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Communication

Bio-glycidol conversion to solketal over acid heterogeneous catalysts: synthesis and theoretical approach

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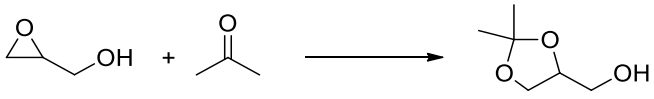
Table S1. Glycidol conversion to solketal.



Experiment	Catalyst	Conversion [%]	Selectivity to Solketal [%]	Yield [%]
1	Montmorillonite K10	0	-	-
2	AC-SO_3H	0	-	-
3	MS-SO_3H	0	-	-
4	MS	0	-	-
5	AC	0	-	-

Reaction conditions: glycidol/acetone moles ratio 1:43, t=24 h, reflux, catalyst loading 10 % wt.

MS: mesoporous silica; AC: activated carbon.

The catalyst recyclability test

After the reaction, catalysts are removed by filtration, washed with fresh acetone (10 mL), dried overnight at 40°C and then reused a second time for solketal synthesis. Under the optimized reaction conditions (glycidol/acetone moles ratio 1:43, catalyst loading 20 % wt, reflux 18 h) the catalyst is stable and retains high efficiency during four consecutive cycles (Figure S1).

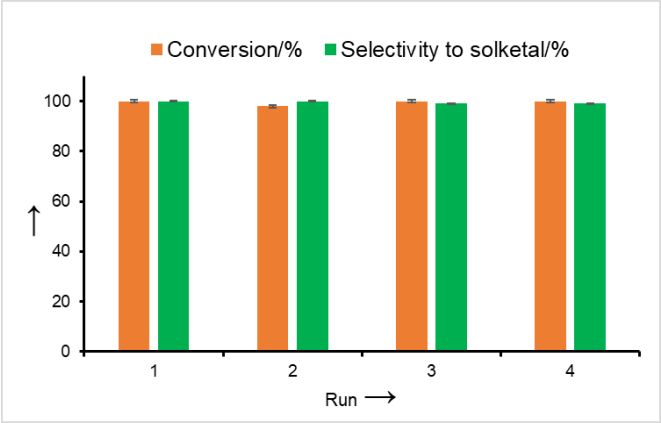


Figure S1. Nafion NR50 recyclability.

Characterization of the reaction mixture at low conversion

350 μL of glycidol and 15.0 mL of acetone (1:43 moles ratio) were mixed together in a round bottom flask under magnetic stirring (300 rpm) for 1 h under reflux conditions in the presence of 0.09 g of Nafion NR50.
Afterwards, Nafion NR50 was removed by filtration, acetone was removed using a rotary evaporator and the reaction products were analysed by ^{1}H and ^{13}C NMR.
The spectra were collected on Bruker Avance-400 spectrometer [400(^{1}H) e 100(^{13}C)] using $CDCl_3$ as solvent.

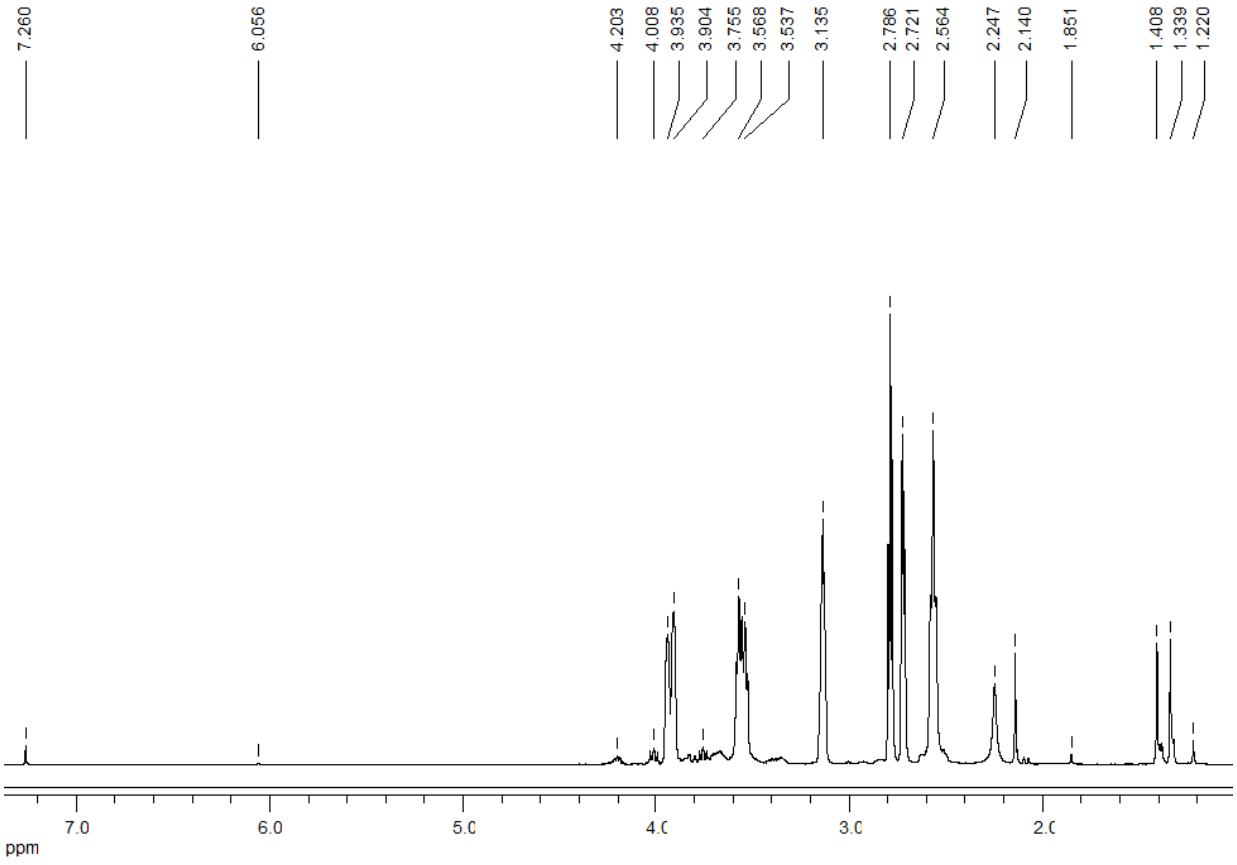


Figure S2. ^{1}H-NMR ($CDCl_3$, 400 MHz) spectrum of reaction mixture.

