

**Z-isomerization of retinoids through combination of monochromatic photoisomerization
and metal catalysis**

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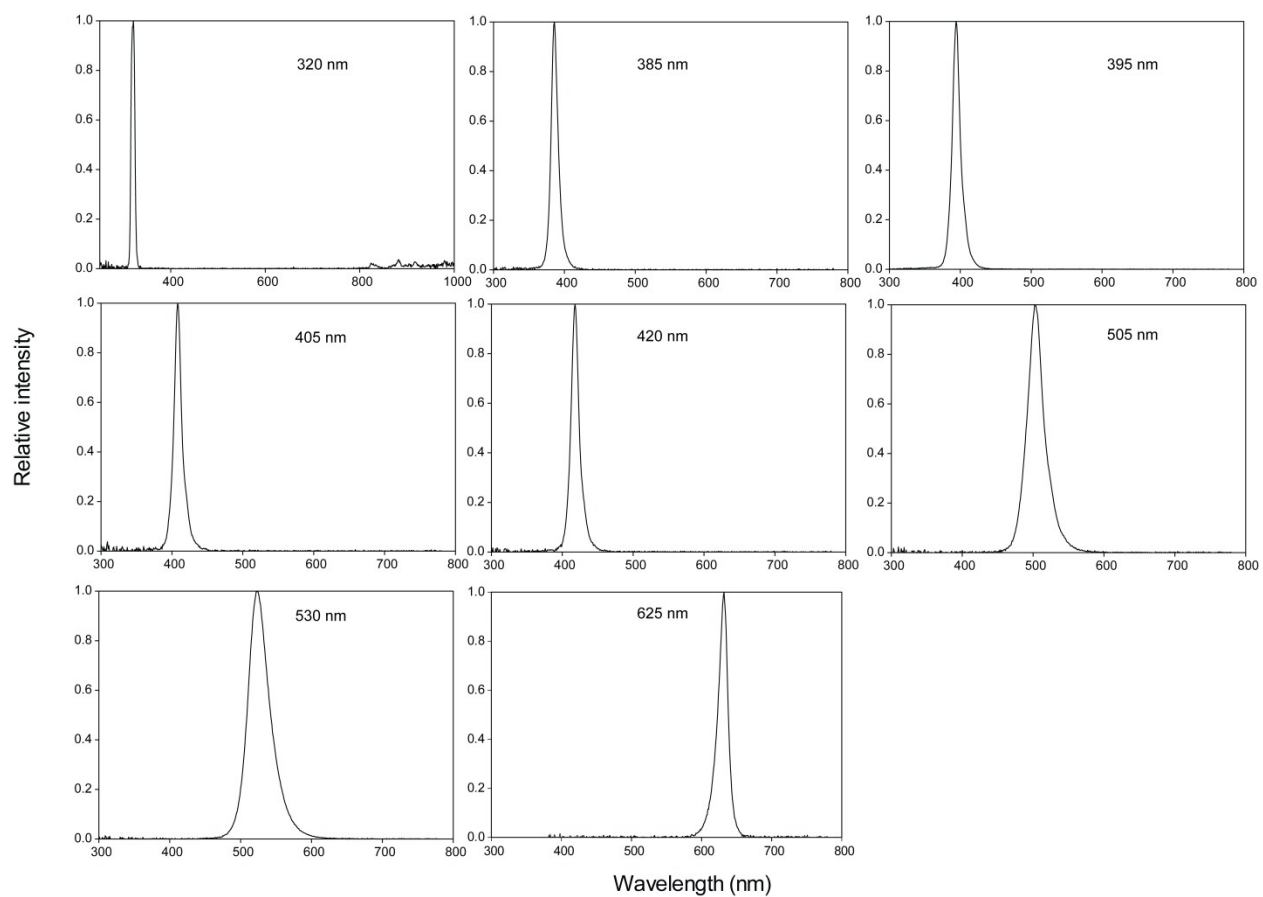


Figure S1. Emission spectrum of the screened UV wavelength (320, 385, 395, 405, 420, 505, 530 and 625 nm)

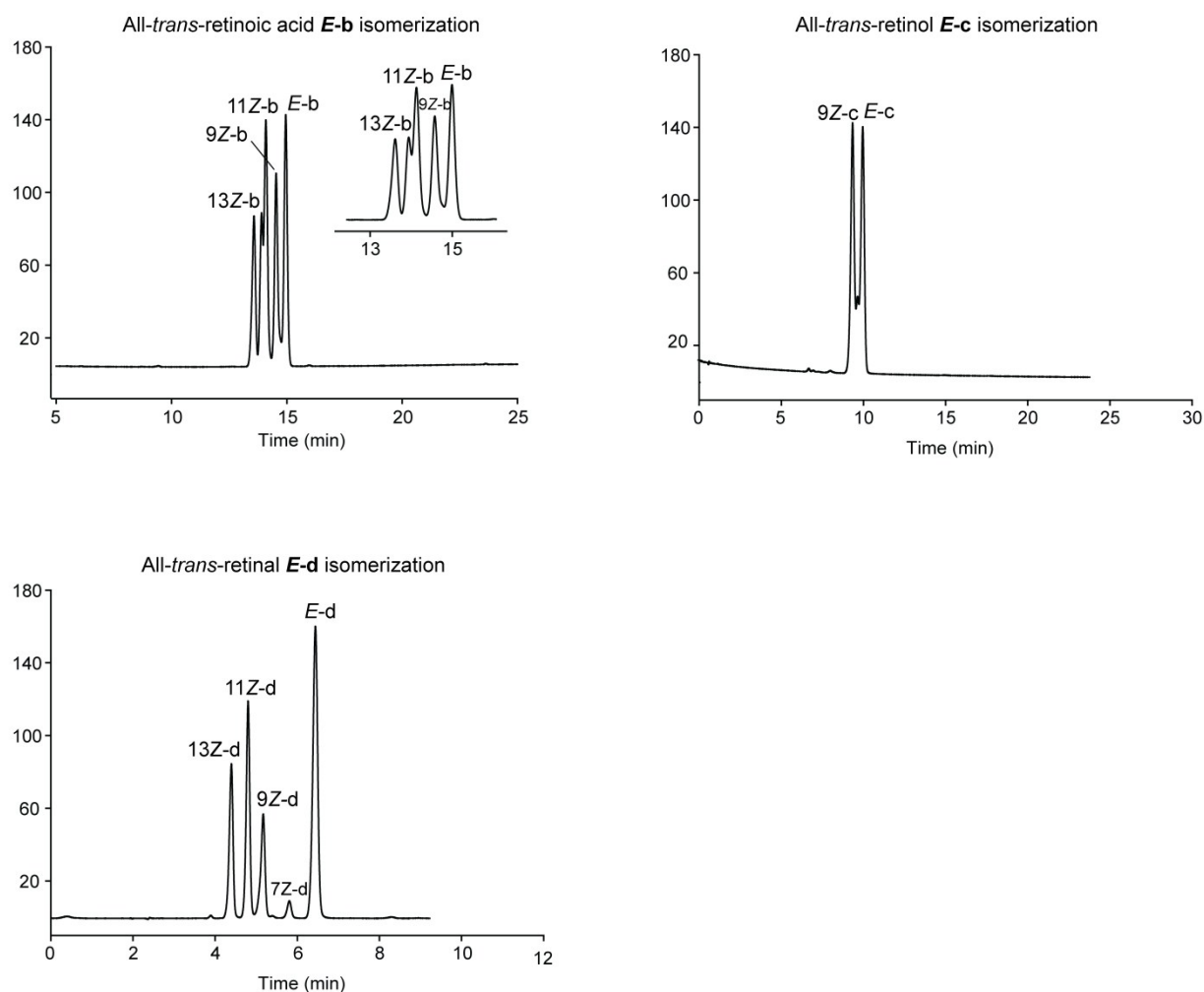


Figure S2. Representative HPLC chromatograms of a mixture of all-*trans*-retinoic acid **E-b**, all-*trans*-retinol **E-c** and all-*trans*-retinal **E-d**, obtained following irradiation treatment. **9Z-b**, **9Z-c** and **9Z-d** represent the 9-*cis* isomer, **7Z-d** represents the 7-*cis* isomer, **13Z-b** and **13Z-d** represent the 13-*cis* isomer, and **11Z-b** and **11Z-d** represent the 11-*cis* isomer.

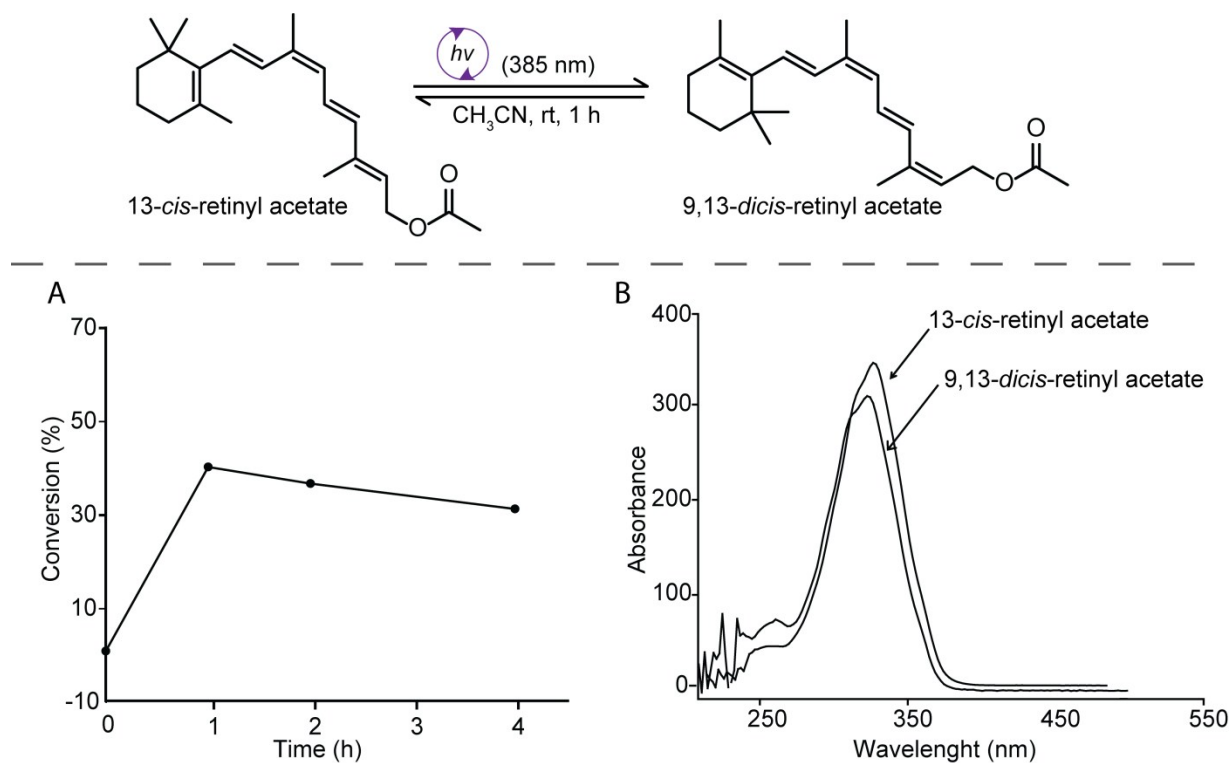


Figure S3. The relationship between the distribution of *cis*-retinyl acetate isomers. A) Time course of the reaction from 13-*cis* to 9,13-*dicis*. B) Absorbance spectra of 13-*cis* and 9,13-*dicis* isomers.

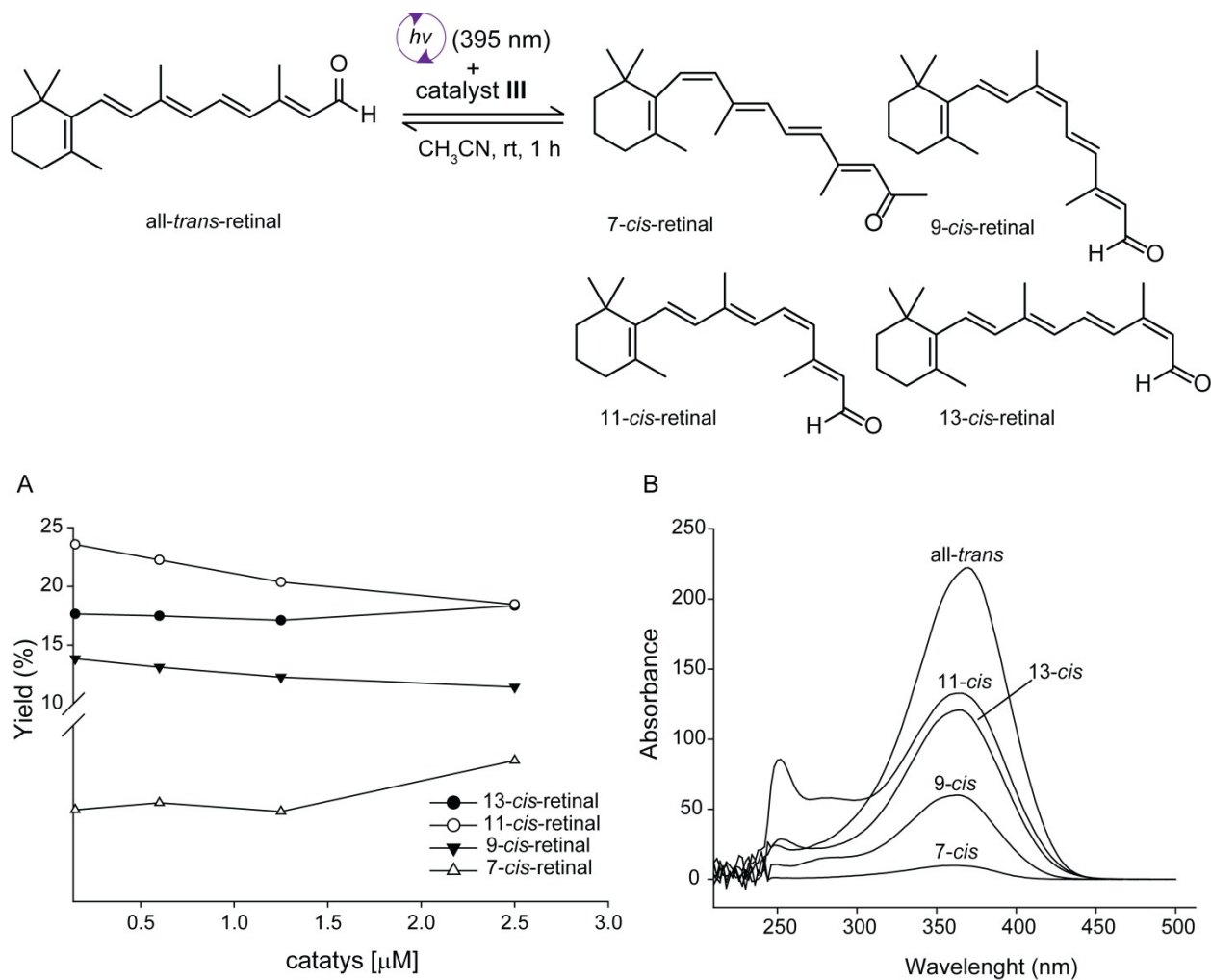


Figure S4. A) Catalyst **III** effect on the distribution of *cis*-retinal isomers. B) Absorbance spectra of all isomers.

