956	8.821502686
O	9.530913353	6.607845783	6.762314320	O	9.531936646	6.625264168	6.727293491	O	9.520335197	6.623496532	6.672986507
O	14.479973793	8.528560638	8.901637077	O	14.458735466	8.512035370	8.864173889	O	14.466836929	8.583073616	8.887024879
O	10.795670509	6.271127224	9.092381477	O	10.865950584	6.257495403	9.030368805	O	10.772766113	6.316706657	9.011185646
O	8.685584068	2.012169361	6.694440842	O	8.686926842	2.017080784	6.641011238	O	8.691465378	2.015722275	6.643001556
O	15.641790390	9.171888351	2.200827122	O	16.296968460	-0.166108981	2.160607815	O	16.219789505	-0.148635626	2.178585529
O	15.531282425	1.742200851	9.103469849	O	15.534072876	1.741334438	9.078145981	O	15.453433990	1.837057233	9.050531387
O	8.722639084	6.795496941	2.364237070	O	8.618877411	6.882349491	2.349076986	O	8.676043510	6.886732101	2.289054632
O	11.426672935	-0.401315928	6.652303696	O	11.443022728	-0.396535963	6.590310574	O	11.411768913	-0.376844019	6.596692085
O	9.961421013	7.824323177	4.459144592	O	9.990856171	7.799662590	4.402043343	O	9.976611137	7.862113476	4.382895947
O	13.456161499	0.836767614	7.767048359	O	13.461631775	0.850882649	7.738799095	O	13.448876381	0.884446859	7.701896667
O	16.997234344	4.574660778	1.103084087	O	17.050659180	4.599616051	0.989103794	O	16.971445084	4.619252205	1.027525663
O	16.994567871	1.057507873	4.446166992	O	17.002122879	1.052455425	4.414551258	O	16.980442047	1.100792408	4.399996758
O	13.382565498	8.145156860	1.161913872	O	13.384772301	8.165777206	1.159496069	O	13.375039101	8.143008232	1.102395058
O	9.854921341	4.172587395	7.767539978	O	9.883424759	4.170289040	7.699464798	O	9.872880936	4.190468311	7.698404789
O	13.192711830	4.809796333	8.776857376	O	13.198360443	4.589677811	9.166090012	O	15.126607895	4.392337322	6.978439808
O	14.398751259	4.042540550	7.068141937	O	14.816473961	4.186621666	7.285434723	Cu	4.795157433	5.284216404	7.855251312
Cu	4.830347061	5.221511841	7.752637386	Cu	4.856901169	5.274768353	7.946799755	H	5.679315090	7.288332939	6.682787895
H	5.684352398	7.259094238	6.622986317	H	5.734469891	7.257204533	6.724892139	H	6.864923477	6.325895786	7.304791451
H	6.869990349	6.365970135	7.333458424	H	6.931061268	6.319294930	7.356138706	H	6.177119255	5.965127945	5.833637238
H	6.305262566	5.953998089	5.829193592	H	6.237615108	5.920512676	5.900054932	H	4.868408680	4.608322620	0.327712625
H	5.010333538	4.603217602	0.282980144	H	4.824250221	4.571620464	0.368171155	H	2.858731747	4.776160717	9.236694336
H	2.963468790	4.729351997	9.228731155	H	2.845111609	4.755897045	9.223444939	H	3.217841864	3.381179333	8.430926323
H	3.310549736	3.317337036	8.447588921	H	3.234581470	3.368799686	8.420397758	H	12.524885178	4.220276833	8.895798683
H	15.015783310	6.324695110	0.222650096	H	14.616074562	5.970446587	0.212802574	H	13.981546402	3.313204288	9.085670471
H	12.275386810	5.195951939	8.841098785	H	12.351723671	5.107643127	9.096516609	H	14.678177834	5.746303082	0.072935499
N	6.022113323	6.301082611	6.747756481	N	6.040246964	6.285834312	6.833711147	N	5.977285385	6.313016891	6.773297787
N	3.730306387	4.153249264	8.863466263	N	3.633958578	4.175408363	8.910810471	N	3.633430481	4.196286201	8.892095566
N	13.313948631	4.412539482	7.309959412	N	13.697338104	4.391494274	7.353643417	N	14.010404587	4.629130363	7.158101559
				N				N	13.546985626	4.224853039	8.879023552