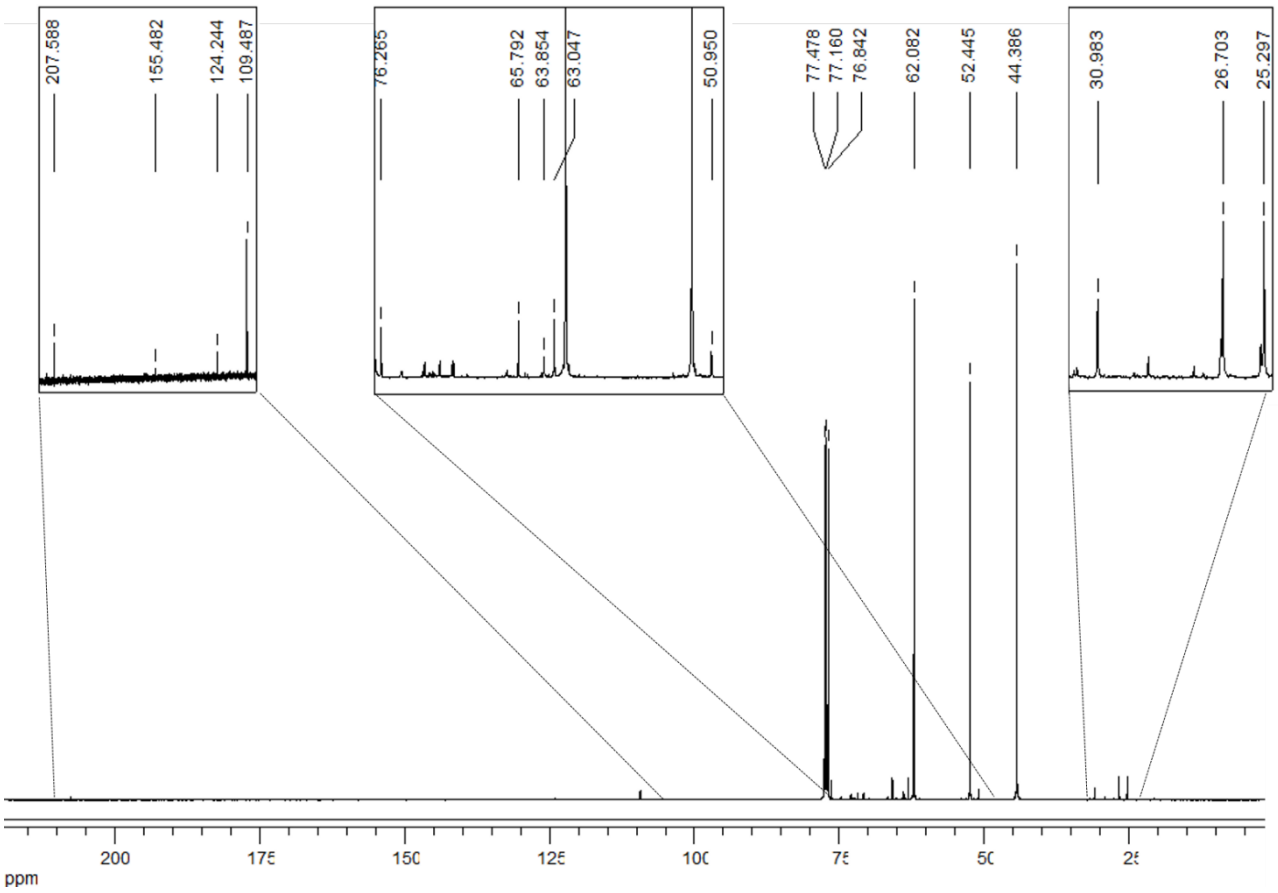


Figure S3. ^{13}C-NMR ($CDCl_3$, 100 MHz) spectrum of reaction mixture. .

^{1}H-NMR spectrum (Figure S2) clearly shows the formation of solketal (characteristic singlet at 1.3 and 1.4 ppm; three doublets of doublets from 4.0 to 3.5 ppm and one multiplet at 4.2 ppm) in the presence of 80% of unreacted glycidol (doublet of doublets at 3.9 ppm, doublet of doublets 3.6 ppm, multiplet at 3.5 ppm, doublet of doublets at 3.1 ppm, doublet of doublets at 2.8 ppm, doublet of doublets at 2.7 ppm and triplet at 2.6 ppm).

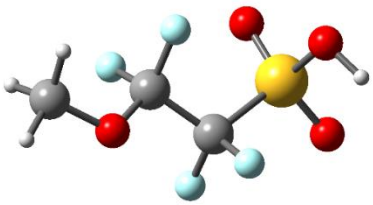
^{13}C-NMR spectrum (Figure S3) confirms the presence of solketal (109.5, 76.3, 65.8, 63.0, 26.7 and 25.3 ppm) and glycidol (62.1, 52.4 and 44.4 ppm).

Characteristic signal of 2,2-dimethyl-1,3-dioxan-5-ol (P2 product in Figure 3) is not observed to the rapid isomerization of this compound to solketal, the more stable isomer as confirmed by DFT calculations. The other signals observed was attributed acetone impurities (207.6 and 30.98 ppm at ^{13}C and 2.14 ppm at ^{1}H) and to the products of aldolic condensation of acetone (4-hydroxy-4-methylpentan-2-one and mesityl oxide), in the presence of an acidic heterogenous catalyst such as Nafion, that don't affect the reaction yield.