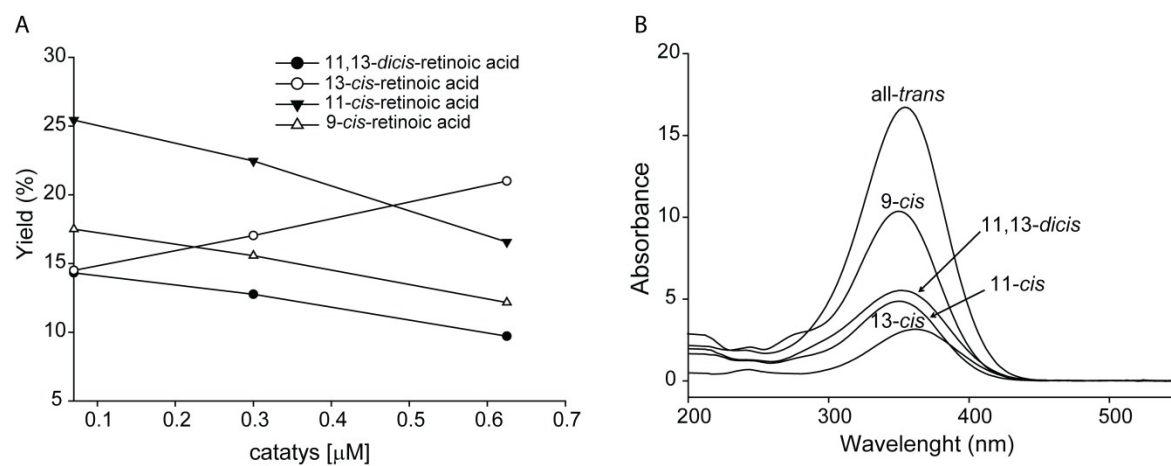
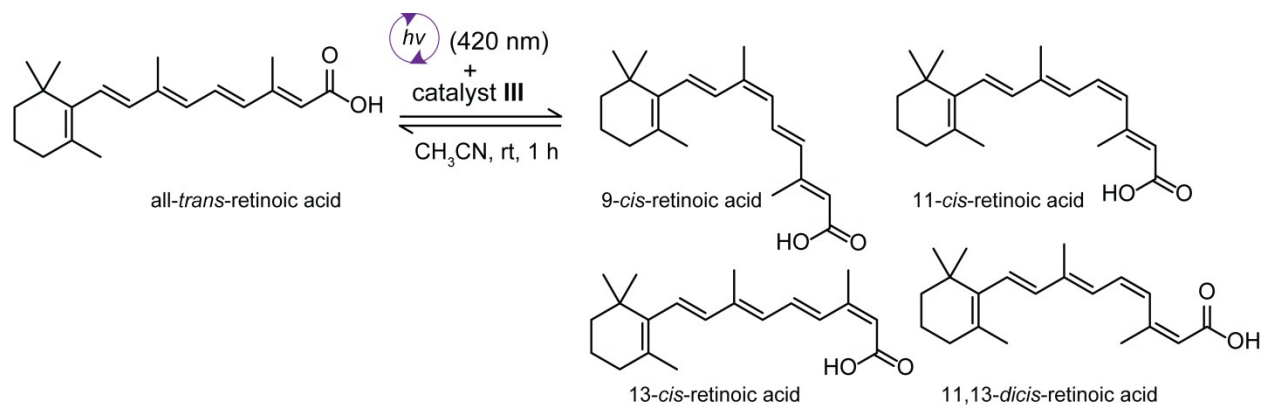
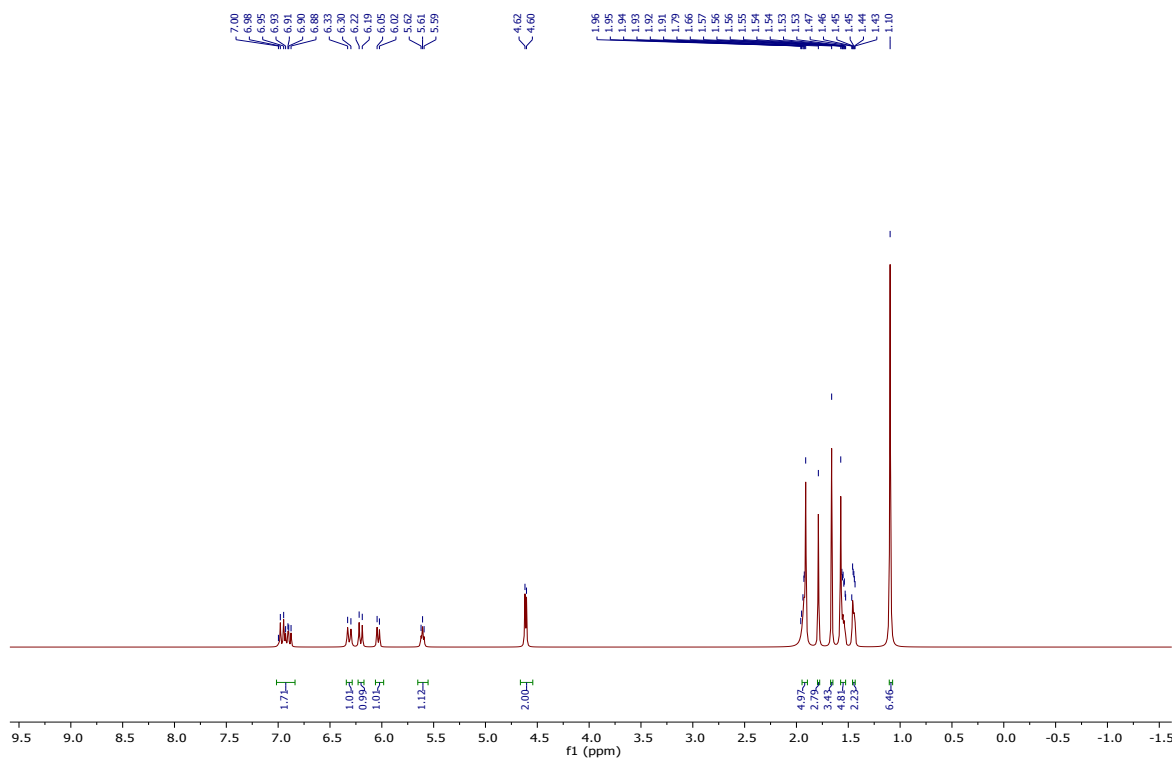
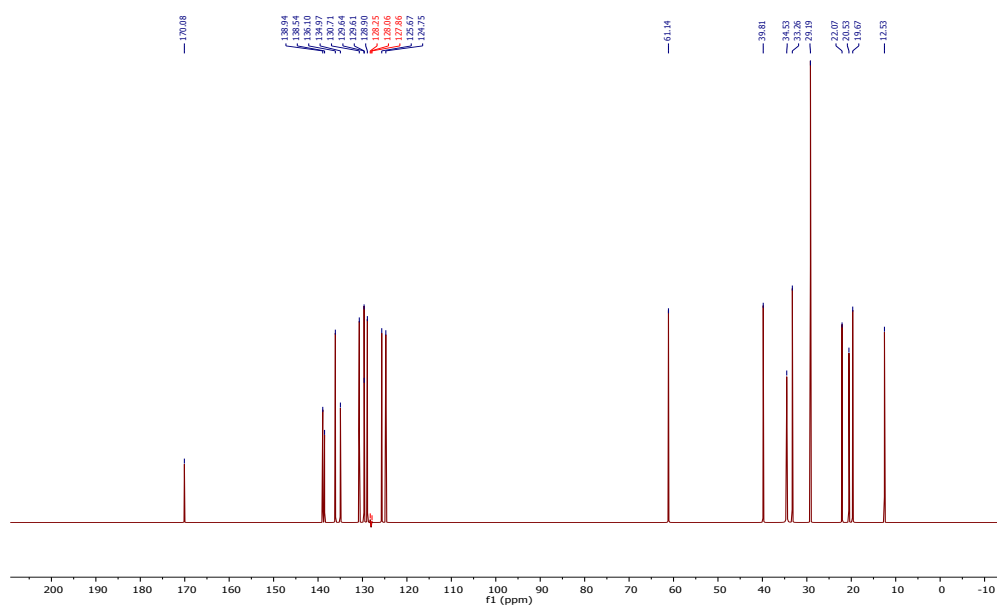


Figure S5. A) Catalyst III effect on the distribution of *cis*-retinoic acid isomers. B) Absorbance spectra of all isomers.

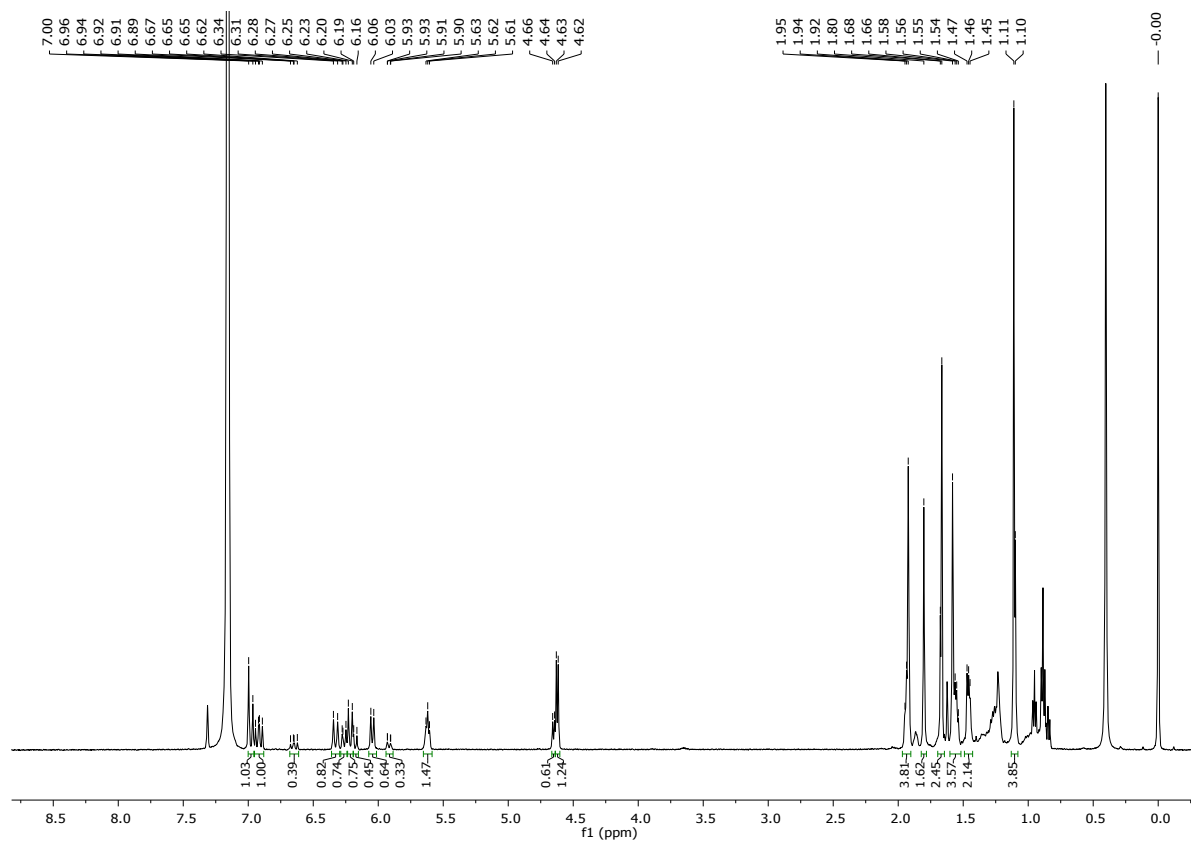
9-*cis*-retinyl acetate **9Z-a**- ¹H-NMR



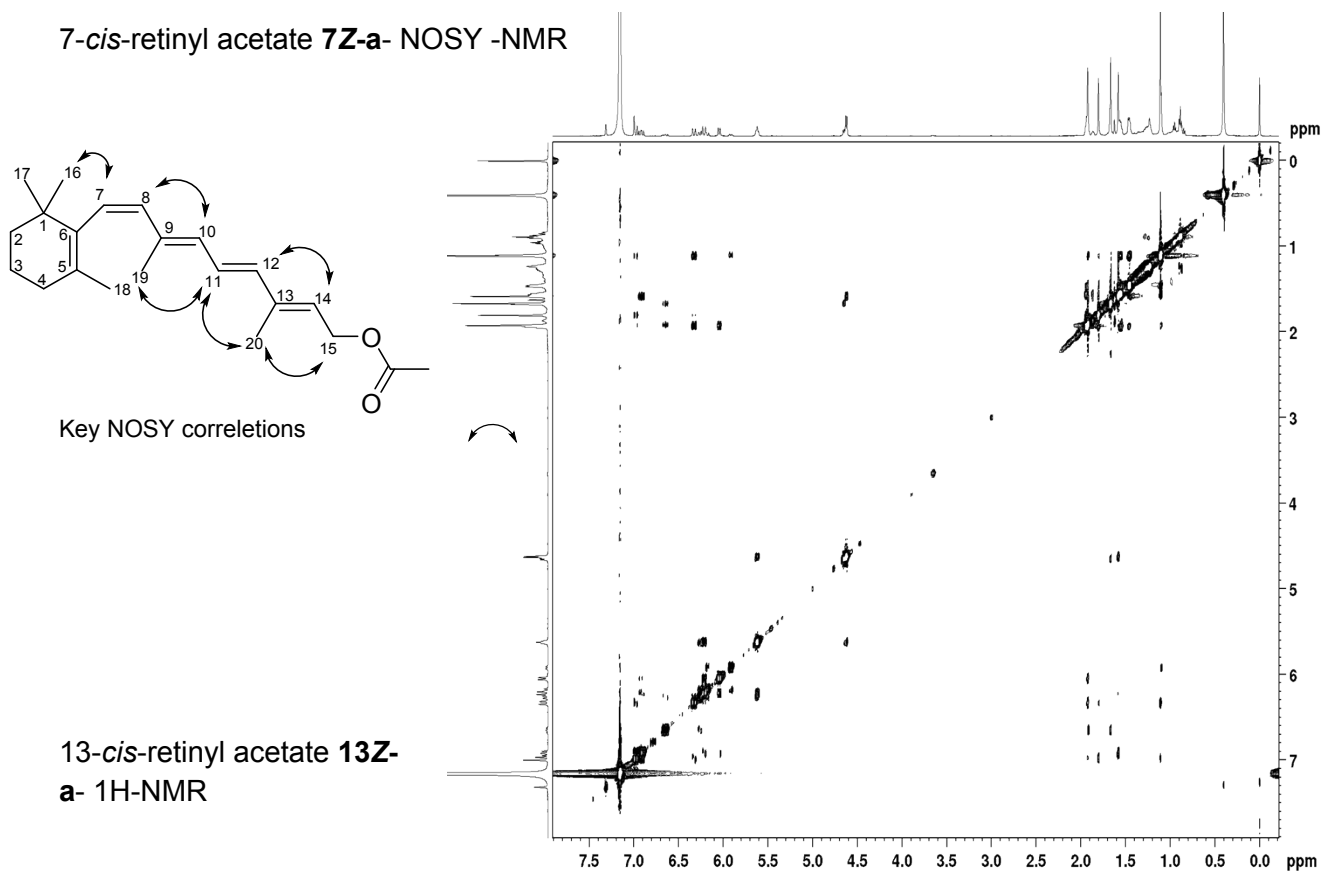
9-*cis*-retinyl acetate **9Z-a**- ¹³C-NMR



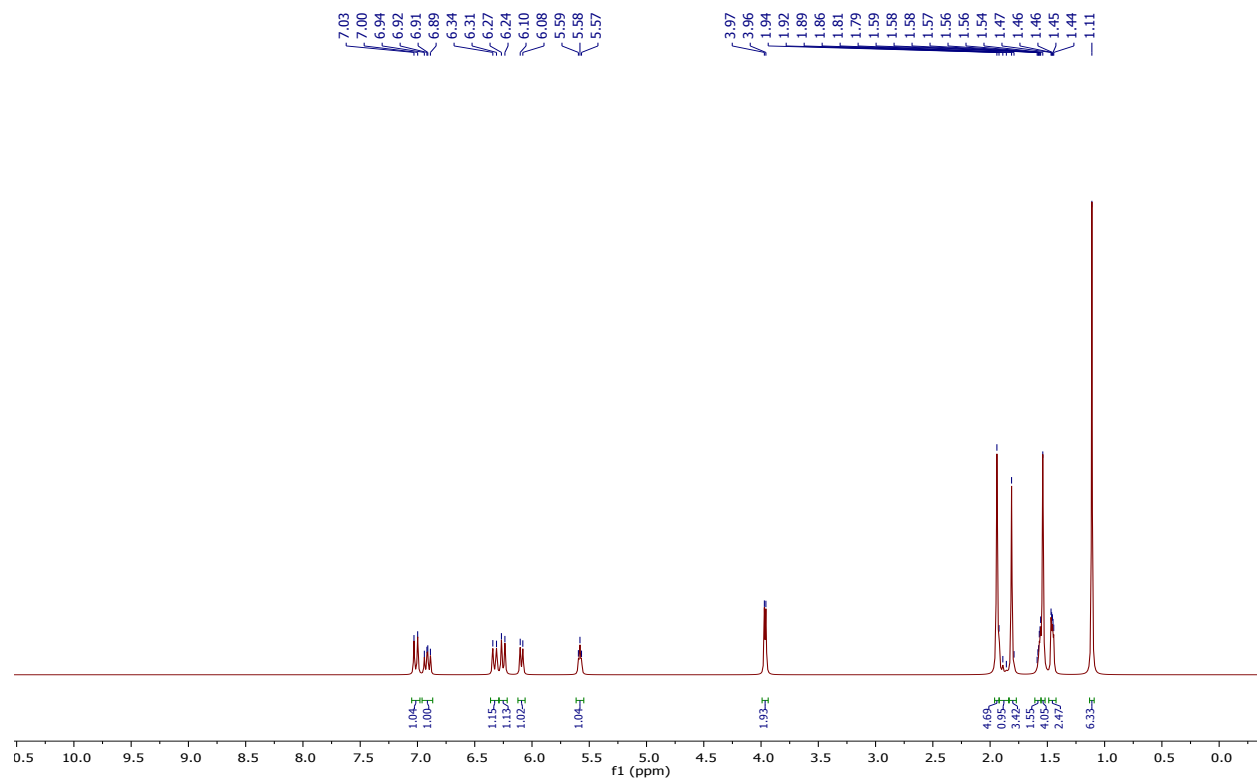
7-*cis*-retinyl acetate **7Z-a**- ¹H-NMR