ts			Structure D				
Si	0.179807663	2.621118307	7.847490311	Si	0.136190772	2.605375528	7.869923592
Si	7.977144241	0.840496182	2.766021967	Si	7.950939178	0.837282777	2.800278902
Si	2.467324018	8.292108536	0.600917876	Si	2.434429646	8.296873093	0.628937244
Si	5.566685200	8.458027840	0.843452334	Si	5.540981293	8.461464882	0.862829447
Si	7.945686340	0.782588363	5.900082588	Si	7.913362503	0.772564650	5.936984539
Si	0.169882655	5.782789707	8.021180153	Si	0.128044724	5.777682781	8.053009987
Si	0.200984120	8.102880478	5.887551308	Si	0.169896960	8.081576347	5.920477867
Si	5.633836269	0.548781931	8.036094666	Si	5.593335629	0.570887983	8.068721771
Si	2.504315376	0.499720097	7.864661217	Si	2.468091965	0.493683636	7.890377998
Si	0.164494798	8.164602280	2.791909218	Si	0.146375999	8.150172234	2.836333036
Si	8.028182983	3.117599487	0.631462991	Si	7.987623692	3.121599913	0.670131028
Si	9.613094330	2.622784138	7.857358932	Si	9.575696945	2.609365940	7.892416477
Si	17.446794510	0.870266676	2.762745142	Si	17.426301956	0.836093783	2.810434103
Si	11.880929947	8.341546059	0.616847336	Si	11.835726738	8.321336746	0.642829776
Si	15.012454033	8.518127441	0.809214532	Si	14.950757027	8.512127876	0.848173797
Si	17.392515182	0.800973058	5.880435944	Si	17.355819702	0.779808223	5.913623810
Si	9.581744194	5.769589424	8.046754837	Si	9.549149513	5.763961792	8.065501213
Si	9.615722656	8.086187363	5.888034344	Si	9.582540512	8.078267097	5.918791294
Si	15.051058769	0.664330900	8.000746727	Si	15.017431259	0.620245934	8.039501190
Si	11.927081108	0.508338273	7.824563980	Si	11.887948990	0.492170870	7.863083363
Si	9.597497940	8.053595543	2.782201052	Si	9.568382263	8.065880775	2.811612368
Si	17.378570557	3.186417103	0.593935370	Si	17.353958130	3.136334419	0.636635065
Al	7.922665119	6.273797035	0.857843280	Al	7.892683506	6.285037518	0.872876823
Al	17.366672516	6.353588581	0.838089228	Al	17.389980316	6.294619083	0.888513148
O	1.638761759	1.880704403	8.016698837	O	1.600411057	1.875239253	8.031314850
O	0.088825583	0.220062181	2.694360971	O	0.076838568	0.207964301	2.765223742
O	8.190616608	2.254945040	2.002636671	O	8.124507904	2.263244390	2.049074888
O	2.301221132	-0.414083064	9.193867683	O	2.251151085	-0.408913583	9.226884842
O	1.523845911	8.288649559	1.904385090	O	1.493469238	8.280301094	1.936555147
O	-0.711747348	2.318764448	9.178212166	O	-0.748301685	2.285555363	9.202949524
O	6.399427891	7.105843067	0.766368926	O	6.357367992	7.100975037	0.756721258
O	8.145518303	8.807289124	6.022197723	O	8.110049248	8.796555519	6.066104412
O	6.520221233	0.491869152	6.657876015	O	6.481441975	0.511644125	6.694742680
O	8.149806023	5.898378849	8.751697540	O	8.112688065	5.911257744	8.762052536
O	0.177539021	6.665326595	6.643126011	O	0.140577763	6.639818668	6.667510033
O	5.009391785	8.485187531	8.749981880	O	4.977330208	8.506914139	8.780436516
O	1.441128969	6.300055981	8.953215599	O	1.396118641	6.302887917	8.984948158
O	-0.600499153	2.039912224	6.531453133	O	-0.630826712	2.021598101	6.549356937
O	6.736604691	0.046837986	2.063436270	O	6.724559307	0.020899057	2.096863270
O	6.216272831	1.686714649	9.019873619	O	6.159023762	1.706106186	9.063000679
O	18.049888611	6.991806984	2.286246300	O	18.012277603	6.992382050	2.322736025
O	2.028732777	-0.319139063	6.550053120	O	2.000778675	-0.347192228	6.585050583