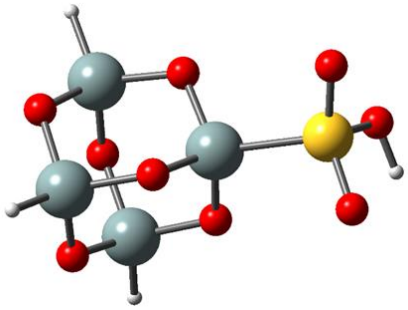
Computational methods

All the DFT geometry optimizations were performed at the GGA BP86 level [1–3] with the Gaussian09 package[4]. The electronic configuration of the systems was described with the SVP basis set[5]. All geometries were characterized as minimum or transition state through frequency calculations. The reported free energies were built through single point energy calculations on the BP86/SVP geometries using the M06 functional and the TZVP basis set[6]. Solvent effects were included with the PCM model using acetone as the solvent[7,8]. To this M06/TZVP electronic energy in solvent, thermal corrections were included from the gas-phase frequency calculations at the BP86/SVP geometries. In order to simplify the calculations, the catalyst structure has been modeled

as in Chart 1: the polymeric chain has been modeled as a $–CH_3$ group and the chain end $–O-CF_2-CF_2-SO_3H$ has been explicitly considered.



Scheme S1. Nafion NR 50 modeled structure.



Scheme S2. Sulfonated-silica modelled structure.

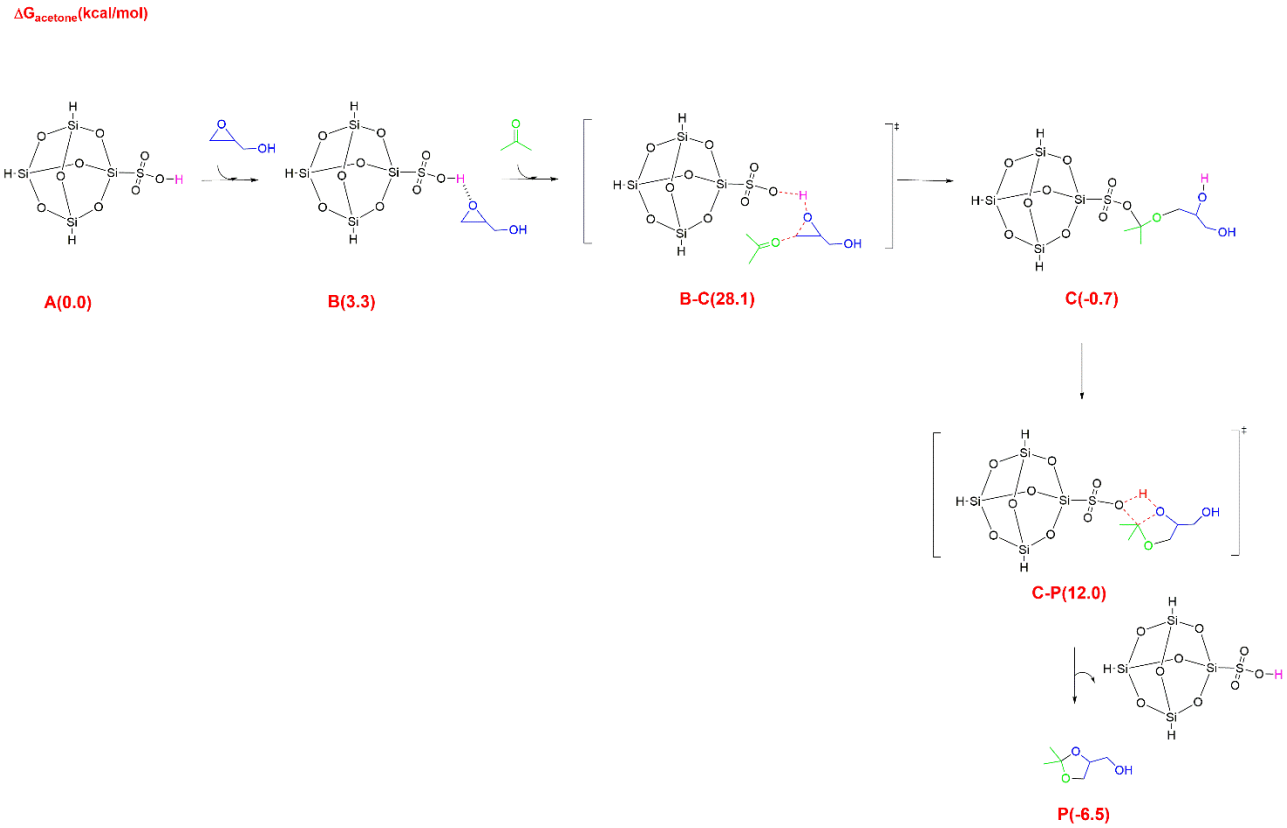


Figure S4. Mechanistic pathways investigated and corresponding free energies (kcal/mol in acetone) for the sulfonated-silica catalyzed reaction.

Optimized xyz coordinates of species in Figure 3 and Figure S4

A

S	-1.715228	-0.240009	-0.126792
O	-1.837407	-0.725933	1.449935
O	-1.562817	-1.455554	-0.925205
O	-2.728807	0.795636	-0.385403
C	-0.046794	0.710081	-0.041123
C	1.217339	-0.202521	-0.059680
F	-0.081928	1.435892	1.099760
F	-0.030009	1.540317	-1.098726
F	1.300973	-0.812543	-1.280204
F	1.056166	-1.204993	0.862930
O	2.293033	0.569722	0.205688
C	3.573039	-0.097287	0.186085
H	4.320103	0.679700	0.426761
H	3.606704	-0.901167	0.949075
H	3.779297	-0.520744	-0.817525
H	-2.242803	0.021692	1.944720