7-*cis*-retinyl acetate **7Z-a**- NOSTY -NMR







9-*cis*-retinal **9Z-d** ¹H-NMR

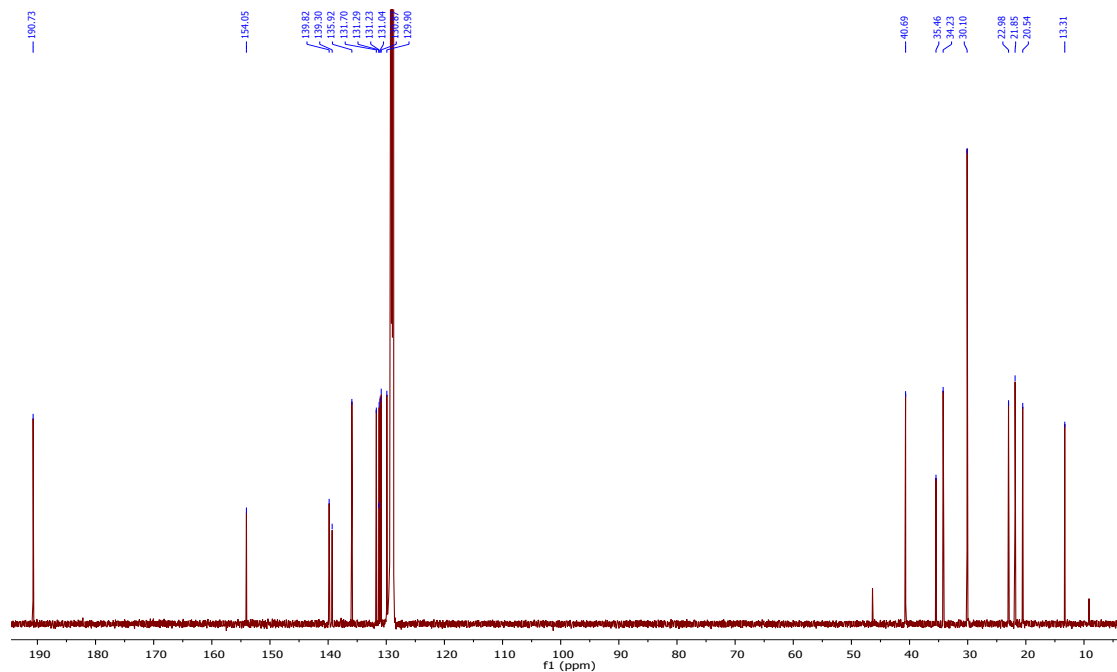
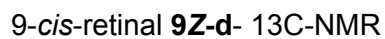


Table S1. Relative energies of key intermediates in the *E/Z* isomerization of retinyl acetate **E-a** and retinal **E-d**. All energies are relative to the all-*trans* isomer and are given in kcal/mol.

Isomer	Retinyl acetate (E-a)	Retinal (E-d)
7- <i>cis</i>	3.8	4.9
9- <i>cis</i>	0.4	1.1
11- <i>cis</i>	5.0	5.7
13- <i>cis</i>	0.0	0.7
T1-all- <i>trans</i>	34.1	29.0
T1-7- <i>cis</i>	32.2	28.8
T1-9- <i>cis</i>	32.9	30.9
T1-11- <i>cis</i>	30.2	27.2
T1-13- <i>cis</i>	33.0	29.6
MECP-7- <i>cis</i>	38.3	38.0
MECP-9- <i>cis</i>	37.4	38.4
MECP-11- <i>cis</i>	39.8	37.3
MECP-13- <i>cis</i>	39.1	41.6
T ^{TS} -7- <i>cis</i>	36.2	38.3
T ^{TS} -9- <i>cis</i>	37.9	38.1
T ^{TS} -11- <i>cis</i>	38.7	38.6
T ^{TS} -13- <i>cis</i>	41.3	41.7

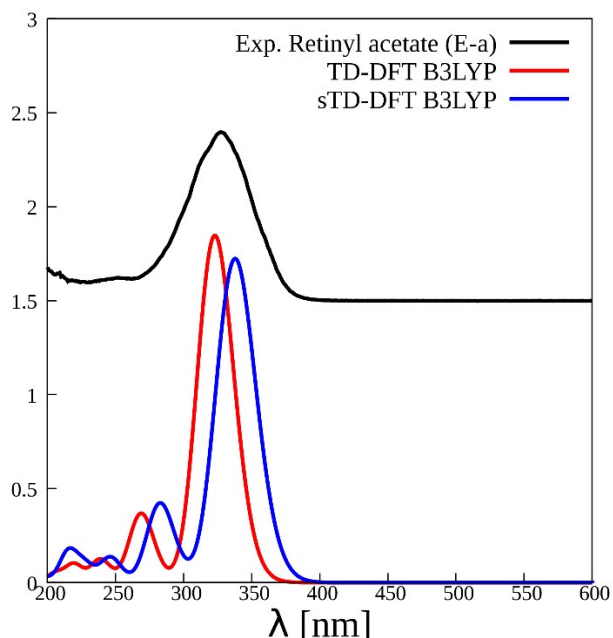


Figure S6. Comparison of computed UV-Vis spectra of retinyl acetate **E-a** using two methods: TD-DFT (red) and sTD-TDF (blue). Experimental spectrum is given in black for reference. Calculated spectra were shifted uniformly by -30 nm to match experimental spectrum visually.

Cartesian coordinates

acetate_all_trans.xyz

C	1.80741391495912	2.72702421465758	1.28064562728124
C	0.48146393394764	2.43715719567247	1.34390021294061
H	2.49248500490877	1.99724181935786	1.70461463459238
C	2.41778298625291	3.86741712861820	0.65721887963365
H	1.76226142063543	4.59645795577960	0.19953180750323
C	3.75232127760939	4.05141631820905	0.56012529382721
H	4.41098463966579	3.32021524139655	1.02126807921953
C	4.40495531768196	5.12385752178792	-0.17342172890832
C	5.75111548794767	5.14105943989787	-0.24785324408617
H	6.29874984013205	4.37924654638963	0.29878648334750
C	6.58371932417189	6.08243978729759	-1.04587283949326

O	7.15795130000596	7.08602723836880	-0.15860516708977
H	7.40691262037998	5.55853511193361	-1.53502063420330
C	3.52880511635922	6.15140086677868	-0.83588254834467
H	2.84595513686142	5.68122305094358	-1.54798236163826
H	2.91460452049820	6.66141892307675	-0.08966107277512
H	4.10231284583327	6.90826547311471	-1.36379701467812
C	-0.58996712547859	3.35329389395743	0.82149381262690
H	-1.16841524174529	2.86319735636929	0.03413152914080
H	-1.29329325088165	3.61355269119481	1.61648571637312
H	-0.19061123494212	4.27935228704433	0.41688034480531
C	0.06992346444721	1.15961037945924	1.89946184890429
H	0.87077764967891	0.49962046437101	2.21916629227014
C	-1.19618587935895	0.72381289832104	1.99777749585631
H	-1.99441688478641	1.40394148421474	1.71857574589898
C	-1.26678285183008	-1.73025816188316	1.78234051567013
C	-1.74944487317970	-3.10743746223314	2.17097746295997
C	-2.44836690077606	-3.18070764506141	3.52361220632861
C	-3.34217298173573	-1.96426147563597	3.70852715963212
C	-2.54918549349394	-0.64940179955542	3.67026235112952
C	-1.62670087676306	-0.61346142348159	2.44216878166017
H	-0.90315912645696	-3.80214069902785	2.13589158546458
H	-2.43247826913096	-3.45252687426505	1.38267935399547
H	-3.03261235860231	-4.10085566143547	3.60037102767027
H	-1.70355995022186	-3.21799034322347	4.32249393624242
H	-3.88970308323412	-2.02336366513486	4.65320236761577
H	-4.09086879473773	-1.94489013831284	2.90834260015260

C	-0.42841288391086	-1.74379522672156	0.53245613171614
H	-0.94505596897625	-2.31194009982009	-0.24908945178866
H	-0.20679994348121	-0.75039479329378	0.15310319366349
H	0.52205878185322	-2.25742613974800	0.70909114057551
C	-1.69573896787527	-0.50793487435693	4.94385118022261
H	-1.14936344024969	0.43662626263311	4.93882188980815
H	-2.33741848122661	-0.52816932037587	5.82941547620316
H	-0.96452196117861	-1.31137398297515	5.03045848637735
C	-3.55206890174076	0.51328180394894	3.64864918019560
H	-4.25956000662321	0.40207483489147	4.47334420038549
H	-3.05590296070719	1.47755449210953	3.76832461264848
H	-4.12345211180415	0.53166551681686	2.71799200231708
H	6.02185644841235	6.59967793755045	-1.82010951045816
C	7.97000233673973	7.98654255103712	-0.74746263618976
O	8.22065710345022	7.99009557477081	-1.92712667936139
C	8.51669153582496	8.96328370775701	0.25950800364708
H	9.07097525701036	9.74280499840689	-0.25660515896123
H	7.70805329299540	9.39672330007894	0.84871875166170
H	9.17855201986620	8.43578923332810	0.94954472281153

acetate_cis7.xyz

C	2.15593878731766	1.84973677789394	1.59944888104652
C	1.05931908598295	1.33186286089363	2.20475220980900
H	1.99805894653637	2.51950387202353	0.75820473900625
C	3.52778121676056	1.52730853444619	1.88664528002641

H	3.72473365084321	0.69651568313972	2.55499549697383
C	4.55915111168155	2.17101128411466	1.30183406842330
H	4.32511135000992	3.02826550390232	0.67643846435203
C	5.97057052295650	1.83103015337029	1.37860543089783
C	6.85217080133569	2.72655032967057	0.89849067631507
H	6.45657351598577	3.65696531094220	0.50273902807948
C	8.33071939849550	2.62714699577042	0.80576414107347
O	8.66254145179395	2.99708401646686	-0.55890292385454
H	8.83669295933014	3.32486429244068	1.47747534840066
C	6.35450466280502	0.49366912125369	1.95213150655229
H	6.27193161803656	0.48793113808952	3.04267780557825
H	5.68879622080476	-0.28338496465368	1.57386186877321
H	7.37531718339045	0.21753437506132	1.69469083994532
C	1.17143819868885	0.52826514987889	3.47608374528820
H	0.25010047686012	0.59468570289808	4.04888272529816
H	1.36813682876507	-0.53130289842760	3.29904956468362
H	1.98124958800507	0.91825666349224	4.09309106446081
C	-0.23991099678729	1.62985736230384	1.61535845144093
H	-0.25763503001041	2.54197383557069	1.02501863663805
C	-1.38837998371351	0.92873926915383	1.65780040729202
H	-2.24063328769437	1.40349979857006	1.18217009403361
C	-0.88139857397595	-1.46788054176236	1.96180008460106
C	-1.03970342958468	-2.78831236205219	2.67366591012971
C	-1.89242041174306	-2.69372350038527	3.92923813416918
C	-3.15882158451023	-1.92428978271437	3.59935463447823
C	-2.87075207225620	-0.47331258194020	3.17380567407763

C	-1.64007914697510	-0.39297394039130	2.25324312836429
H	-0.03947415673396	-3.16689118770170	2.91555745135137
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H	-3.85023090340182	-1.91360109649443	4.44628376325722
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H	0.01917665645860	-2.36846895033491	0.25445834821034
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C	-2.64678868374840	0.39837293855279	4.42009723073908
H	-2.38675476892268	1.42014782603153	4.14107251205906
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H	-1.83750140336958	0.00651539956368	5.03886453324255
C	-4.12177952683285	0.03740748182445	2.43291514328159
H	-5.00544299970151	-0.14061705465521	3.05063368561339
H	-4.07770588253469	1.10592554686464	2.22060911573923
H	-4.25627786283793	-0.49408862372205	1.48886748635976
H	8.72088952235785	1.63120977207632	1.01348037811752
C	9.93337398926976	3.36217133115189	-0.81793481661723
O	10.81961227488725	3.34061402107187	-0.00286390422330
C	10.06714121587703	3.80216964615299	-2.25258805950194
H	11.09780829965131	4.07827606493940	-2.45858621843968
H	9.74934784409570	2.99935133401480	-2.91915425003546
H	9.41065475032973	4.65332633410245	-2.43760113200037

acetate_cis9.xyz

C	2.12427708520592	2.15337994283015	0.89244187841562
C	0.78522621979884	1.94108084878905	0.87684314817753
H	2.48031203977954	3.07181507191776	0.43375800479988
C	3.15961073615416	1.33426344624953	1.46369141257116
H	2.89314401012437	0.38511372652291	1.91256835233873
C	4.44691700582607	1.73499726989039	1.46150447401133
H	4.66477516708675	2.70139201932625	1.01565589430227
C	5.60854110636502	1.02302704817447	1.96367534590233
C	6.79659762282285	1.64611085457657	1.84643927862426
H	6.79549156499968	2.64435901244861	1.42384941827399
C	8.16062681584456	1.14085201308017	2.15344114145818
O	8.94447861726308	1.08131711198897	0.92338423979564
H	8.68047176013396	1.79935930233367	2.85054514742184
C	5.41027015492164	-0.34820160026769	2.54894026141849
H	4.71570529389250	-0.30974501778990	3.39213228946523
H	4.97313174887880	-1.02121865885556	1.80725449356007
H	6.33876794531495	-0.78822317322761	2.90546959735413
C	-0.11149734174803	2.98022647689083	0.26217007240873
H	-0.74687725139190	2.54869614141505	-0.51609454852719
H	-0.77962528501402	3.42197456498320	1.00783117249700
H	0.47563609976385	3.78381562905909	-0.18119325663111
C	0.17151450512190	0.75875520581628	1.45283298190787
H	0.83291571653220	-0.02161857334893	1.81161969651417

C	-1.14852077189636	0.56443285925132	1.58370807004604
H	-1.82199766314801	1.35591822104382	1.27267067568434
C	-1.72649890389834	-1.83455851043728	1.61920321275944
C	-2.38019747010687	-3.05342602356042	2.22559033227283
C	-2.80939356041903	-2.87271699836554	3.67679370808068
C	-3.46080943650137	-1.50823369047029	3.85595597738800
C	-2.50358084016527	-0.35404212258382	3.52301311783906
C	-1.78079405707958	-0.62083421050422	2.19312322761024
H	-1.69863425536348	-3.90523371184014	2.12946107979278
H	-3.25173925268216	-3.31450852925203	1.60993318042470
H	-3.50022992362268	-3.66694524947947	3.96972974414203
H	-1.94069722855619	-2.96157426528639	4.33449415489418
H	-3.83024788053502	-1.38259843014050	4.87758666648220
H	-4.33020855417573	-1.44148670213459	3.19303670428561
C	-1.08394748894243	-2.10673032861824	0.28493366589975
H	-1.80259947606272	-2.60078221583304	-0.37785045856801
H	-0.72067497741860	-1.20584942377128	-0.20228343400163
H	-0.24131037808708	-2.79746435878541	0.39118236882482
C	-1.44976022240904	-0.18177266228897	4.63338035275908
H	-0.73973837327505	0.60215573654917	4.36718201127109
H	-1.93284737459871	0.10498761625006	5.57157863045446
H	-0.88418552515769	-1.09855919889564	4.80038940034953
C	-3.32347860578993	0.94515633038690	3.45857609730865
H	-3.91997245333203	1.04528156189447	4.36801865462723
H	-2.68184525580346	1.82437143180937	3.38813031103130
H	-4.00666861282741	0.94591482814543	2.60626726861769