O	0.617682815	7.900412083	4.339146614	O	0.595273376	7.859370232	4.376565456

O	4.078613281	0.926446199	7.690256119	O	4.034403801	0.935790420	7.713606834
O	7.513742447	4.590057373	0.934405386	O	7.499303818	4.601442337	0.971786082
O	7.622119427	1.126933813	4.343523979	O	7.587181091	1.099409223	4.378424168
O	3.996220350	8.105622292	1.100015163	O	3.965104818	8.120903015	1.117973208
O	0.487793028	4.208357811	7.654383659	O	0.425066471	4.198719501	7.700874329
O	11.072130203	1.889506817	7.958711624	O	11.032659531	1.870575666	8.000827789
O	9.361701965	0.003700018	2.677007914	O	9.351795197	0.029109374	2.694947243
O	17.437349319	2.258285999	1.931108356	O	17.423433304	2.220247507	1.979057312
O	11.710581779	-0.391576171	9.166682243	O	11.680757523	-0.401337177	9.212937355
O	10.977375984	8.361119270	1.949149489	O	10.953837395	8.353242874	1.986108184
O	8.794800758	2.348030567	9.231782913	O	8.748847008	2.325737476	9.262103081
O	15.744739532	7.083444118	0.527510107	O	15.687613487	7.011227131	0.620153546
O	17.574129105	8.822152138	6.011474609	O	17.545177460	8.803887367	6.032430172
O	15.970712662	0.600807250	6.663490295	O	15.947670937	0.579152167	6.714134216
O	17.622371674	5.953535080	8.785394669	O	17.585073471	5.969607830	8.829276085
O	9.574237823	6.656594753	6.667852402	O	9.545899391	6.643128395	6.683889389
O	14.482387543	8.654506683	8.809949875	O	14.477375984	8.587873459	8.832188606
O	10.827687263	6.312539101	9.006086349	O	10.784825325	6.309944630	9.029328346
O	8.752602577	2.029321909	6.590595245	O	8.726292610	2.019207001	6.617369652
O	16.327295303	-0.133156002	2.104014397	O	15.647991180	9.198936462	2.125515461
O	15.493821144	1.905919075	8.951552391	O	15.455140114	1.824261069	9.040642738
O	8.844908714	6.757514477	2.244940281	O	8.810556412	6.780657291	2.257997990
O	11.439915657	-0.335645676	6.529550552	O	11.409987450	-0.349261701	6.565124035
O	10.013239861	7.837079048	4.347641945	O	9.982398987	7.849713802	4.375763416
O	13.487545013	0.920656145	7.605981350	O	13.458568573	0.877327681	7.653359413
O	16.983249664	4.676725388	0.970803618	O	16.972085953	4.634816647	1.014883757
O	17.045038223	1.137920618	4.324041843	O	16.989782333	1.102261066	4.357680321
O	13.437904358	8.176402092	1.055458546	O	13.399232864	8.149348259	1.098073125
O	9.939475060	4.212656498	7.647580624	O	9.887933731	4.199667931	7.690377235
O	14.334037781	4.274907112	6.443473339	O	14.731296539	4.266901970	6.743935108
Cu	4.945633411	5.246953011	7.529996395	Cu	4.845593452	5.238053799	7.667246819
H	5.790972710	7.270095348	6.362223625	H	5.711875916	7.267743111	6.539731979
H	6.966878414	6.410374165	7.131922722	H	6.892642021	6.352433205	7.235634327
H	6.450595856	5.950685024	5.625473499	H	6.307154179	5.958754063	5.731994152
H	5.195934296	4.680465698	0.104830764	H	5.042111397	4.643210888	0.217351422
H	3.115148306	4.758890152	9.059382439	H	2.987443924	4.758541107	9.160028458
H	3.487286091	3.337340832	8.303897858	H	3.341230392	3.341187954	8.390142441
H	12.575368881	5.012569904	8.821769714	H	12.539816856	4.638821125	8.796536446
H	13.808905602	3.800014496	8.762913704	H	13.933792114	3.565286160	8.838024139
H	14.271198273	5.512885571	9.148211479	H	15.099140167	6.347154140	0.108229622
N	6.136734962	6.320787907	6.525416374	N	6.038503170	6.304879665	6.655232430
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