B

C	4.716829	0.683233	-0.884239
O	3.707447	-0.181625	-0.323203
C	2.465288	0.341038	-0.226186
F	1.945215	0.676060	-1.448859
C	1.551954	-0.733408	0.447212
F	1.895523	-0.870966	1.742545
S	-0.311193	-0.295525	0.474193
O	-0.954973	-1.259898	1.390710
O	-0.642131	-0.639270	-1.058216
O	-0.460618	1.158830	0.735750
F	1.678392	-1.913580	-0.182334
F	2.437696	1.481314	0.528457
O	-3.180134	-0.455618	-1.403239
C	-4.177977	0.221398	-0.573329
H	-4.903749	0.775852	-1.198265
C	-4.143494	-1.254222	-0.675971
H	5.648831	0.090654	-0.893006
H	4.448800	0.977724	-1.919168
H	4.851128	1.587718	-0.257186
H	-1.674010	-0.549868	-1.186336
H	-3.718586	-1.836504	0.162905
H	-4.866020	-1.789548	-1.317540
C	-3.702535	0.951927	0.670918
H	-4.613130	1.138534	1.290558
H	-3.046174	0.273248	1.264214
O	-3.083089	2.180748	0.376346
H	-2.111853	2.020016	0.412849

B-C

C	3.896352	-2.180971	1.646222
O	3.682242	-1.123415	0.694155
C	2.395781	-0.856453	0.374821
F	1.665712	-0.472570	1.480493
C	2.376084	0.281498	-0.693614
F	2.830877	-0.224774	-1.863843
S	0.661820	1.053358	-1.044020
O	0.845447	1.819276	-2.289420
O	0.427078	1.937718	0.195139
O	-0.294718	-0.110240	-1.085610
F	3.195642	1.278111	-0.294087
F	1.751582	-1.963521	-0.121394

151	O	-1.018957	1.152854	2.128892
152	C	-2.367935	1.172489	1.596357
153	C	-2.587471	2.037766	0.340219
154	O	-2.033244	3.321084	0.483617
155	C	-2.058643	-0.261490	1.436114
156	O	-3.687989	-1.090782	0.556005
157	C	-3.629676	-1.860068	-0.421906
158	C	-2.345302	-2.466712	-0.912229
159	C	-4.906270	-2.184877	-1.154628
160	H	4.989957	-2.240569	1.791208
161	H	3.404078	-1.947395	2.612536
162	H	3.517563	-3.147766	1.255622
163	H	-0.353278	1.406723	1.352807
164	H	-2.131102	-0.919488	2.313052
165	H	-1.381634	-0.516461	0.603239
166	H	-5.079786	-3.282341	-1.138222
167	H	-5.766932	-1.654553	-0.708086
168	H	-4.796285	-1.903039	-2.224468
169	H	-1.668496	-1.660697	-1.287986
170	H	-1.800240	-2.943898	-0.071607
171	H	-2.511523	-3.209216	-1.714214
172	H	-2.185458	1.494631	-0.546324
173	H	-3.685708	2.140350	0.195677
174	H	-1.068383	3.205375	0.310396
175	H	-3.062592	1.430354	2.419784
176				**B-C-2**
177	C	4.164953	-2.484173	1.023805
178	O	3.904937	-1.198991	0.431115
179	C	2.616650	-0.935014	0.115502
180	F	1.807977	-0.945213	1.237183
181	C	2.549096	0.466860	-0.568114
182	F	3.074632	0.362548	-1.810865
183	S	0.792203	1.196942	-0.759521
184	O	0.949906	2.313105	-1.710433
185	O	0.473388	1.672604	0.677539
186	O	-0.079650	0.046829	-1.179128
187	F	3.280731	1.347072	0.149050
188	F	2.089243	-1.880993	-0.723227
189	H	5.251426	-2.511225	1.222515
190	H	3.608723	-2.599139	1.976811
191	H	3.891203	-3.303894	0.328289
192	O	-0.877689	0.270761	2.306598
193	C	-2.616751	0.364782	1.383230
194	C	-2.577936	1.567093	0.437807
195	O	-2.059690	2.716345	1.054755
196	C	-1.572681	-0.678214	1.485920
197	H	-0.234109	0.800297	1.671451
198	H	-1.851403	-1.581290	2.064180
199	H	-1.026314	-0.918976	0.553233
200	H	-2.030070	1.291230	-0.490403
201	H	-3.637823	1.770762	0.169645
202	H	-1.074036	2.633706	0.969125
203	H	-3.227480	0.497694	2.291120
204	O	-4.255588	-0.610288	0.476353
205	C	-4.297144	-1.206430	-0.612376
206	C	-3.105191	-1.433871	-1.504191
207	C	-5.626403	-1.759408	-1.073748
208	H	-5.513491	-2.793754	-1.459468
209	H	-6.371013	-1.723688	-0.257603
210	H	-5.989073	-1.142047	-1.925036
211	H	-2.264474	-0.732378	-1.335243
212	H	-2.729809	-2.463653	-1.305149

213	H	-3.403229	-1.418129	-2.571807	
214					**C**
215	C	-4.825218	1.677071	0.138026	
216	O	-3.467142	1.373473	0.522653	
217	C	-2.926535	0.267442	-0.026791	
218	F	-3.650788	-0.860758	0.241496	
219	F	-2.840690	0.348923	-1.395704	
220	C	-1.486695	0.091286	0.556228	
221	F	-0.817310	1.257847	0.512382	
222	F	-1.559612	-0.345972	1.824590	
223	S	-0.465841	-1.175848	-0.473061	
224	O	-1.244282	-2.414325	-0.614153	
225	O	0.696614	-1.352774	0.679950	
226	O	0.070330	-0.482107	-1.666551	
227	O	1.858141	1.782296	-1.335429	
228	C	3.105942	1.600857	-0.681453	
229	C	3.032987	0.473923	0.351529	
230	C	3.406717	2.952548	-0.013040	
231	O	2.328872	3.338737	0.819202	
232	O	2.746769	-0.742171	-0.361452	
233	C	2.108382	-1.777670	0.305401	
234	C	2.697766	-2.118581	1.675364	
235	C	2.062224	-2.967585	-0.649917	
236	H	-5.083255	2.613259	0.663890	
237	H	-4.895529	1.829197	-0.957937	
238	H	-5.511918	0.865424	0.452341	
239	H	1.445795	0.904990	-1.511969	
240	H	2.228916	0.710466	1.080215	
241	H	4.001269	0.382184	0.895331	
242	H	3.772109	-2.364621	1.556343	
243	H	2.597370	-1.269010	2.377500	
244	H	2.174579	-2.990685	2.111526	
245	H	1.667565	-2.648108	-1.633556	
246	H	3.090535	-3.351274	-0.800721	
247	H	1.426357	-3.775249	-0.241737	
248	H	4.324510	2.888110	0.611144	
249	H	3.604768	3.701236	-0.820856	
250	H	1.538657	3.142232	0.267913	
251	H	3.919495	1.354281	-1.411171	
252					**C-2**
253	C	-5.450265	-0.786905	0.452167	
254	O	-4.339863	0.102314	0.204495	
255	C	-3.124021	-0.474024	0.116877	
256	C	-2.067639	0.655815	-0.114775	
257	S	-0.382284	-0.045391	-0.713811	
258	O	-0.497719	-0.346842	-2.140272	
259	F	-2.786723	-1.163343	1.250044	
260	F	-3.043854	-1.376023	-0.914532	
261	F	-2.491038	1.512780	-1.056986	
262	F	-1.856395	1.317959	1.042318	
263	O	0.035977	-1.061988	0.282862	
264	O	0.451200	1.377491	-0.559720	
265	C	1.687542	1.480746	0.248069	
266	C	1.320880	1.483476	1.735860	
267	O	2.467491	0.393793	-0.192381	
268	C	3.600401	-0.080765	0.564913	
269	C	4.706486	-0.448981	-0.439685	
270	H	4.971644	0.458930	-1.027993	
271	O	4.342404	-1.467411	-1.337280	
272	C	2.291392	2.808870	-0.217466	
273	H	-6.348971	-0.145376	0.471236	
274	H	-5.539310	-1.535650	-0.360572	