H	8.17518907517928	0.12308728184944	2.53263232941227
C	9.44521178989790	2.24928630553636	0.47395965632928
O	9.32700355173127	3.29891905112508	1.05595304014989
C	10.12835230610309	2.08632034428449	-0.85887956238159
H	10.97612885336524	2.76549344094185	-0.91592173010236
H	10.44330772824626	1.06012082195923	-1.03545652790780
H	9.41607145265447	2.37183894241702	-1.63679803983600

acetate_cis11.xyz

C	2.02864467859831	2.66901182242621	1.83718646448287
C	0.71268211122828	2.37633927301780	1.66013059307164
H	2.63478798802231	1.87834308483414	2.25479029550010
C	2.67498281501987	3.92500786683478	1.55563734835190
H	2.01385597836714	4.78024187444270	1.46909819305715
C	3.98846265787633	4.20909879155423	1.38494965875933
H	4.22066409838142	5.25680691437207	1.22213580073146
C	5.15175820956407	3.34089848518656	1.27237395744841
C	6.33432351453810	3.91408976671854	0.96702598899472
H	6.36520555588874	4.99162477768759	0.84488187010241
C	7.59799953635717	3.18139671009533	0.66606573885728
O	7.52116473748304	2.75905187078044	-0.73013504322856
H	8.47333831140048	3.82001247682634	0.78450425628410
C	5.01131689664199	1.85053162143822	1.41167829002688
H	4.74459575369993	1.57587927908325	2.43452661853630
H	4.22121801152899	1.47789329759645	0.75993011817060

H	5.92805115142642	1.32916891959901	1.15083110071094
C	-0.27732996162213	3.33260612276865	1.06055377705474
H	-0.74738072466446	2.89667859149706	0.17542136208055
H	-1.07844698680598	3.55145078300191	1.77130784285500
H	0.17974046496450	4.27087050909421	0.75825780693510
C	0.24436424748565	1.06928976376230	2.07306759650562
H	0.96381616759002	0.48212144839726	2.63007310468168
C	-0.98679312563716	0.56309659383585	1.86564374490262
H	-1.70041832508993	1.18933028009125	1.34480021121984
C	-0.75516792069231	-1.82042007728876	2.52532484114767
C	-1.24593844824630	-3.03947526825306	3.26656935720050
C	-2.49295307227465	-2.77224588627501	4.09462169676039
C	-3.50060155776605	-2.04265841493876	3.22443017277267
C	-2.99577131256421	-0.66201790965524	2.76892004248074
C	-1.50578523460825	-0.70625636632824	2.37906938538103
H	-0.43118447223145	-3.40435611979167	3.90176309610416
H	-1.43684046491597	-3.84773127689505	2.54807643280592
H	-2.91163313874492	-3.70598537230214	4.47714268429991
H	-2.23368064050709	-2.16217782001918	4.96449551799626
H	-4.45562576507511	-1.91297845489363	3.73980784135547
H	-3.70278053076045	-2.65610146424541	2.33996508368776
C	0.63413978102501	-1.99231151199205	1.97506783134463
H	0.73522713408248	-2.99813580415806	1.55529990222966
H	0.87274596362039	-1.26788263762266	1.20067273828309
H	1.39269844572338	-1.91099173596923	2.76123935597161
C	-3.20090772929704	0.37039296068072	3.89140344993440

H	-2.87955936581168	1.36305768146251	3.57273467691689
H	-4.25617346555125	0.43032772783771	4.16964627455077
H	-2.62476239608779	0.10858319393194	4.78026740341144
C	-3.85769651943023	-0.25381170592318	1.55933151032783
H	-4.91369219047247	-0.36648349967030	1.81808554803257
H	-3.70691020081876	0.78381601028217	1.25949640753926
H	-3.64973784380457	-0.89199442914349	0.69867874780000
H	7.75132765768414	2.29661983846870	1.28186776472175
C	8.44419408392708	1.87669532139315	-1.15700387639348
O	9.35951928635480	1.47684324094618	-0.48287289121485
C	8.15197832396919	1.44086314768426	-2.56986913459208
H	9.04530035520274	1.00101373774434	-3.00609144384554
H	7.36249602530470	0.68590045571262	-2.54937175689706
H	7.79401721552348	2.27609267627867	-3.16996923120608

acetate_cis13.xyz

C	1.80228295932451	2.77443603665299	1.27212778301156
C	0.48388718585916	2.44216845345009	1.30978307071607
H	2.50204323445206	2.05020068008673	1.68157705476312
C	2.39534778634526	3.95448500871851	0.70838365722266
H	1.73358079015537	4.74352319244884	0.37512473856373
C	3.72790782196102	4.11049887206157	0.54256061995471
H	4.36803970581015	3.29748982747805	0.86446132690974
C	4.37278238501813	5.26316258405076	-0.06153763428770
C	5.68934356070017	5.30082274015897	-0.35104541845057

H	6.08229304006772	6.19986692840062	-0.81540072865113
C	6.69625477984763	4.22267966372368	-0.15577977443926
O	7.13180155827122	3.79777848928131	-1.47795268381621
H	7.57423456504944	4.58753455118445	0.38203962359559
C	3.51952181808075	6.46159877027800	-0.39038217645088
H	2.73026235154188	6.19857342867423	-1.09881799284347
H	3.03054094628755	6.85826797001675	0.50326673853909
H	4.11994085893783	7.25417160640920	-0.83513065382904
C	-0.60458713616393	3.32538771550770	0.76852044828920
H	-1.13987944180658	2.82974880783680	-0.04531175233432
H	-1.34009767810826	3.54619122501356	1.54592158419777
H	-0.22469984231270	4.26951601568755	0.38761763386746
C	0.11065728156159	1.16013617058068	1.87555370097962
H	0.91931085908037	0.60698313786237	2.33909093583361
C	-1.12536010696016	0.62522966363496	1.86714742107102
H	-1.92240928294586	1.22231248553419	1.44191781065941
C	-0.78644642459398	-1.77993830385654	2.37611421136992
C	-1.15920667549933	-3.05688468218620	3.08813191700235
C	-2.23721541700907	-2.87325468730759	4.14310334750822
C	-3.36404432674487	-2.04369720686643	3.55387418474200
C	-2.90774563379900	-0.63028446610908	3.14692837117578
C	-1.53707530691232	-0.65948749404291	2.44257127759450
H	-0.25226259425160	-3.47856133856618	3.53571936076523
H	-1.48225662764656	-3.79568022286793	2.34250951226908
H	-2.60820508501327	-3.84100527288174	4.48888547158948
H	-1.81449486166631	-2.36904602602453	5.01646734679964

H	-4.19835396151058	-1.95360460233020	4.25442105495793
H	-3.75272161204280	-2.55964578982125	2.66930210488297
C	0.48834849655291	-1.91343018347794	1.58966399725183
H	0.50292922896083	-2.88216105798120	1.08065607503342
H	0.61695856297845	-1.12944911321205	0.84793176629976
H	1.36140479289481	-1.90141325202787	2.25127319353341
C	-2.80980731259211	0.26793123318787	4.39348524980348
H	-2.45729351757628	1.26567582073534	4.12717898424332
H	-3.78606125239688	0.36618664874514	4.87423498512120
H	-2.10843939448954	-0.14114035942984	5.12208571108565
C	-3.99778142637167	-0.06781571695370	2.21425968860837
H	-4.97374488985728	-0.19530370624367	2.68932866960938
H	-3.87504544874306	0.99536174026354	2.00504392090162
H	-4.01209892104583	-0.60461775050542	1.26420299870132
H	6.31961121047636	3.35451230491748	0.37880265342007
C	8.07504863349620	2.83627874935684	-1.51623590210585
O	8.55856436563112	2.33239896799859	-0.53399110264640
C	8.42638899258933	2.49069293610457	-2.94045228543185
H	9.16909094073711	1.69787539537882	-2.95385152112085
H	7.53141337351379	2.17307431315087	-3.47724797733212
H	8.81818936587709	3.37352103312068	-3.44844864170458

acetate_mecp7.xyz

C	1.72860594091496	2.58292150988842	0.23552012577409
C	0.53227020563345	1.78667825234457	0.24875363153933

H	1.97175659914176	3.07983063838916	1.17084583759640
C	2.61394580816340	2.73967173593963	-0.80951005103769
H	2.38270560116096	2.28058955633966	-1.76327812758134
C	3.81137535632733	3.44060603503037	-0.67812947304516
H	4.03406302349169	3.84185025656794	0.30659770840166
C	4.79824136810606	3.66886887893411	-1.68057047497029
C	5.96191902468505	4.27094979296029	-1.30004341371660
H	6.06152548724658	4.55704049566278	-0.25724560134843
C	7.11943257632961	4.63806483745755	-2.15344044147269
O	7.26867243359967	6.09210928773633	-2.18365676899972
H	8.05764681101930	4.29782534323746	-1.71477891400310
C	4.53511829405751	3.23997238348671	-3.10139762942360
H	4.69633656486568	2.16480384979174	-3.22532786222445
H	3.50330642066218	3.45511796218614	-3.38281923210089
H	5.17448152378480	3.77036054857603	-3.80054857550460
C	0.16066998679513	0.99311304853750	-0.97377395139795
H	0.01561425876312	1.64972273960649	-1.83511261672976
H	0.95149967935292	0.28640309885099	-1.23900458709772
H	-0.75853228008475	0.43266390838498	-0.80946883577688
C	-0.19632511779658	1.73243601185157	1.38451670706958
H	0.12295845247869	2.37442465870861	2.20369147970044
C	-1.42761881808839	0.96801673542880	1.65312334310194
H	-2.33113187585653	1.54233666619653	1.48489134206552
C	-0.48712430965386	-1.04242716095451	2.72019731808970
C	-0.62237225122488	-2.15823241988132	3.71484034555266
C	-1.95245635317970	-2.18181305931389	4.44976003712913

C	-3.06413965893479	-1.99557851493805	3.43185119160260
C	-3.01194835652437	-0.61307875536607	2.75216426025081
C	-1.56510145474483	-0.22837875299418	2.34292980863314
H	0.21229269010818	-2.09344933341596	4.42394427874871
H	-0.47503024295903	-3.11480719367813	3.18956372226850
H	-2.07193706780870	-3.12123378744258	4.99422385087816
H	-1.98469032257274	-1.38164190392102	5.19437005277379
H	-4.04874946075085	-2.12107755909126	3.89001609376804
H	-2.97359340478774	-2.77563647193234	2.66807753489585
C	0.90783730381708	-0.88887181286527	2.18109114871590
H	1.48932823727593	-1.78466750155075	2.40958059641904
H	0.93020315942049	-0.73949447574840	1.10385761966215
H	1.43602233342055	-0.04200390314449	2.62823052719899
C	-3.57913166939021	0.44129223892097	3.72089848212940
H	-3.64257195393273	1.42053717224689	3.24664348308148
H	-4.58374860489673	0.15968119474414	4.04631310328139
H	-2.95055349701769	0.54493427356222	4.60563545212617
C	-3.91023511026135	-0.68321656818321	1.50688366502174
H	-4.90827032068937	-1.02840198437656	1.79033012496929
H	-4.01873316890684	0.28624867509761	1.02046296476989
H	-3.50289848552102	-1.38417076324241	0.77613748785754
H	7.04189363951899	4.26628783950846	-3.17123261284846
C	6.47012126417770	6.74670892922700	-3.04841602192919
O	5.80285975058796	6.20328340443555	-3.89232040098746
C	6.49056324695914	8.22797368023575	-2.79512868841721
H	6.18779051398247	8.75732170701930	-3.69528631086983

H	5.76698965494344	8.44463113401513	-2.00575456668399
H	7.46811856179191	8.56066501393305	-2.45076720090610

acetate_mecp9.xyz

C	2.08805739171649	2.64564412473690	1.43210525603783
C	0.64474144615908	2.33997187692934	1.57572674163436
H	2.63873382145671	2.91212803032449	2.33162675651894
C	2.74989431285872	2.57612606438517	0.24892809412065
H	2.16453724951956	2.33939969856762	-0.63379712226339
C	4.14258940214269	2.74952966942404	0.09746198221944
H	4.72474111210665	2.89829734290446	1.00211497433043
C	4.85334585891359	2.71244901781519	-1.12678442743359
C	6.22173297389420	2.78975160590288	-1.10623789573743
H	6.70455715024512	2.92444556375158	-0.14384349904674
C	7.12175723020273	2.69250465166957	-2.28220023734448
O	7.54803376931622	4.03438993020663	-2.66980572238608
H	8.02051609633678	2.12053836239458	-2.04419268672812
C	4.07745353262707	2.58664765415320	-2.41655991983022
H	3.63078784076775	1.59456108336320	-2.51986977456754
H	3.26067438617884	3.30945812104928	-2.44113867422413
H	4.70155899809932	2.76979601065682	-3.28729180942647
C	-0.29931340669286	3.49129876396052	1.40835330129047
H	-1.31478343704747	3.25236533249711	1.72125388544240
H	0.04388173773905	4.34899807041245	1.99428043133919
H	-0.32914539831100	3.82548778152638	0.36547680971499
C	0.27947459242987	1.05664593815319	1.85786741671355
H	1.09667958130710	0.37103838333434	2.02179357457088

C	-1.04451461903203	0.57682063086294	1.99558068996143
H	-1.81489843113000	1.31358692853543	1.81619488570202
C	-0.74758243185090	-1.82240334625262	2.57969934540743
C	-1.20870255588781	-3.03942571637284	3.33645388704295
C	-2.46810301472070	-2.80819122962831	4.15511175775958
C	-3.47920038673882	-2.09216331342153	3.27814732904383
C	-3.00604568153819	-0.68649567609218	2.86712666443799
C	-1.51110789490748	-0.68135514054054	2.46185839122302
H	-0.38508192083894	-3.37914157442918	3.97590791050867
H	-1.37453729800865	-3.86127979143753	2.62511063258724
H	-2.86885372163477	-3.75581522012094	4.52224127372946
H	-2.23463473169859	-2.20278445922057	5.03501865562696
H	-4.44877652385509	-2.00328520973059	3.77464564250862
H	-3.64398211152972	-2.69145925906778	2.37629106277560
C	0.61378695314173	-1.99908034062424	1.96735468390600
H	0.76201601505092	-3.05005753564787	1.70438637499156
H	0.75056559885692	-1.40483935653843	1.06696906313731
H	1.41620182465542	-1.74053209525968	2.66824644696557
C	-3.23233719604256	0.29326539810708	4.03273181642204
H	-2.95209307836130	1.30953555044173	3.75502021681646
H	-4.28526069582195	0.30146408963434	4.32689948772471
H	-2.63583908364916	0.01762674467803	4.90331170074193
C	-3.88356833900208	-0.25811676130030	1.67748551258607
H	-4.93712670940138	-0.37796494655060	1.94396787448044
H	-3.73449835805265	0.78377139996018	1.39253235514019
H	-3.68155418263573	-0.87966360186357	0.80349712194405

H	6.65465552014234	2.22173548208931	-3.14299818770880
C	8.25935789591600	4.11231400559931	-3.81151126516966
O	8.53992670176242	3.15713332878816	-4.49101683293167
C	8.63070874598699	5.53804748813771	-4.12384664430536
H	9.33966505896424	5.55671172773083	-4.94722450396474
H	7.73356805206863	6.09244315425116	-4.40524784435499
H	9.05751323582666	6.02117635416416	-3.24486835968084

acetate_mecp11.xyz

C	2.41206520576703	2.04491892458918	1.49843192789794
C	1.05425481331183	2.04057392942776	2.01534096295427
H	2.83235548275238	1.06942436554444	1.26965003442215
C	3.16575705604647	3.12128080215128	1.26679442902469
H	2.77808432159910	4.11350287138669	1.46961901224112
C	4.54393093873648	3.06123330635779	0.73813970105087
H	5.33674767896640	3.01107529347868	1.47608793683066
C	4.89991633715547	3.13604080014462	-0.58704578586368
C	6.25940490786945	3.15122222322840	-0.92917396564507
H	6.98168403087941	3.12665716556398	-0.12016437504674
C	6.80436944302344	3.29288488886370	-2.29652117070411
O	7.18284877815654	4.69645761836511	-2.48804613166059
H	7.70009597263719	2.69057660797826	-2.44667798672759
C	3.84111231057265	3.20621105517727	-1.66153633599099
H	4.04393303866755	2.49936638941140	-2.46669201321525
H	2.86048571059728	2.97634081872473	-1.25065804106506