H	-5.331641	-1.299953	1.427843	
H	3.745514	-2.074126	-0.835573	
H	3.998806	0.719449	1.234358	
C	3.180098	-1.296288	1.418908	
H	3.255303	2.975916	0.305716	
H	2.477670	2.760282	-1.307006	
H	1.618448	3.660010	0.004804	
H	0.800104	0.550518	2.018929	
H	2.228319	1.597491	2.362013	
H	0.654140	2.341651	1.946381	
H	5.615868	-0.710377	0.169581	
H	2.497980	-0.980381	2.241318	
O	2.591585	-2.318085	0.624176	
H	4.086684	-1.727280	1.897620	
H	1.710226	-1.973030	0.340467	
				C-P
S	0.365780	-0.663653	-0.314923	
O	0.087737	0.515975	-1.244982	
O	0.063059	-0.354503	1.131959	
O	-0.183813	-1.959470	-0.806082	
C	2.259208	-0.867211	-0.415637	
C	3.079635	0.229256	0.335319	
F	2.588546	-0.862419	-1.724967	
F	2.558572	-2.075897	0.112753	
F	2.929686	0.055968	1.685276	
F	2.567064	1.469616	0.052079	
O	4.375942	0.120237	-0.046440	
C	5.293525	1.036811	0.577258	
H	6.283112	0.822905	0.134780	
H	5.007336	2.087066	0.363879	
H	5.330504	0.875278	1.674227	
H	-1.504603	0.476669	-1.226352	
O	-2.490171	0.471179	-0.980690	
C	-4.102949	1.084416	0.627915	
C	-2.677439	1.368299	0.095065	
H	-1.922757	1.180469	0.896719	
C	-2.469095	2.834636	-0.332149	
H	-3.027789	2.983102	-1.293562	
H	-2.921889	3.518966	0.423286	
O	-1.104433	3.157293	-0.422221	
H	-0.610202	2.393741	-0.804670	
H	-4.182252	1.232071	1.725288	
H	-4.880365	1.685577	0.118467	
O	-4.460583	-0.288609	0.262324	
C	-3.597129	-1.244639	0.467156	
C	-3.645706	-2.384622	-0.478466	
H	-2.600063	-2.491336	-0.860262	
H	-3.892992	-3.332762	0.043426	
H	-4.341780	-2.192476	-1.313449	
C	-2.707152	-1.275965	1.635504	
H	-2.567801	-2.321930	1.972175	
H	-1.652703	-0.929157	1.368859	
H	-3.062336	-0.637848	2.466951	
				C-P2
S	0.841032	-1.630494	0.091365	
O	-0.126204	-1.168627	-1.011144	
O	0.382579	-1.176266	1.452887	
O	1.260993	-3.039601	-0.026729	
C	2.433288	-0.635780	-0.311407	
C	2.467071	0.823677	0.235978	
F	2.566145	-0.605126	-1.657244	
F	3.474298	-1.315202	0.220386	

F	2.535756	0.804112	1.602292	
F	1.276495	1.459125	-0.068482	
O	3.523258	1.467034	-0.314725	
C	3.740280	2.820631	0.120391	
H	4.624806	3.179658	-0.435967	
H	2.864629	3.457961	-0.120783	
H	3.943268	2.859708	1.210385	
H	-0.870727	0.349702	-1.399824	
O	-1.410539	1.169682	-1.591007	
C	-3.599760	1.677740	-0.673255	
C	-2.780126	0.878727	-1.713427	
H	-3.146743	1.270973	-2.697378	
C	-3.112984	-0.633677	-1.690253	
H	-4.212444	-0.769634	-1.797259	
H	-2.634249	-1.103386	-2.580628	
O	-2.689572	-1.270269	-0.495597	
H	-1.696540	-1.411851	-0.606549	
H	-3.063159	2.605146	-0.386328	
H	-4.604575	1.933739	-1.058492	
O	-3.926529	0.903511	0.538303	
C	-3.032729	0.461655	1.367256	
C	-3.564619	-0.520161	2.352926	
H	-4.666451	-0.463388	2.426312	
H	-3.293706	-1.520155	1.946302	
H	-3.080248	-0.412860	3.341718	
C	-1.653944	0.940972	1.454271	
H	-1.494430	1.361706	2.472213	
H	-0.934241	0.058930	1.427984	
H	-1.356683	1.639051	0.653115	
				P
O	-0.032871	-0.683355	0.224193	
C	1.306170	-0.208007	0.035755	
O	1.199130	1.203384	-0.263974	
C	-0.161610	1.586930	-0.139510	
C	-0.925563	0.270953	-0.352975	
C	2.070527	-0.412882	1.345617	
C	1.970105	-0.896641	-1.162593	
H	-0.392848	2.359930	-0.902453	
H	-0.381476	2.012243	0.872969	
H	-1.066791	0.071068	-1.444838	
C	-2.287080	0.206498	0.319482	
H	2.090662	-1.981402	-0.969151	
H	1.347657	-0.763817	-2.069729	
H	2.967559	-0.453866	-1.357524	
H	2.093857	-1.487684	1.616099	
H	3.111720	-0.046560	1.246678	
H	1.569961	0.144611	2.161636	
O	-2.969115	-0.953197	-0.123543	
H	-2.121043	0.211994	1.425236	
H	-2.841125	1.146354	0.058274	
H	-3.790588	-1.028622	0.394734	
				P-2
C	-1.089490	-0.068970	-0.077343	
O	-0.344329	0.950662	-0.803044	
C	0.834390	1.393263	-0.155682	
C	1.712115	0.218073	0.302989	
C	0.851106	-0.650474	1.248306	
O	-0.527326	-0.274546	1.213809	
O	2.140354	-0.608964	-0.778550	
C	-1.076351	-1.339767	-0.940148	
C	-2.498422	0.471167	0.166592	
H	2.455871	-0.026735	-1.496171	