H	3.80178004171467	4.20242764224038	-2.10915434944698
C	0.43978060365836	3.35794608349601	2.37114505197764
H	-0.55744791524432	3.26141886559191	2.79212081180057
H	1.05763633593363	3.89275183438892	3.09799910886774
H	0.37084879581020	3.99880753186637	1.48626834445718
C	0.40621398517972	0.82434531561758	2.11919240014232
H	0.97337020084410	-0.02074990100042	1.75994730489299
C	-0.89390377340704	0.60893036766980	2.58912125971216
H	-1.42911946448031	1.50513974509948	2.86517387726702
C	-1.14187514910930	-1.86560059241393	2.71643226586212
C	-2.00211926693123	-3.10225935740657	2.76549013664028
C	-3.43944069738607	-2.88013864629963	3.21743241639503
C	-3.98932155514604	-1.61145829425556	2.59314938412744
C	-3.16921774655192	-0.35584130384060	2.93499222425799
C	-1.65664114684131	-0.59289712468457	2.71095453381624
H	-1.51545937667326	-3.84656600859956	3.40317081734444
H	-2.00052049401009	-3.54821364862294	1.75951800428326
H	-4.05504533513424	-3.73761792928973	2.93401907708897
H	-3.48148584948399	-2.81182134211830	4.30793549263751
H	-5.02411658904616	-1.44674365106009	2.90603311464805
H	-4.00432669410241	-1.73032747478497	1.50389479694336
C	0.32875395270769	-2.17650200276889	2.64569427110126
H	0.52438132289609	-3.17118056736449	3.05008380561293
H	0.69998561772208	-2.17718963959616	1.61438221670678
H	0.93022243988043	-1.46304816707565	3.20686890078343
C	-3.38410100598951	0.04143194356498	4.40803784336373

H	-2.80323873262814	0.93055066228747	4.65962276305114
H	-4.43744595646954	0.26521990703424	4.59818100193802
H	-3.07135028691869	-0.75260015518400	5.08661142793433
C	-3.71377163103687	0.76999221208876	2.03839609228407
H	-4.80223333615777	0.81082782847092	2.12807429092334
H	-3.32990825915904	1.75275555005913	2.31099195378575
H	-3.46406932323535	0.58846698767209	0.99116735997881
H	6.08836382535626	3.03233018073932	-3.07410007257301
C	8.04055638495675	4.95523268137518	-3.49262294566349
O	8.43291239328584	4.12529571869956	-4.27459247041291
C	8.46216447040691	6.40225107235466	-3.47402742009680
H	8.83379079618275	6.68956245062603	-4.45465460225518
H	7.64016677426494	7.04581234946387	-3.16349255481880
H	9.26816524660342	6.52165605656608	-2.74660382586141

acetate_mecp13.xyz

C	1.91648395481208	2.83481089885024	1.09630277048840
C	0.54520425400820	2.50606120818094	1.05083564792479
H	2.56540337495017	2.03107358115629	1.43720105153132
C	2.55011045618135	4.00904648425577	0.77376623545474
H	1.97764801448630	4.87458723688446	0.46532579955438
C	3.98552022851091	4.08636961017154	0.77915136262049
H	4.48632332736021	3.14800931727803	1.00074711462674
C	4.78235906562896	5.13421076272312	0.49044923735198
C	6.23616795940502	4.90168365471690	0.39113744022170

H	6.87987078317255	5.10614389885151	1.23702778729427
C	6.87369008653572	4.61769661892246	-0.92068124696027
O	6.18192703756374	3.55100444277937	-1.62342533953280
H	6.88433526288099	5.49390839689843	-1.57737016083395
C	4.32072362717639	6.52791337285879	0.17523544737114
H	3.27152564493733	6.68192026724336	0.42847293508423
H	4.91458942049961	7.25533235975695	0.73438634740509
H	4.46391543928388	6.74354290476345	-0.88778021151632
C	-0.48286472045387	3.46824890769080	0.53111618537406
H	-1.19673138475038	2.96486209252916	-0.12495554826708
H	-1.05801934982657	3.91304754182532	1.34988051039743
H	-0.02858120402271	4.28022974444972	-0.03387604375531
C	0.17062204614708	1.23761387811853	1.54533454830607
H	0.98129143508234	0.66029513441434	1.97015276360480
C	-1.09165968514404	0.70391387506418	1.59769112846296
H	-1.90270957337799	1.32297571052824	1.23506776372804
C	-0.66125587020989	-1.64023258269621	2.29862071961341
C	-1.00070452052188	-2.84778671417952	3.13539256625738
C	-2.12714938866474	-2.59434588890547	4.12261849112429
C	-3.27765298638090	-1.94544690927507	3.37473293980935
C	-2.90451609040411	-0.56812686977964	2.79257151330347
C	-1.47522268221141	-0.55558899686317	2.21152634438667
H	-0.09296006511141	-3.17148320138215	3.65763497096527
H	-1.26379143896146	-3.68293056109835	2.47165448045807
H	-2.44735650504842	-3.52585352572459	4.59539297238507
H	-1.77394932841897	-1.93814875740500	4.92312126704016

H	-4.15474111571768	-1.82747737201661	4.01588083670417
H	-3.57737224334860	-2.61050912245970	2.55774571579103
C	0.64915603177480	-1.78887824987635	1.57474490069804
H	0.75465385868854	-2.82038047146580	1.22536178305195
H	0.74068639137674	-1.12481143970918	0.71879654211322
H	1.49953671709525	-1.60389642219399	2.24076971873358
C	-3.01716228344491	0.50366504035846	3.89140957541039
H	-2.74807967271295	1.48876225805134	3.50840912159261
H	-4.04011694854742	0.55510348288036	4.27252827837083
H	-2.35072470170635	0.28451360358782	4.72674737335632
C	-3.93511426374752	-0.26223598337818	1.68984324795076
H	-4.94171350138210	-0.40721542244236	2.09063030613986
H	-3.87487984622272	0.76270162974607	1.32220831065104
H	-3.80645521634892	-0.93610797229998	0.84078666772555
H	7.89319787634136	4.25737886845444	-0.79128398984416
C	5.21794517812529	3.91335969873149	-2.49513745018364
O	4.95172380128008	5.05612711445676	-2.77200523513809
C	4.53210629245031	2.70576342093229	-3.07179833620635
H	3.82177084361946	3.02173662525658	-3.83078230959903
H	5.26491785901958	2.02203231961839	-3.50194882877353
H	4.00665882629380	2.17482197016542	-2.27625930082462

acetate_triplet_all_trans.xyz

C	2.06400744006354	2.88366147317617	2.06678644129278
C	0.66899192403924	2.56376838119448	2.31587035696163

H	2.78427114764526	2.11213764615580	2.32613199191910
C	2.52971942914359	4.01577571472684	1.45777485662911
H	1.80696699100700	4.76872582093667	1.16982679180115
C	3.88011977741021	4.22908019708799	1.09766434749781
H	4.60909291515647	3.50269919716487	1.44465363860392
C	4.34408357756350	5.22944810551065	0.20796685325662
C	5.65819368352720	5.21893587030319	-0.19311783418854
H	6.32038241250890	4.49171938662505	0.26668266441767
C	6.24252986944009	6.00380449717689	-1.30749679753712
O	7.26591858515326	6.91210922054794	-0.80086106861568
H	6.73031217949320	5.34360170070354	-2.03038474961285
C	3.34978139591881	6.22852954013415	-0.33295617526704
H	2.60985288315599	5.73533149173469	-0.96942183143159
H	2.80729395748688	6.71166840522531	0.48152222174478
H	3.82525613906109	7.01227254347469	-0.91679973450390
C	-0.35365990627333	3.65446850220253	2.16135143227985
H	-1.33680224497244	3.34146426741455	2.50308767258744
H	-0.05537606591202	4.54775816083057	2.71591176481674
H	-0.45924802155278	3.95314189185419	1.11466704242452
C	0.33584239740260	1.27195981681923	2.60242722347324
H	1.15940139967435	0.57168952026798	2.65495624912387
C	-0.98724000218236	0.76405875713144	2.83999065647879
H	-1.68508099168557	1.48933478396125	3.23104769630479
C	-0.86086154876399	-1.53540919531933	1.92417323486440
C	-1.41610527311054	-2.92417590573494	1.75375608626456
C	-2.63494703462303	-3.25484533060628	2.60029939863863

C	-3.54882977598496	-2.04490218305313	2.66684270236750
C	-2.87119043409262	-0.82119832077038	3.30684249709100
C	-1.50001108208814	-0.53233127725107	2.64792757596080
H	-0.61095574670536	-3.64637662453419	1.93792913739818
H	-1.66781786743703	-3.05319446892925	0.68944827625246
H	-3.16224909103234	-4.11107283106327	2.17350256051315
H	-2.32477800522606	-3.54877731374725	3.60601987418647
H	-4.45488399604267	-2.27726954915111	3.23248910652212
H	-3.87208595765791	-1.78054825932520	1.65389523602450
C	0.42281934532138	-1.33699910273184	1.16611548918347
H	0.49022399381063	-2.05807462209804	0.34876042099779
H	0.51612736981640	-0.33762400464625	0.74341052057062
H	1.29787361273463	-1.50460670285939	1.80416223579343
C	-2.63516703973643	-1.07758499352845	4.80647063952223
H	-2.22517990030727	-0.18549331031867	5.28434468304993
H	-3.57153900033748	-1.34040758366058	5.30592776137166
H	-1.92247043091742	-1.88571020929540	4.97052176196394
C	-3.86020873348825	0.34945015320520	3.16747491247044
H	-4.83969654437055	0.03596926460790	3.53569202514902
H	-3.56965261998445	1.22361190090995	3.74918456344562
H	-3.97157770104626	0.65281329706398	2.12512616057770
H	5.51014339176399	6.59112118818313	-1.85566979735212
C	7.79851513264143	7.73665247268515	-1.72414992670059
O	7.47337769614020	7.73754591606940	-2.88566697197021
C	8.81578468774425	8.65786356605922	-1.10764864017691
H	9.34106408392049	9.19950576459552	-1.89038710872560

H	8.30416129384494	9.36697302534391	-0.45304040973866
H	9.51862807594161	8.09252606253993	-0.49531363897265

acetate_triplet_cis7.xyz

C	2.36685595740793	1.89053494881342	1.69956025930051
C	1.21321920861431	1.21210344091557	2.25334763589774
H	2.15867604299959	2.70119763657961	1.00604903846313
C	3.67754208374458	1.56752233504775	1.92222305284626
H	3.90517663682894	0.71213084229243	2.54830720823445
C	4.74731914648004	2.28932345018409	1.35938256476701
H	4.49046835428938	3.21083205832686	0.84566503944517
C	6.12127408089457	1.94675135634649	1.37388535918847
C	7.00948662657140	2.85577653930637	0.86343167804676
H	6.60379019338191	3.79516470187788	0.50153807875796
C	8.47625544786873	2.73497141274383	0.69269717070317
O	8.74847149991419	3.10488803957275	-0.68900838648330
H	9.03131230773163	3.42370030631801	1.33518015527115
C	6.54545151359469	0.60726610256069	1.92418016302086
H	6.55757073051057	0.60999745031575	3.01761389244754
H	5.85365412244851	-0.17337910738762	1.60665764838576
H	7.54039624179474	0.32613958024963	1.58486373912263
C	1.42777105705080	0.32921159721021	3.44712244011476
H	0.48785756091168	-0.02126955214848	3.86289933138004
H	2.03523080033894	-0.545796666666264	3.20077949818865
H	1.97119097297730	0.88294259288456	4.21709211927966
C	-0.00454769280382	1.44326570250364	1.68563735306574

H	-0.02034534198171	2.22989929069250	0.93219933926459
C	-1.29827143030151	0.88887079373287	1.97818737769218
H	-2.09395101008630	1.62160490164573	1.89411549385198
C	-0.96729097986248	-1.55772539486751	2.15836867157322
C	-1.28194553462085	-2.86411145093731	2.83112952413805
C	-2.32146290418797	-2.75202485759918	3.93366780718013
C	-3.48012595269755	-1.91848834344739	3.41656887522906
C	-3.06629314600842	-0.46712706396619	3.10738078706159
C	-1.69551590681401	-0.40022950980940	2.38798690234248
H	-0.34622663982402	-3.28357596665479	3.22193639012791
H	-1.61931566002989	-3.58493197605921	2.07290006777008
H	-2.66083385040925	-3.74212075544542	4.24602991683934
H	-1.87939145041614	-2.28015414249273	4.81555300650223
H	-4.30747092343937	-1.89834094723139	4.13076071124908
H	-3.86700850486009	-2.38526026305840	2.50439778427669
C	0.16500558782075	-1.66232349210516	1.18295572553850
H	-0.02580657713440	-2.50459618193291	0.50872057997289
H	0.30797125977687	-0.76984863900820	0.58349102405968
H	1.10826837013513	-1.89217668589430	1.68927525219562
C	-2.98761472499436	0.32824627133148	4.42301871901147
H	-2.67346148124774	1.35656075639495	4.24075130302802
H	-3.96269033531258	0.34681236768173	4.91585159022879
H	-2.26799834179207	-0.11631497178029	5.11221585389797
C	-4.17636522061540	0.13057784456545	2.22425485615415
H	-5.14617653701555	-0.04864478409107	2.69571700586829
H	-4.07720311817105	1.20679859429450	2.08222220250032

H	-4.18474115667216	-0.34262689851674	1.24111248484245
H	8.86243605744574	1.73318459607849	0.87866738799911
C	10.00953686386723	3.45190231245470	-1.00936298761279
O	10.93914476091592	3.40251360996768	-0.24502908962751
C	10.07919679091025	3.91260241107075	-2.44216233375511
H	11.10098051975310	4.18706626544871	-2.68997263413489
H	9.72901253025893	3.12010912681703	-3.10494225940448
H	9.41861336706026	4.76844164787018	-2.58650859030520

acetate_triplet_cis9.xyz

C	2.28369673720196	2.48383067829052	1.75831739181847
C	0.84814445129637	2.22515692036698	1.77575905880354
H	2.56438573928620	3.52871912790189	1.65439911358810
C	3.30446652716450	1.58337660736561	1.83189357127515
H	3.07039002469423	0.52794269629135	1.91683969357961
C	4.67042505606526	1.95616307741290	1.77458255302643
H	4.88310489519231	3.01445064186911	1.65472656230747
C	5.77932385620417	1.08863788143347	1.81501775189545
C	7.04088120731604	1.61981129005725	1.64881191226242
H	7.11903292727056	2.69075541033182	1.49541069695715
C	8.33017580585297	0.88722774022460	1.57991661593376
O	8.83080554209448	0.82505697480708	0.20246887842943
H	9.09295664258997	1.38376861555647	2.17930406091204
C	5.54083924123206	-0.38770269308545	2.01559103718814
H	4.84391362379948	-0.56418044797672	2.83641031991614

H	5.10505800788568	-0.83590666437610	1.11897537682098
H	6.45652227107763	-0.92722176988859	2.24330437874748
C	-0.04965826603839	3.40261562278664	1.49769726383679
H	-0.85185032484771	3.14669111974129	0.80411423253740
H	-0.52327173007516	3.77186161537884	2.41478807409146
H	0.51302540923776	4.22972242082813	1.06494011733262
C	0.33264283848147	0.98429880435053	2.05203836946876
H	1.03890111847657	0.19624542328892	2.26619775355003
C	-1.04452630568711	0.68559102307669	2.15461092370998
H	-1.70371760795275	1.54042726158015	2.09672569693528
C	-1.08975930743461	-1.79078675803939	2.26463471125755
C	-1.72022172100806	-3.06954685910533	2.74393176159210
C	-2.89916341609952	-2.87137677451265	3.68124700386373
C	-3.80786583561566	-1.79905986214183	3.10798931720530
C	-3.11504917344500	-0.42922245282347	2.99670783068699
C	-1.67590155230283	-0.55375980392472	2.43999919877737
H	-0.94440205844172	-3.68104833948242	3.22096748003817
H	-2.04095813225036	-3.65094513202347	1.86676070686521
H	-3.44288502766632	-3.81026639579676	3.81053839912226
H	-2.54030365400038	-2.57579924751549	4.67085223762308
H	-4.71019371619964	-1.68086057832459	3.71332044816967
H	-4.13880868738639	-2.11604742817789	2.11292131846381
C	0.20682690747883	-2.02004868829636	1.53951560979494
H	0.16699739753360	-2.98040824545983	1.01771356776878
H	0.43175221156217	-1.24513568955295	0.81067760052501
H	1.05258053430654	-2.08390721689196	2.23518880119967

C	-3.06810204867674	0.22934618230824	4.38935330568698
H	-2.57945611643915	1.20324287648484	4.35034882018659
H	-4.08038630315773	0.36993859848140	4.77680176767353
H	-2.51286022839575	-0.38490018598053	5.09995462564350
C	-3.99273631105935	0.43635681561845	2.07379001581729
H	-5.03114424488427	0.37899826350371	2.40871285235030
H	-3.71008330519721	1.48906052501818	2.08488915812886
H	-3.94629109730504	0.07843716191635	1.04386931607915
H	8.25329081643140	-0.15427043754967	1.87662777990599
C	9.52141903964104	1.90010685758321	-0.22381256248193
O	9.77033748953696	2.85621502566903	0.46716108693358
C	9.92092580135045	1.76494038563928	-1.66915880986568
H	10.74388602081409	2.44329551516538	-1.87835733917363
H	10.19399735958622	0.73970274620664	-1.91457443043077
H	9.06998822390582	2.04790656839123	-2.29335860233158

acetate_triplet_cis11.xyz

C	1.98069433334999	2.72328609992105	1.39774249278798
C	0.56777941359407	2.44840467156758	1.58379131917432
H	2.60862790171139	1.84631311075797	1.42686148741352
C	2.54587319326337	3.94847237199623	1.19676124318737
H	1.87275134295817	4.79978676883627	1.19009139076726
C	3.91551591865865	4.30269334554518	1.00201018750732
H	4.09135962085565	5.37020508166801	0.91637520390336
C	5.07538307990072	3.50863311399505	0.91106145703548

C	6.30049201810988	4.12941618968192	0.76236950224746
H	6.32296901565985	5.21072747582204	0.68698737180351
C	7.60512545857936	3.41717752805737	0.69279470436749
O	7.74516278681464	2.75477305523554	-0.60684359642497
H	8.43770471857585	4.11378701558659	0.78796464381369
C	5.00050883249744	2.00638544859208	0.96382910083818
H	4.63615754556685	1.66631722074000	1.93577659504911
H	4.30811574453138	1.63256794034754	0.20814559562109
H	5.96423107192338	1.53893746842779	0.78796796656841
C	-0.40755251557841	3.58702251968240	1.55532747204080
H	-1.40594202922906	3.28413581599620	1.86189657051626
H	-0.08378497221890	4.38458472435098	2.22893176125301
H	-0.47846152009715	4.02616057890224	0.55563763600607
C	0.20857548011864	1.13959479395752	1.79458517240694
H	1.03484292673349	0.44812124388258	1.85686441838001
C	-1.09892624383280	0.63382583832709	1.98786909245125
H	-1.88649438042213	1.37127039091423	1.92538952551173
C	-0.73045900307979	-1.79673747519458	2.38133564455463
C	-1.12975845629133	-3.06359763596602	3.08722516524776
C	-2.35265276877327	-2.91410798634106	3.97613056597712
C	-3.41823972626223	-2.16708679335261	3.19408085621059
C	-2.99128850708803	-0.72583252657922	2.86061656395300
C	-1.51942782579545	-0.65771246073173	2.38099234973390
H	-0.26807459450090	-3.42316892728118	3.66299170069981
H	-1.31385813886846	-3.84479726696888	2.33553139688600
H	-2.71560790169034	-3.89236298607299	4.29901802412123

H	-2.09003168285439	-2.36155723943385	4.88235939348511
H	-4.36484051946175	-2.13349245140044	3.73892079903373
H	-3.61462503686472	-2.70931271809709	2.26248048559293
C	0.59449740876306	-1.91542373018068	1.68334574093232
H	0.74496154053774	-2.94841572128005	1.35917596215694
H	0.67167566832034	-1.27432257616017	0.80818060151058
H	1.43029857663017	-1.67884467724064	2.35291083780298
C	-3.17328737181534	0.15760664211620	4.10888891845492
H	-2.91441726376479	1.19586983637555	3.90098047425204
H	-4.21206076005017	0.12801170263374	4.44796174486032
H	-2.53664555765527	-0.17886985451424	4.92774028864097
C	-3.93582615506343	-0.22846588695566	1.75189188078754
H	-4.97211971637858	-0.39179781596315	2.05959260733800
H	-3.82090976643440	0.83521815444962	1.54195228472206
H	-3.76584512997324	-0.77728889347305	0.82407896488219
H	7.71736833727884	2.65402614293975	1.46207707135750
C	8.39148098367311	1.57246784895296	-0.63568799642824
O	8.87535915338427	1.03590374187368	0.33044588806174
C	8.39808131727045	1.00203768173975	-2.03045386516064
H	9.03519768903951	0.12276543108768	-2.06277073599368
H	7.38074741696130	0.72518522419939	-2.31434745645523
H	8.74644481378274	1.74853456602748	-2.74429834644482

acetate_triplet_cis13.xyz

C	1.58728186710859	2.99382197441976	0.66334199878845
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C	0.20987377780311	2.72740934425489	1.03733750227036
H	2.27229139452118	2.15897899211256	0.79053238368681
C	2.11517704241452	4.17074258732369	0.23630606083673
H	1.45308420884637	5.00966278767307	0.05035253306051
C	3.51620117505774	4.36229202629638	0.04437620926820
H	4.15605687982155	3.55604370928580	0.38128561330396
C	4.12970792689991	5.47394433174606	-0.54937410212343
C	5.50703596696660	5.61397055169578	-0.57199026398063
H	5.94356486122450	6.42937590041422	-1.13478553674125
C	6.45415170527145	4.74645256028460	0.18619485819717
O	6.46304175136925	3.35809594783547	-0.26450143779817
H	7.46878162681164	5.13331228353470	0.12152325583510
C	3.28024436418598	6.53652867270887	-1.20481946606590
H	2.63637277426781	6.10580206678754	-1.97519368132536
H	2.63042580285431	7.03431368908078	-0.47974982958309
H	3.90351979072114	7.30097906000908	-1.66749445796960
C	-0.73738278052605	3.88322494581090	1.14783818951572
H	-1.68060067148113	3.60222770831467	1.60951827124939
H	-0.29541805606683	4.69855880189197	1.72589776611701
H	-0.97070510318026	4.28914675997631	0.15794002541123
C	-0.16145159303522	1.42773180656763	1.30382303543458
H	0.58031394021772	0.66849628849947	1.07653023126052
C	-1.35240172968918	0.98958484090161	1.90876430925436
H	-1.96982333221205	1.75949920789384	2.34959508325254
C	-1.47441814385779	-1.39656288713290	1.30851196006069
C	-1.80457175706568	-2.83040406492155	1.63263591946173

C	-2.21025345629204	-3.05496465572060	3.08240955790491
C	-3.21587898555182	-1.98333367701676	3.46426801207400
C	-2.60467184438385	-0.57280257473403	3.42875853892477
C	-1.77042360991907	-0.35519110099982	2.14756304410499
H	-0.95238651861357	-3.45927103709666	1.34829944124475
H	-2.62192040425839	-3.15340248865574	0.97174333816114
H	-2.63981025274406	-4.05137934634256	3.21107790572599
H	-1.33206542779686	-3.00291275206981	3.72985061648163
H	-3.62824999940472	-2.16396464026816	4.46010183653142
H	-4.05571424503824	-2.02674185570926	2.76160492713488
C	-0.89035543987881	-1.22006781398875	-0.06386531020288
H	-1.36075051476883	-1.92766608407880	-0.75388977460952
H	-1.03479230477847	-0.21400268922746	-0.45502069670566
H	0.18358533669114	-1.44027913874309	-0.08562330691251
C	-1.68871852519373	-0.38114358372600	4.65023233635893
H	-1.29850840003702	0.63664183685592	4.69096940931013
H	-2.24227851805079	-0.57814203233160	5.57265143587381
H	-0.83238379902119	-1.05554040063389	4.61432312820708
C	-3.76396988148955	0.43439573828876	3.51366046524003
H	-4.42834370386159	0.15358964325737	4.33264183643781
H	-3.42158017937292	1.44977479918296	3.71288110038792
H	-4.34686486562851	0.44028340067002	2.59058906961411
H	6.16245586889502	4.66034718436117	1.23356615519616
C	7.30618419455433	3.03825437428072	-1.26252098151180
O	8.02847514621909	3.82422208783393	-1.81950902216053
C	7.22913337772901	1.56117757189473	-1.54167555839024

H	7.62420909876272	1.34767138108532	-2.53178705810926
H	7.83041163539609	1.03304076547846	-0.79932296194936
H	6.20369303658744	1.20718866488846	-1.44726719604033

retinal_all_trans.xyz

C	1.62693325601274	2.70405526314090	0.88763846319186
C	0.31003027915178	2.36184837606015	0.92644756131617
H	2.32611106427795	2.02060086985703	1.36185637577174
C	2.20896750800243	3.86126661484543	0.28132438915083
H	1.54428925962843	4.57554616029185	-0.18668509727983
C	3.54172537136269	4.09958232822406	0.25742024577788
H	4.20364810461222	3.37557659526759	0.72354904638070
C	4.18217421118929	5.24375030694796	-0.34911847977985
C	5.53942081710477	5.31579730079218	-0.32318669688365
H	6.10115536722068	4.51362157476854	0.14482498531233
C	6.36229514081449	6.38414030445938	-0.86382399879741
O	7.57888182868225	6.38269509678561	-0.81953848863300
C	3.30615704692842	6.29431566215875	-0.97642853407152
H	2.68330179470478	5.85135399808066	-1.75714850968051
H	2.63289362553993	6.72376295669305	-0.23080627684630
H	3.87321932425899	7.10471605034186	-1.42278384030042
C	-0.78067716683868	3.19849208614076	0.32115843729322
H	-1.32897271918972	2.62987847161643	-0.43409127675945
H	-1.50410475817778	3.49493995604700	1.08434411631004
H	-0.40308975382816	4.10184422865751	-0.15004079470844

C	-0.05129493246321	1.12128292249359	1.58170109307823
H	0.77645659491162	0.55419361705671	1.99478479923186
C	-1.29408562219716	0.62906931079242	1.72973721611764
H	-2.12970128774186	1.21867718131978	1.36988952320408
C	-1.01777882055843	-1.79843166468917	2.09041844370073
C	-1.27141815910420	-3.08265970295277	2.83955466929111
C	-2.01642520292513	-2.89668182462051	4.15324472844162
C	-3.16465814579867	-1.92497860909152	3.94501330145718
C	-2.68162771479235	-0.53056845043006	3.51446253117952
C	-1.61933798077733	-0.63464573282130	2.40718798755627
H	-0.30943942752040	-3.57939573665487	3.00836135946003
H	-1.83172344861757	-3.76079537642676	2.18271784550484
H	-2.38783858879108	-3.85602965095172	4.52112589843409
H	-1.33190687140066	-2.51404235836447	4.91493286478820
H	-3.76564056263300	-1.82419671889145	4.85242736152250
H	-3.82842411028672	-2.32424821988107	3.16980545675848
C	-0.06809561753186	-1.98023562484434	0.93986404696878
H	-0.36301803856827	-2.86070112986124	0.35876997705514
H	-0.03397472063884	-1.12235283507521	0.27381850027027
H	0.94752217596432	-2.17830108438033	1.29997443220826
C	-2.07354388298507	0.20585985580103	4.72327226229615
H	-1.70082617229725	1.18945423240209	4.43398739439292
H	-2.82442874853931	0.33819967676631	5.50594142369409
H	-1.23545784910238	-0.34931897090328	5.14480842693645
C	-3.91065924248003	0.25618719989193	3.02388025121997
H	-4.70422199835687	0.19696236909426	3.77235674766865

H	-3.69080523417098	1.31195749475400	2.86112157179620
H	-4.29651977824350	-0.16128125074111	2.09114470772014
H	5.83577561718872	7.23469536703232	-1.33542102171780

retinal_cis7.xyz

C	2.12645125474909	1.89717183788258	1.48882657892476
C	1.05425182940233	1.33022706276771	2.10372555252100
H	1.93921131231160	2.59426736252844	0.67700814093582
C	3.49911359580227	1.57966535303236	1.74965775261090
H	3.69607108689556	0.73575375204939	2.40062554473191
C	4.54440979315147	2.23222173613755	1.18868887021239
H	4.33770377616664	3.11461452974726	0.59054745153859
C	5.93829566522866	1.86352124166633	1.31040289700396
C	6.88288081624282	2.75307273840269	0.90604057010955
H	6.56318595192248	3.71228196233700	0.51201434386293
C	8.32584769869732	2.58403973184076	0.96487765616468
O	9.11782462138613	3.44010398635411	0.61595358635057
H	8.70331348104659	1.62322562427692	1.36193077494987
C	6.25816550041223	0.49890099500771	1.86144111740244
H	6.05995141111895	0.45513430128554	2.93619985739828
H	5.62489644492937	-0.25125401649895	1.38692659469030
H	7.29371733508375	0.21662314186955	1.69691717676411
C	1.22797000403719	0.48623524678346	3.34170633341891
H	0.29502708891317	0.39816825223032	3.88942447249854
H	1.57006246332074	-0.52669507232796	3.11727779312057

H	1.96628343189204	0.94442769119705	4.00048642224813
C	-0.26565895119320	1.61229060554072	1.56251101729255
H	-0.31222372198764	2.52002755744700	0.96739223409582
C	-1.41010595453182	0.90551657230991	1.65183122125313
H	-2.27813449240091	1.37898686241063	1.20443043619207
C	-0.90312183682003	-1.49113518621796	1.97404082615094
C	-1.05335665075606	-2.80123824898849	2.70587340281877
C	-1.88042385647354	-2.68740358017252	3.97687272341942
C	-3.14889576747341	-1.91538818258779	3.66296229798983
C	-2.86215092647809	-0.47061483460059	3.21600584662723
C	-1.65063980633194	-0.40816639617489	2.26691457741932
H	-0.05009826939133	-3.18120130020882	2.93205387504075
H	-1.49908498553851	-3.54367447194776	2.03156612293984
H	-2.11832222167171	-3.67691060777988	4.37375194437971
H	-1.30340316546413	-2.16745630748619	4.74709044788806
H	-3.82299276006402	-1.89115693028174	4.52321297008514
H	-3.68433175124689	-2.43556817438226	2.86185174077810
C	0.12938129050926	-1.53937385562787	0.88416381917176
H	-0.07202602470006	-2.39954811913807	0.23752215497051
H	0.14770431398651	-0.64277780182851	0.27226673862910
H	1.13277760452564	-1.69662982691011	1.29236582950457
C	-2.60291210245279	0.41115347566807	4.44855190526962
H	-2.33613983780982	1.42751825883508	4.15595615418778
H	-3.49641209792382	0.45800197219747	5.07563295208727
H	-1.78711344083963	0.01590111575339	5.05649395172232
C	-4.12759152000458	0.03951263043113	2.49948331781726

H	-4.99771021109891	-0.13557719216888	3.13669206658079
H	-4.08835563583464	1.10740689288481	2.28322850112397
H	-4.28391505824435	-0.49512410054572	1.56054245610612

retinal_cis9.xyz

C	2.08820750629383	2.26199237267607	0.78157854812029
C	0.74657332389920	2.04831680133930	0.85119791736722
H	2.42400059109899	3.16387555338727	0.27836060908493
C	3.12506401742743	1.44638366083366	1.34037714614181
H	2.83302598753250	0.55653121640178	1.88258368424912
C	4.44001307566379	1.75110864889815	1.25177242090327
H	4.72648427335242	2.64578977141420	0.70707362743707
C	5.52381663631808	0.99528037362821	1.83794743107445
C	6.79587371912307	1.43397713828608	1.64443625289491
H	6.95809641957522	2.32945029163337	1.05359291441329
C	8.01528395103041	0.81881818064589	2.14211043580571
O	9.12909982084156	1.24285381467798	1.89453240268453
H	7.90374234780413	-0.08054362586904	2.77601822942890
C	5.17740009356705	-0.23750954522878	2.63032947408542
H	4.51890272125115	0.02061865972302	3.46282787575086
H	4.63754401447452	-0.95095501404281	2.00318371873813
H	6.05082006253886	-0.73696532408213	3.03692560462375
C	-0.18927856314357	3.07943236879241	0.28544249169526
H	-0.87032714726730	2.63840465146300	-0.44714358523024
H	-0.81036850466225	3.52133784821102	1.07016167803243