399	H	2.595649	0.625474	0.857179
400	H	0.618581	2.043392	0.729483
401	H	1.375373	2.023030	-0.896764
402	H	1.006060	-1.723175	0.986832
403	H	1.155456	-0.507912	2.304805
404	H	-2.442146	1.366234	0.816930
405	H	-2.963208	0.756395	-0.797143
406	H	-3.129854	-0.291811	0.664344
407	H	-1.620178	-2.163767	-0.434978
408	H	-1.568056	-1.131548	-1.911203
409	H	-0.033221	-1.646553	-1.149319
410				**B'**
411	S	-0.119975	1.380723	0.033804
412	O	-0.779785	0.781739	-1.300202
413	O	0.782243	2.476232	-0.330867
414	O	-1.138057	1.533730	1.097533
415	C	0.936754	-0.115635	0.595496
416	C	2.275033	-0.299459	-0.183970
417	F	0.166433	-1.224119	0.446309
418	F	1.197871	0.061417	1.906516
419	F	3.114426	0.733777	0.125856
420	F	2.030515	-0.207783	-1.529938
421	O	2.799512	-1.500925	0.155870
422	C	4.071092	-1.824831	-0.441018
423	H	4.338503	-2.825511	-0.057066
424	H	3.989242	-1.856603	-1.546648
425	H	4.845339	-1.088911	-0.143211
426	H	-1.722267	0.386645	-1.124309
427	O	-3.185602	-0.142917	-1.125855
428	C	-3.824422	-0.673100	-0.207761
429	C	-3.184840	-0.991140	1.121549
430	H	-3.919331	-1.278950	1.897496
431	H	-2.472662	-1.832352	0.978116
432	H	-2.577933	-0.121249	1.450206
433	C	-5.278152	-1.025495	-0.413856
434	H	-5.903458	-0.447892	0.301637
435	H	-5.589408	-0.803308	-1.450843
436	H	-5.450918	-2.097972	-0.179403
437				**B'-C'**
438	S	-0.347210	-0.698087	0.469121
439	O	0.257223	0.200591	-0.651363
440	O	-0.580162	-2.085163	0.014990
441	O	0.357962	-0.496051	1.770296
442	C	-2.042955	0.139847	0.733870
443	C	-3.113460	-0.174035	-0.355646
444	F	-1.820154	1.481194	0.773157
445	F	-2.502569	-0.262195	1.936357
446	F	-3.449761	-1.497184	-0.282873
447	F	-2.567593	0.015872	-1.600232
448	O	-4.180518	0.634312	-0.144258
449	C	-5.298117	0.446062	-1.033115
450	H	-6.055204	1.191074	-0.729226
451	H	-4.998443	0.624657	-2.086151
452	H	-5.715787	-0.576354	-0.931390
453	H	0.600811	1.765978	-0.607037
454	O	1.304848	2.475573	-0.857906
455	C	2.380651	2.294272	-0.128106
456	C	3.588775	3.029998	-0.635848
457	H	4.519883	2.634580	-0.188603
458	H	3.636685	2.970768	-1.738678
459	H	3.494625	4.098012	-0.342570
460	C	2.224069	2.085298	1.353875

461	H	1.916063	3.065477	1.780494	
462	H	1.437735	1.338836	1.593729	
463	H	3.175584	1.792280	1.835740	
464	O	2.818331	0.489625	-0.725145	
465	H	1.833284	0.199235	-0.822162	
466	C	3.464462	-0.471434	0.139284	
467	H	4.404856	-0.004986	0.501811	
468	H	2.820419	-0.721712	1.010354	
469	C	3.774899	-1.735733	-0.643265	
470	C	2.811794	-2.859005	-0.682063	
471	O	3.980186	-2.901558	0.155457	
472	H	4.478313	-1.604566	-1.491144	
473	H	1.836055	-2.771532	-0.166046	
474	H	2.827502	-3.541793	-1.553209	
475					**C'**
476	C	5.580222	-0.631876	-0.656968	
477	O	4.467586	-0.382792	0.227055	
478	C	3.265745	-0.213477	-0.362863	
479	F	3.261698	0.828018	-1.251423	
480	F	2.871397	-1.319905	-1.073036	
481	C	2.212579	0.073761	0.755198	
482	F	2.342722	-0.813321	1.756861	
483	F	2.385453	1.324029	1.227610	
484	S	0.414214	-0.055809	0.113709	
485	O	0.281517	0.796689	-1.088108	
486	O	-0.319788	0.611451	1.370759	
487	O	0.089116	-1.498581	0.065374	
488	H	6.460198	-0.762496	-0.002444	
489	H	5.411057	-1.554627	-1.247997	
490	H	5.741453	0.228246	-1.338002	
491	O	-3.399352	-0.010231	0.296159	
492	C	-3.537795	-1.417513	-0.070736	
493	C	-4.907088	-1.657250	-0.720108	
494	C	-3.159581	0.892140	-0.765931	
495	C	-3.036445	2.274613	-0.169122	
496	C	-1.951035	3.194137	-0.578698	
497	O	-1.890200	2.519372	0.700686	
498	C	-3.372092	-2.157463	1.261149	
499	O	-2.569925	-1.798508	-1.011182	
500	H	-1.685114	-1.822245	-0.572426	
501	H	-5.719857	-1.307290	-0.054065	
502	H	-4.977303	-1.124411	-1.689862	
503	H	-5.044948	-2.737065	-0.926288	
504	H	-3.470455	-3.249853	1.105593	
505	H	-2.368413	-1.937472	1.677193	
506	H	-4.131284	-1.824812	1.996608	
507	H	-2.237521	0.624682	-1.328086	
508	H	-3.997094	0.921287	-1.508807	
509	H	-3.963290	2.703642	0.256088	
510	H	-1.204891	2.843865	-1.314511	
511	H	-2.094045	4.286826	-0.502793	
512	H	-0.936050	1.393656	1.052875	
513					**C'-P**
514	S	0.670695	-1.343308	1.036496	
515	O	-0.440040	-0.248513	0.930865	
516	O	1.503678	-1.178752	2.243325	
517	O	0.136435	-2.672952	0.667952	
518	C	1.760974	-0.861364	-0.464852	
519	C	2.677142	0.383089	-0.269498	
520	F	0.932223	-0.617939	-1.525786	
521	F	2.535879	-1.926094	-0.760798	
522	F	3.591721	0.139248	0.708195	

F	1.907694	1.445524	0.189510	
O	3.260725	0.683108	-1.454023	
C	4.255628	1.723935	-1.427241	
H	4.563857	1.874079	-2.477560	
H	3.832210	2.666910	-1.023712	
H	5.131385	1.418779	-0.819361	
H	-0.779017	0.938164	1.838085	
H	-2.016082	-0.449222	0.791425	
O	-2.998888	-0.197347	0.674666	
C	-3.414985	-0.488034	-0.637933	
C	-2.620775	-1.641812	-1.255396	
H	-2.951114	-1.808426	-2.299250	
H	-1.533549	-1.435407	-1.246115	
H	-2.779459	-2.571180	-0.673453	
C	-4.923682	-0.710107	-0.642164	
H	-5.171251	-1.642961	-0.099024	
H	-5.430487	0.138832	-0.142963	
H	-5.295410	-0.786644	-1.682481	
O	-3.206856	0.732064	-1.463050	
C	-2.137737	1.494393	-1.023306	
H	-1.134369	1.001542	-1.103290	
H	-2.071194	2.391401	-1.704889	
C	-2.287515	2.113178	0.304107	
C	-1.156904	2.708440	1.059690	
O	-1.239320	1.805425	2.157008	
H	-3.300686	2.258918	0.712737	
H	-0.181923	2.671659	0.528687	
H	-1.360470	3.745271	1.402748	
				Glycidol
C	-1.679254	0.437054	0.000722	
H	-2.526942	0.461583	0.713706	
H	-1.767454	1.145238	-0.848147	
C	-0.341990	0.024038	0.472732	
O	-1.156746	-0.855305	-0.317535	
C	0.919538	0.563495	-0.157392	
H	-0.222231	-0.286552	1.531402	
O	1.968212	-0.365830	0.064665	
H	0.718488	0.735738	-1.244413	
H	1.138036	1.561992	0.304777	
H	2.778607	0.003551	-0.330739	
				Acetone
C	-0.000004	0.187324	-0.000003	
O	-0.000001	1.408730	0.000000	
C	1.295801	-0.617695	-0.002292	
H	1.300384	-1.367629	-0.821806	
H	2.160860	0.063467	-0.107398	
H	1.390417	-1.186537	0.948318	
C	-1.295799	-0.617695	0.002292	
H	-2.160870	0.063454	0.107369	
H	-1.390394	-1.186580	-0.948296	
H	-1.300374	-1.367611	0.821824	
				A-silica
S	2.802520	-0.146145	-0.072948	
Si	0.575506	-0.070273	-0.002297	
O	-0.081034	-1.230678	-1.020161	
Si	-1.779483	-1.235244	-1.080772	
O	-2.293912	-1.426043	0.517526	
Si	-1.736278	-0.285577	1.631922	
O	-2.183808	1.225402	1.019472	
Si	-1.665971	1.586979	-0.547740	
O	-2.221978	0.332510	-1.532908	
O	3.282350	-1.315994	0.676326	