H	0.36421489870815	3.88434145242746	-0.19655956389294
C	0.17607723271683	0.85930340849886	1.45553048003539
H	0.86169318506080	0.07464677860853	1.75156613222757
C	-1.13229611263786	0.64463620968729	1.66532989173748
H	-1.83236323497232	1.43862351860086	1.42843853480668
C	-1.55898197240614	-1.78352223119062	1.66092549587626
C	-2.16526790734311	-3.04609184229411	2.22488757048717
C	-2.68385208803323	-2.91121764795773	3.65080660087999
C	-3.41772221342818	-1.58772191209121	3.81160520387206
C	-2.51111081030139	-0.37752469947802	3.54187132407207
C	-1.71381648327366	-0.57864603851425	2.24237171168527
H	-1.42538130563585	-3.85125915260919	2.15927164384103
H	-2.98113264440964	-3.35634650186661	1.55837386845827
H	-3.34491550203209	-3.74627444658915	3.89445908908570
H	-1.84939837517975	-2.96366918935272	4.35512596600426
H	-3.84029480795195	-1.49781939857696	4.81605329789858
H	-4.25825129556136	-1.55904212743328	3.10975058408879
C	-0.84773445523380	-2.01056601872011	0.35340182777412
H	-1.49666315988875	-2.57505931219523	-0.32441237001505
H	-0.54767481941527	-1.08929019100583	-0.13770891879134
H	0.04739566262520	-2.62365675436126	0.49851792903550
C	-1.52006675177788	-0.17518791174857	4.70361398986064
H	-0.84493487505410	0.65491646631497	4.49089047861694
H	-2.06105421380003	0.05693147188827	5.62509661557466
H	-0.91027937023657	-1.06230130038127	4.87456308403716
C	-3.39829691161658	0.87522419821960	3.46873656669218

H	-4.04770263715528	0.91084338413158	4.34616919553092
H	-2.80752843092982	1.79224703208129	3.46379249308588
H	-4.03398528255549	0.86623108111875	2.58071010313365

retinal_cis11.xyz

C	2.06286512024872	2.57614761973628	1.68664441401656
C	0.73582547267166	2.28357259150406	1.57230711454826
H	2.69318824876258	1.78274948674810	2.06144944292094
C	2.67276392269594	3.84382752501457	1.40318997434427
H	1.98333430069756	4.67462079024931	1.30672261237684
C	3.97902522246921	4.19242046723444	1.26169669797519
H	4.15975926042125	5.25274378131769	1.11977269145197
C	5.18356828587194	3.39097083056914	1.19249555904704
C	6.36491863960121	4.05005069507662	1.04007498954579
H	6.36178169252245	5.13489430641688	1.00480434726864
C	7.68487669844506	3.46109976824440	0.89098173373821
O	8.69587124898801	4.12198523201784	0.73817641392054
H	7.75718095911530	2.35696477839800	0.91914175537171
C	5.09480843120516	1.89162503598514	1.24257727319630
H	4.84263990594732	1.55675004683444	2.25151632598915
H	4.30937451560492	1.53424786275583	0.57775752069544
H	6.02445701228515	1.41031126427250	0.95549699756554
C	-0.27988580649969	3.24954441581572	1.03320744329390
H	-0.80024976085625	2.81979988412367	0.17413673197699
H	-1.03823406883988	3.47021261940138	1.78854218381622

H	0.16304198739216	4.18643636104525	0.70844816706661
C	0.27925754600608	0.97915373244628	2.00198429302272
H	1.02196799546647	0.37376800137816	2.50575215350499
C	-0.97868276936291	0.50961036703912	1.87160136060422
H	-1.69856858894225	1.16634511883652	1.40058048981323
C	-0.81840245518634	-1.88246385770940	2.52587847956577
C	-1.34881722759025	-3.08934899530914	3.25922687546417
C	-2.56483107106935	-2.78191225382909	4.11839869200345
C	-3.56007745090008	-1.99873022924367	3.28110904193557
C	-3.00664608394854	-0.63683095168111	2.82386682169300
C	-1.52777535853795	-0.73852927349258	2.39968781133351
H	-0.53799944282120	-3.50368564029395	3.86856199909094
H	-1.59258952443039	-3.87357516774297	2.53039408850460
H	-3.01411876062727	-3.70328469913341	4.49586410936554
H	-2.26056723481277	-2.19744310038292	4.99124819260078
H	-4.49369002353583	-1.83046984770019	3.82351495658574
H	-3.81508135480193	-2.59467991949525	2.39812931262273
C	0.55432815580673	-2.10023427463743	1.95147589100857
H	0.62060630112729	-3.11269594693228	1.54200940761253
H	0.79830696318593	-1.39188558385448	1.16400857952587
H	1.32823129854003	-2.03044110552451	2.72365205129162
C	-3.14240120400214	0.39045616793250	3.96142009228770
H	-2.77670457122570	1.37067379724813	3.65199065225550
H	-4.18864024984166	0.49948769128651	4.25702039428538
H	-2.56749103759031	0.08767021538497	4.83781361599466
C	-3.87910499774055	-0.18265231377683	1.63797103487308

H	-4.93220623305949	-0.26276409565751	1.91896981133998
H	-3.70156988647826	0.85322515278459	1.34678552481511
H	-3.71180681137713	-0.81665358170132	0.76547680787292

retinal_cis13.xyz

C	1.70786539791247	2.77974908282572	1.14745776260678
C	0.38830566904792	2.44457825090449	1.15026604521097
H	2.38804055444478	2.07967677097632	1.62534773593496
C	2.32952716557069	3.92792637628980	0.56001788023884
H	1.69678512327597	4.66963630599448	0.08950293296015
C	3.67292241724094	4.10403328174100	0.55396909519199
H	4.27175658598929	3.33826453844104	1.03023057812883
C	4.37588126253303	5.21452334422354	-0.04536061698050
C	5.73351303292343	5.31475132943406	-0.04811378595905
H	6.19918336317372	6.17376501504052	-0.51918700930798
C	6.68005591125371	4.36501806297293	0.51828263757048
O	7.88640423411974	4.51830586710071	0.47982827244978
H	6.26428288077050	3.46213153132446	1.00329908166712
C	3.56940376830321	6.30278359813293	-0.70029587396715
H	2.92401204485358	5.89583899074505	-1.48257172397115
H	2.92113833331029	6.80040331004715	0.02591043233128
H	4.21954562560351	7.05172544344491	-1.14935170951549
C	-0.68500207412108	3.30066251811631	0.54176257447312
H	-1.21160763670027	2.76162178375083	-0.24943773401462
H	-1.42976397508726	3.56821404394527	1.29523754307960

H	-0.29393254123513	4.22107869412826	0.11610566456312
C	0.01289456050778	1.18528940073091	1.76053616494025
H	0.82605499293718	0.63808938093492	2.22429397556687
C	-1.22103756653034	0.64881170859562	1.79534758894477
H	-2.03822357447662	1.22710688794704	1.38085017715417
C	-0.84558640898348	-1.75734607120436	2.23602828604739
C	-1.14338205255802	-3.04773216311290	2.95830782552292
C	-2.09695576078352	-2.88376544746543	4.12992130301259
C	-3.27374838803927	-2.03105362497823	3.69105643412573
C	-2.85145845715479	-0.61137050688858	3.27267651349855
C	-1.57875677368406	-0.63728826690165	2.40730165473847
H	-0.19454542685227	-3.48185601281742	3.29253656538375
H	-1.55100748780945	-3.76765133087704	2.23616675973827
H	-2.43815560150194	-3.85713214226438	4.48998952193764
H	-1.57557077650438	-2.40542738399044	4.96341575029051
H	-4.02275615514382	-1.95538620661505	4.48384987781384
H	-3.76517311418846	-2.51944453904705	2.84274353590953
C	0.32686400296391	-1.87946286255662	1.30387358719443
H	0.24998289288707	-2.81564636562830	0.74185294019182
H	0.39975820943986	-1.05602397108859	0.59846051399295
H	1.26639032304287	-1.93570793683218	1.86442978569038
C	-2.58035440042560	0.24183448731672	4.52533914306472
H	-2.24009049449313	1.24199740114975	4.25245316737432
H	-3.48755402853183	0.33917808123702	5.12668197148726
H	-1.80477078351420	-0.20753410283599	5.14712452722935
C	-4.03530452097544	0.00075517793546	2.50088430991625

H	-4.94734106954159	-0.11858541721830	3.09052689168350
H	-3.90923178679524	1.06628152058618	2.30598501892384
H	-4.18349443147427	-0.50668416569086	1.54564593693483

retinal_mecp7.xyz

C	1.44858811820267	2.99027678450442	0.61749042141700
C	0.31125769123891	2.10229142190862	0.72900470366549
H	1.57937096712287	3.71178640233025	1.41975200181139
C	2.36579582795673	2.97356278303669	-0.40053974973177
H	2.26840066290006	2.20480842500028	-1.15817403715232
C	3.41427224198268	3.89657265793720	-0.53738411202372
H	3.45350290172348	4.72230446857558	0.16711072839261
C	4.40571058289149	3.86407507200341	-1.54260135606495
C	5.27613678523096	4.93041666653098	-1.64789467079350
H	5.16767285197708	5.75612737922166	-0.95160759050046
C	6.30669787578355	5.12074397756473	-2.64065299563012
O	6.97547859721304	6.14069574468024	-2.72626537848789
H	6.48036786242321	4.29793344970461	-3.35896311716770
C	4.46941630890259	2.66557525455878	-2.45703878325442
H	4.57151369924165	1.75115323378643	-1.86901974626707
H	3.55373520081367	2.57240380033741	-3.04549954035227
H	5.30240413717492	2.71061070736079	-3.15204899905077
C	-0.08399757935092	1.27735881625103	-0.46527076261214
H	-0.19591757137770	1.90618408072025	-1.35099458158850
H	0.67471631445225	0.52519079645906	-0.69703033098337

H	-1.01936548702769	0.75252593831852	-0.28136703589718
C	-0.32647528261963	1.99394081891260	1.90865624189516
H	0.03563856255505	2.60417554166831	2.73183581031730
C	-1.51227702612879	1.15710448974661	2.18361687204216
H	-2.43500461244396	1.68134654642792	1.97606232806986
C	-0.47418681043563	-0.95173391768991	2.89975616176157
C	-0.55352241121061	-2.44797144651382	3.00013084617995
C	-1.93917550318825	-3.02044018003803	3.27257982154728
C	-3.00149380175786	-2.25736668675569	2.50541517853862
C	-3.01274594116231	-0.74724594805233	2.81272197876857
C	-1.60045974826483	-0.14496055345926	2.61500473728734
H	0.15451156709565	-2.79641332290610	3.75814180144284
H	-0.17105619689694	-2.86082116438736	2.05184139011256
H	-1.96438878618964	-4.07701389112512	2.99434777710077
H	-2.15492850770731	-2.97373866423429	4.34285310788416
H	-3.99039479292712	-2.66248308561815	2.73947353456432
H	-2.84648967299154	-2.39775548364381	1.42940202988837
C	0.92113802250887	-0.40671018598350	2.93954129856368
H	1.59234064297018	-1.12500905692716	3.41263132747600
H	1.31508838642454	-0.20644778965349	1.93684225243768
H	0.99416644195123	0.52817073639997	3.49249297646541
C	-3.43351816207204	-0.51584133329530	4.27733490727781
H	-3.51863698018375	0.55206818537915	4.48538346006707
H	-4.40338961602954	-0.98017136941712	4.47547714749918
H	-2.70791233783779	-0.92908860270208	4.97656869170773
C	-4.07587781347325	-0.11982971437564	1.90042308957418

H	-5.01394672009882	-0.66741614007258	2.01332381627861
H	-4.28318487767688	0.92206018225719	2.14687624355269
H	-3.77865203368463	-0.17153491473187	0.85123095897082

retinal_mecp9.xyz

C	2.52480458263984	2.10670937346732	1.35521448644932
C	1.08633883774847	1.99812324892757	1.70372170254201
H	3.23375190495009	2.18932057070750	2.17510103156232
C	2.97687973055110	2.11781929343237	0.08836219077535
H	2.24397239108112	2.05742483868516	-0.70898691711943
C	4.35737030116643	2.17479219157854	-0.25954570562696
H	5.06990386487783	2.17008448389363	0.55972318792102
C	4.87170064665145	2.21893141640738	-1.55773296438073
C	6.25249867119492	2.21484513192021	-1.71832616027020
H	6.87585690292210	2.18845817702248	-0.83020839606368
C	6.98380555804647	2.21495664514075	-2.95859698497200
O	8.20635553385140	2.19133148041196	-3.01512896912474
H	6.39482028405917	2.23177157462292	-3.89408033112326
C	3.91921670702016	2.25604094465431	-2.72932892261410
H	3.41449661654225	1.29416127034240	-2.84904395977313
H	3.14527327636296	3.00811039135829	-2.57178047429261
H	4.41960365696835	2.49019297729595	-3.66358225416531
C	0.36936983703711	3.30832465829440	1.79163203189324
H	-0.63893685557779	3.21638483587670	2.19084189732161
H	0.92579482104282	4.00069541896397	2.43160829617120

H	0.31448864397899	3.78255289981978	0.80609506818460
C	0.55194841006299	0.76838476546375	1.90935912933256
H	1.24457360850726	-0.05416852251810	1.83186081919740
C	-0.81789868652347	0.49161679789775	2.19171642738470
H	-1.47320307521660	1.33877000428911	2.04431450444659
C	-0.85469968349549	-1.84238612788756	3.06807291636368
C	-1.59545395911732	-2.96644245340778	3.74310786766432
C	-3.01107507681915	-2.61729519272581	4.17148431621959
C	-3.69794125971081	-1.89238544082229	3.02936551850102
C	-3.01872995508705	-0.55179436537916	2.69120153529456
C	-1.47304220036810	-0.67759011842252	2.65220265583400
H	-1.00255702788104	-3.29915810047581	4.60252904517128
H	-1.62008579560497	-3.83164894308102	3.06367798366791
H	-3.55708258919007	-3.52115352835470	4.45097037347751
H	-2.98667863667394	-1.97986135327769	5.05925834123099
H	-4.74846511101741	-1.70012881874732	3.26175436460794
H	-3.68480837926368	-2.53633183349541	2.14369983678394
C	0.61724564528202	-2.11277844252416	2.92249480391274
H	0.86057803993834	-3.10052178524872	3.31511383798887
H	0.94017607741649	-2.08824680183192	1.87901824497443
H	1.22771869074910	-1.38746047645101	3.46711596605585
C	-3.44982943942679	0.49862519394221	3.73063939497265
H	-3.00962946210341	1.47410690119719	3.52357955358442
H	-4.53662857484572	0.61393049192469	3.72155259500118
H	-3.14373628327348	0.21061496734431	4.73759082236479
C	-3.53685589658506	-0.13247866372678	1.30124761563232

H	-4.62727764121979	-0.20381610978402	1.27448383695545
H	-3.26299018745355	0.89080385932308	1.04340699599656
H	-3.13564368919458	-0.79159216804395	0.52965487008819

retinal_mecp11.xyz

C	2.07040832380744	2.06613260623505	0.90624455241431
C	0.63849158934231	1.93136295411242	1.01351063797857
H	2.63675196300543	1.16249490776086	1.11812897572826
C	2.77113705417846	3.18053619118241	0.63374807927814
H	2.26557528372763	4.12846364701388	0.48509584267807
C	4.24686606726352	3.21478751326703	0.64431634776890
H	4.70698686082724	3.42299900480933	1.60519900025397
C	5.08463109368017	3.02611929800901	-0.41985883359335
C	6.48006837476486	3.03498889398078	-0.17946923731972
H	6.82697266214428	3.16922460525136	0.83992297894176
C	7.51108571054784	2.87818902049456	-1.16142204975470
O	8.70896016037729	2.88014943008987	-0.88545502601050
H	7.19313916870259	2.74614006800107	-2.21155217006524
C	4.54896823737074	2.82033901872140	-1.81557775030669
H	4.70349344519879	1.79216164478620	-2.15113886997394
H	3.48142490536543	3.03111777619766	-1.85613942401228
H	5.05619541601946	3.47121440681653	-2.52757888142062
C	-0.26349042820891	3.05729344070609	0.59944517848687
H	-1.13799756429489	2.68500448353168	0.06364913320532
H	-0.63274446867758	3.61476375915733	1.46713427600631