O	3.241801	0.169079	-1.450572	
O	0.028853	1.433638	-0.518737	
O	-0.040788	-0.334263	1.535054	
H	-2.100287	2.920071	-1.008389	
H	-2.232389	-0.521882	3.001136	
H	-2.311043	-2.270486	-1.987508	
H	3.260964	1.942036	0.2625330	
				B-silica
C	4.099066	2.001811	-0.813242	
C	4.916244	1.217689	0.139048	
C	5.139951	-0.276377	-0.037570	
O	5.035906	-0.985122	1.179400	
O	3.552216	1.630589	0.476213	
O	2.117016	-0.457444	0.911646	
S	1.402617	-1.076824	-0.436671	
Si	-0.694732	-0.387927	-0.133409	
O	-1.641124	-0.805758	-1.455343	
Si	-3.264154	-0.316879	-1.343820	
O	-3.849682	-0.985909	0.093450	
Si	-3.006097	-0.592907	1.504449	
O	-2.976742	1.096111	1.580255	
Si	-2.339545	1.898109	0.236604	
O	-3.221014	1.355705	-1.099230	
O	1.443784	-2.543959	-0.316581	
O	1.961226	-0.379537	-1.625814	
O	-0.767761	1.283321	0.033500	
O	-1.399343	-1.067903	1.228554	
H	2.581692	0.442169	0.671000	
H	4.272819	3.086508	-0.929283	
H	3.631805	1.483566	-1.670145	
H	4.444318	-0.659678	-0.821333	
H	6.174507	-0.417298	-0.423195	
H	4.076049	-1.083941	1.361703	
H	5.664222	1.745366	0.761077	
H	-2.354766	3.367064	0.379318	
H	-3.581572	-1.213094	2.713272	
H	-4.054976	-0.706513	-2.527020	
				B-C-Silica
S	0.678303	-0.259637	-0.547513	
O	0.938328	-0.155846	-2.008572	
O	0.972192	-1.675568	0.017690	
O	1.315939	0.809075	0.316083	
O	2.941943	-1.993577	1.596238	
C	4.089886	-1.728051	0.746887	
C	3.862800	-1.855357	-0.772486	
O	3.186477	-3.041355	-1.100996	
C	3.944219	-0.415558	1.402414	
O	5.378170	0.769452	0.553595	
C	5.157923	1.894753	0.067202	
C	3.883482	2.655699	0.304003	
C	6.221348	2.522052	-0.798140	
H	2.072813	-1.828740	1.023314	
H	4.352839	-0.281617	2.413909	
H	3.104805	0.219668	1.068011	
H	6.499860	3.518952	-0.394652	
H	7.112100	1.871573	-0.868029	
H	5.802314	2.702589	-1.812310	
H	2.992754	2.061984	-0.018728	
H	3.748528	2.813420	1.395631	
H	3.880090	3.636845	-0.205370	
H	3.334139	-0.951047	-1.155377	
H	4.865867	-1.871587	-1.253572	

H	2.233729	-2.842934	-0.932709	
H	4.932786	-2.352949	1.101499	
Si	-1.500561	-0.030279	-0.203706	
O	-1.933856	-0.306101	1.403810	
O	-2.439247	-1.071030	-1.141478	
O	-2.006605	1.536475	-0.575151	
Si	-3.577608	-0.111889	1.754107	
Si	-4.112592	-0.920247	-0.942858	
Si	-3.653309	1.842794	-0.338752	
O	-3.976395	1.461378	1.277718	
O	-4.410827	-1.144955	0.706847	
H	-3.890018	-0.370053	3.174559	
O	-4.482810	0.698271	-1.266729	
H	-4.874416	-1.858609	-1.791495	
H	-4.028476	3.230399	-0.679270	
				C-Silica
O	0.843913	-3.156681	-0.953742	
O	1.723951	-1.323784	0.629285	
O	1.685691	-0.955224	-1.945954	
O	2.271132	1.830418	-1.577329	
C	3.049974	2.313788	-0.491965	
C	3.066996	1.313399	0.667824	
C	2.371543	3.632703	-0.078474	
O	0.992248	3.408417	0.153710	
O	3.585957	0.073349	0.160916	
C	3.206235	-1.114311	0.785800	
C	3.370763	-1.104057	2.307996	
C	3.973513	-2.244577	0.102561	
H	2.369816	0.852106	-1.649712	
H	2.028470	1.189051	1.042152	
H	3.708720	1.694858	1.495432	
H	4.424525	-0.868157	2.558607	
H	2.710588	-0.348666	2.775703	
H	3.112322	-2.094670	2.728199	
H	3.840873	-2.183100	-0.994563	
H	5.053527	-2.141537	0.326933	
H	3.617768	-3.228892	0.460740	
H	2.829416	4.042898	0.848624	
H	2.541543	4.380100	-0.893526	
H	0.757968	2.747518	-0.540523	
H	4.105363	2.513967	-0.808134	
S	1.019196	-1.695620	-0.839570	
Si	-0.916416	-0.715816	-0.280110	
O	-2.048289	-0.923218	-1.499709	
O	-0.725699	0.933216	-0.043104	
O	-1.554723	-1.373314	1.123061	
Si	-3.559961	-0.209691	-1.177623	
Si	-2.153196	1.764340	0.381414	
Si	-3.034975	-0.688479	1.605045	
O	-4.075574	-0.876930	0.287526	
O	-3.244276	1.419112	-0.865322	
H	-4.522034	-0.415915	-2.277100	
O	-2.744645	0.968620	1.751680	
H	-1.936417	3.207113	0.582963	
H	-3.557548	-1.295212	2.844563	
				C-P-Silica
O	-1.232230	0.746558	0.448696	
O	-0.778669	-1.622118	1.192744	
O	-0.930441	-1.084737	-1.281885	
H	-2.672181	0.841957	-0.142654	
O	-3.598973	0.799656	-0.575110	
C	-5.751005	0.074232	0.283107	

C	-4.616217	1.163103	0.318601
H	-4.220105	1.255479	1.357871
C	-5.196878	2.530378	-0.097909
H	-5.647932	2.405054	-1.118076
H	-6.013823	2.835318	0.593965
O	-4.209901	3.529257	-0.059911
H	-3.460758	3.176199	-0.584641
H	-6.081997	-0.227729	1.297726
H	-6.632091	0.414315	-0.294176
O	-5.297149	-1.084231	-0.461733
C	-4.261152	-1.772058	-0.076575
C	-3.598516	-2.567413	-1.116017
H	-2.611449	-2.024567	-1.295743
H	-3.310116	-3.574228	-0.755860
H	-4.176050	-2.599829	-2.056870
C	-3.780463	-1.814947	1.316097
H	-3.863309	-2.865700	1.671933
H	-2.663748	-1.624471	1.345152
H	-4.307174	-1.141867	2.013272
S	-0.585349	-0.593208	0.103489
Si	1.586868	-0.167250	0.050380
O	1.974479	1.039264	-1.064220
O	2.476132	-1.531900	-0.391874
O	2.201122	0.340717	1.538358
Si	3.618736	1.410711	-1.190995
Si	4.149994	-1.311771	-0.479983
Si	3.859716	0.670546	1.566881
O	4.130123	1.830486	0.365516
O	4.403842	-0.039618	-1.565354
H	3.887785	2.473097	-2.181467
O	4.630722	-0.739544	1.037097
H	4.866351	-2.542497	-0.873090
H	4.330697	1.109403	2.896458

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