H	0.24761858383369	3.76309592545382	-0.05324596497696
C	0.13018947399105	0.75958347556173	1.57143482679188
H	0.86469133118082	0.02349619581492	1.87201233127978
C	-1.20680001537311	0.50381986447357	1.84041262451611
H	-1.89051463494261	1.31436136974912	1.62877603379295
C	-1.26073455213386	-1.90569790413607	2.43539736442882
C	-1.81749059516801	-3.05713355620831	3.23295800843134
C	-2.77813996942318	-2.62999154850633	4.32980397827018
C	-3.77640652573649	-1.65132889732360	3.73875930788356
C	-3.10975685543117	-0.35979530147259	3.23223157274432
C	-1.79431054390088	-0.65108328161272	2.47504812808380
H	-0.97822676215409	-3.62635396402151	3.64875247015840
H	-2.32423656551715	-3.74961155267948	2.54555428539381
H	-3.28919059329200	-3.49800587689340	4.75302868581392
H	-2.22117605561105	-2.16159471683499	5.14615551244072
H	-4.54699296480507	-1.38130925319453	4.46444260073219
H	-4.28975766802116	-2.14176036981477	2.90406479120851
C	-0.09444999397137	-2.31057598492887	1.57928495498841
H	-0.27511961226338	-3.30999711417437	1.17128706940744
H	0.08566840770621	-1.63152583359011	0.75057613180032
H	0.82681481907995	-2.38089302080209	2.16925238478088
C	-2.80840348707490	0.55876429683504	4.43083798617369
H	-2.32709741236578	1.48292686212922	4.10905176285619
H	-3.73138991988038	0.81952220916958	4.95459125068072
H	-2.13778401235880	0.07303543225697	5.14077635374468
C	-4.13316985409848	0.33170000869906	2.31191119481808

H	-5.08903198526019	0.41483566218356	2.83409212493585
H	-3.83764798403649	1.33872954255421	2.01925657717833
H	-4.29319174011413	-0.25265987381165	1.40446514035861

retinal_mecp13.xyz

C	1.90168210761077	2.89263153557741	1.07565089506512
C	0.52409527848518	2.58618100763941	1.20784004277875
H	2.57535409441340	2.04056408833856	1.13210935993449
C	2.48018207576981	4.11872351201681	0.89535826155256
H	1.86076582301630	5.00601712224485	0.86619997333543
C	3.90510405362033	4.26995962816961	0.73237420165528
H	4.46454262073505	3.33981649218455	0.67981364592793
C	4.60332458747102	5.41352283749716	0.61611789303875
C	6.04567200581775	5.35663832975617	0.31674699552899
H	6.77786002345991	5.37135674665289	1.11715009263006
C	6.54515225624947	5.34582013610503	-1.01506505446552
O	7.74712382042875	5.32622479672145	-1.29249253286835
H	5.78259781191044	5.34779761513283	-1.81608917726872
C	4.04848961357440	6.80531888403453	0.69038272131532
H	4.11070828138662	7.30356164088315	-0.28264411243631
H	3.01196555297158	6.82003595435022	1.02513092668666
H	4.63695417373386	7.41119903416006	1.38544124549772
C	-0.50927324062500	3.66946603588322	1.08956944750325
H	-1.45180966222625	3.28732521539242	0.70019157330228
H	-0.71878936885374	4.12034891685463	2.06542533305175

H	-0.17859475387069	4.46689383046510	0.42528590320754
C	0.17362889269377	1.25810150402930	1.51218991001701
H	1.01332629529505	0.59496813506236	1.66332075821825
C	-1.10158589024145	0.76867459274636	1.70644950179712
H	-1.90270468413470	1.48582965280951	1.58934858318541
C	-0.75463631480944	-1.66420102541974	2.11004367731120
C	-1.12892337419025	-2.94328718426951	2.81387717072220
C	-2.25497497684261	-2.78097076045912	3.81993239180568
C	-3.37131984059905	-1.99203182035561	3.16012685850230
C	-2.93579844249346	-0.56244121299813	2.78439853064195
C	-1.51776178533945	-0.53571566704868	2.16942416024611
H	-0.22957504109704	-3.34129411042543	3.29831514839058
H	-1.40555948642862	-3.69547836906817	2.06246013055565
H	-2.61246040984219	-3.75533282740207	4.16079979323726
H	-1.88930406016222	-2.25248319214724	4.70468676584040
H	-4.25228954655535	-1.92987440932558	3.80371061873642
H	-3.68363316787832	-2.52184261724115	2.25371448943200
C	0.53787012059971	-1.78419134968947	1.35170218552875
H	0.64699380073403	-2.80487862657072	0.97637013397970
H	0.59990297334067	-1.10240917195921	0.50645454148587
H	1.40218295616487	-1.60033560978712	2.00037216739321
C	-2.97168682498001	0.32864105259875	4.03965728895166
H	-2.66763022573967	1.34962212634569	3.80593673775133
H	-3.98118250398915	0.36052186278279	4.45694416424887
H	-2.29536012706471	-0.04501320450070	4.80947890899288
C	-3.97369791178091	-0.04270515378772	1.77222125616749

H	-4.97643036663204	-0.19547378019260	2.17988004509447
H	-3.86921022165209	1.02124097589523	1.55878138913832
H	-3.90383495245436	-0.58811000668208	0.82981381865485

retinal_triplet_all_trans.xyz

C	1.67759863120710	2.72267482884541	0.83638183490933
C	0.28772420011267	2.42173742280347	1.07734904186865
H	2.38101026216639	1.93698202595523	1.10076506577608
C	2.18803956556880	3.86786355757589	0.30723841083058
H	1.51385254916818	4.66671494119402	0.02423937481565
C	3.58483038451763	4.05846727565736	0.09641799239767
H	4.23607774881852	3.24688746587020	0.40746483146938
C	4.19379628069544	5.17641691280028	-0.46395349873137
C	5.58865768638835	5.18045524568880	-0.57568294596230
H	6.13044539505191	4.30209258202843	-0.23949959718572
C	6.42128915327012	6.23605327422427	-1.07488283652669
O	7.64581128236102	6.16120615217700	-1.12995645068839
C	3.34432520881739	6.34111334102525	-0.91261291576893
H	2.54835609382795	6.00432223967748	-1.57950377715024
H	2.86735845542466	6.82569455357086	-0.05692370047927
H	3.91998091418902	7.09451732299984	-1.44235166638610
C	-0.73249862828001	3.49450342614133	0.84012374355905
H	-1.73283058142590	3.18754045962306	1.13345734969773
H	-0.47762308959160	4.39717360614138	1.40237737403244
H	-0.76858080298376	3.78013824489778	-0.21565828257374

C	-0.02802332452793	1.15404094220351	1.52582107334911
H	0.81500207979283	0.48990674714304	1.67249192070860
C	-1.29667804238873	0.67040135750385	1.87797983495991
H	-2.10430273114855	1.38853754066698	1.85732530179886
C	-0.90310329203174	-1.75649681883762	2.16819404877458
C	-1.11197340480744	-3.03618407917929	2.93045900924195
C	-1.95784074595314	-2.87405868719533	4.18238880186427
C	-3.18297395753787	-2.04984813722263	3.83231375963437
C	-2.82334687901295	-0.62152850066843	3.38562226006101
C	-1.61202733732815	-0.61094296733882	2.42771348257438
H	-0.12803656290595	-3.45460037039745	3.17460183540355
H	-1.57644327712778	-3.77272542459380	2.26030017475974
H	-2.24740274605796	-3.84924442371522	4.57991051953730
H	-1.37643809278506	-2.37477724754740	4.96187189693853
H	-3.87264342289998	-1.98746933115385	4.67777069409891
H	-3.72496259672679	-2.55200627511416	3.02382007162296
C	0.11887534819963	-1.88544872043823	1.07732799644483
H	-0.00062786176584	-2.85409407273406	0.58159543164645
H	0.03817759378638	-1.10593727712554	0.32353122000086
H	1.13826851250785	-1.87371093077599	1.48068213734632
C	-2.48377998032877	0.22837381769143	4.62413078600471
H	-2.19520824150795	1.24167629275717	4.34141932166766
H	-3.34438963544367	0.28722868161562	5.29498356565805
H	-1.64853840007276	-0.20202152976037	5.17857046859384
C	-4.07164853761014	-0.03982204124517	2.69662134330233
H	-4.93492060743203	-0.15841768707592	3.35578882000009

H	-3.97907248314735	1.02243549160151	2.46894558246538
H	-4.28208620416184	-0.56898401967828	1.76570624466710
H	5.91978595211987	7.15862127871703	-1.41888152402945

retinal_triplet_cis7.xyz

C	2.27943261785974	1.88335917157563	1.49287688299520
C	1.14685648670233	1.17801280308033	2.05054419226834
H	2.05475039515197	2.69941287547034	0.81047647432715
C	3.58475742370150	1.58009479974819	1.72434012165067
H	3.81559756026616	0.73136792399797	2.35550580491273
C	4.67667374515362	2.32399053654836	1.18717924830848
H	4.43115003964770	3.25324538819183	0.68235271925415
C	6.02397617062795	1.99039516468218	1.27976892907883
C	6.96761282308400	2.91686166433550	0.82242800535049
H	6.60360761843049	3.84869805317510	0.40186394954136
C	8.39748923534846	2.80519004326145	0.87662129131833
O	9.15820692280555	3.68768215903330	0.48913664955842
H	8.81781789254104	1.87695147707377	1.30460833865477
C	6.43110250225950	0.66271816285295	1.87420222506893
H	6.44841467448772	0.70188412690967	2.96678385912053
H	5.72966057253957	-0.11813351463583	1.58169024471150
H	7.41851577605298	0.35657424837927	1.53886498380898
C	1.40572402208153	0.25597522217912	3.20298269381653
H	0.48533323645238	-0.09425030069352	3.65798984964117
H	1.98493066668689	-0.62109017541653	2.89946568149993

H	1.99742014968510	0.77748975929062	3.95978993789525
C	-0.10398349925998	1.43682783469651	1.52347205324955
H	-0.13752239831115	2.28160518705822	0.83791235992064
C	-1.35751680399761	0.84313391122957	1.76024973840648
H	-2.19486298822737	1.48237946231429	1.50478501063142
C	-1.01048073535483	-1.58565376464420	2.05539947192535
C	-1.27189038096309	-2.87919651500182	2.77831366858223
C	-2.15008656492836	-2.71938738025216	4.00810534187652
C	-3.35304903970581	-1.87527988753564	3.63059975222387
C	-2.96143949142155	-0.44602116936170	3.21318262414825
C	-1.70089171454209	-0.43777495951859	2.31984750407389
H	-0.30492872417371	-3.32196564120275	3.04476331824362
H	-1.73117535577243	-3.59234606722373	2.08058397161006
H	-2.46323365691517	-3.69391127582647	4.38905962128354
H	-1.58381466660684	-2.23418711839431	4.80805753913619
H	-4.06982880019256	-1.81458799668270	4.45353797922652
H	-3.87445947895885	-2.36133370395415	2.79910163089288
C	0.03660117142923	-1.71280043304691	0.99033797544746
H	-0.22639918195803	-2.54884924821781	0.33343582707066
H	0.14903511712729	-0.82078764008396	0.38320832785470
H	1.00917387747083	-1.96427177784032	1.42397468946943
C	-2.68349771609156	0.39760382389629	4.46995342242036
H	-2.36511900392524	1.40578612630113	4.20115249541961
H	-3.58237222705846	0.47192308982782	5.08674668014958
H	-1.89301231535771	-0.04570819642231	5.07803598785117
C	-4.17040780914592	0.14885991066392	2.46717586843430

H	-5.06816133341416	0.01013751136294	3.07437847684667
H	-4.06946223762362	1.21682788763614	2.27357455633017
H	-4.32686784868748	-0.35837327381699	1.51352304349307

retinal_triplet_cis9.xyz

C	2.27691622505510	2.45553264824763	1.57351937852760
C	0.84170133416011	2.25828733325715	1.66386338633407
H	2.62110540419349	3.48190113291122	1.67901162486388
C	3.22390047434912	1.50037566465629	1.36611382999126
H	2.90299562881851	0.48015879403657	1.19360050606648
C	4.62294766552461	1.76209252953566	1.37742438179279
H	4.93080696684403	2.78226272942445	1.58704912864276
C	5.63093136740983	0.81758187943597	1.19656887736336
C	6.96142856997308	1.21980044818405	1.34996503100005
H	7.16042140790069	2.26326602204271	1.57339108737278
C	8.12559906694570	0.37886233284131	1.31538643725979
O	9.26569790943595	0.78622131867593	1.51832368208380
H	7.96637506555672	-0.69422388426223	1.10306869841521
C	5.26704316668490	-0.61339549983596	0.87811225318350
H	4.93465326705033	-1.14148065201911	1.77572009379894
H	4.45236652840176	-0.65641064056935	0.15492527665862
H	6.10483737840594	-1.16272943823456	0.45812502603259
C	-0.03878975516571	3.46491684729113	1.47823620489388
H	-0.81857989249432	3.28453185153029	0.73532801910417
H	-0.54551323826810	3.73975357909886	2.41004581724035

H	0.53955718588445	4.32668194620696	1.14684187514211
C	0.31880754959328	1.01591267140407	1.95701688205679
H	1.03331105914678	0.23278100211458	2.15806580291585
C	-1.04349101858897	0.71965486570770	2.10772652920035
H	-1.71575283588679	1.56213599608518	2.01476923049706
C	-1.05172199815873	-1.74610091111362	2.36360835146106
C	-1.62459235850606	-2.99720903605116	2.97227120753115
C	-2.73470753136241	-2.74066577329993	3.97657490276286
C	-3.70971090397695	-1.74466431334214	3.37560381696806
C	-3.06420434371189	-0.37289175763847	3.10221306354281
C	-1.64958433494448	-0.51387571225679	2.49168011998387
H	-0.80401080483768	-3.56006761534102	3.43304781990877
H	-1.99532143879519	-3.64428247908056	2.16437067651501
H	-3.24062605841458	-3.67362078632153	4.23529917375723
H	-2.30991869901910	-2.34590698322984	4.90329862956110
H	-4.57592981073143	-1.59580102305335	4.02475259394794
H	-4.09207407354863	-2.15545568090389	2.43477774101791
C	0.21193559175425	-2.00195906032081	1.59277101828560
H	0.16644002270296	-2.99521870462033	1.13842973644766
H	0.38454851366310	-1.27295204710876	0.80500857651258
H	1.08969275999571	-2.00503332253786	2.25051829331870
C	-2.97109822038975	0.41549536607852	4.42175046213008
H	-2.51995404751139	1.39559807333175	4.26441356240406
H	-3.96610488145195	0.56191185005670	4.84860902140627
H	-2.35879630517868	-0.11176525214043	5.15466697316680
C	-4.00184763709847	0.37596038087575	2.13665072833846

H	-5.02137711671846	0.34292820608844	2.52766672422252
H	-3.73715238059446	1.42636924538008	2.01410647448309
H	-4.00051075909630	-0.09431797321728	1.15219897488835

retinal_triplet_cis11.xyz

C	2.03589643532593	2.58089589641359	1.45950970357056
C	0.63621960104868	2.26476174578853	1.32848258221290
H	2.64999932813902	1.78905860125772	1.86844232050895
C	2.61353434184674	3.77637790143282	1.16798487143973
H	1.96352912557323	4.58789219182732	0.85855277518059
C	3.99997338814013	4.14067032459085	1.28081262714342
H	4.17592292946027	5.20605078051099	1.39648660349685
C	5.14228864765610	3.35381902346397	1.22728008993690
C	6.37888540305396	3.99165351558299	1.42428982383888
H	6.38354258864742	5.06291728518499	1.59810708929672
C	7.67148524020006	3.37412504030003	1.46802902664948
O	8.70971853493780	4.00202937179471	1.66272055451760
H	7.71868105063951	2.27918522419018	1.31949521850397
C	5.07400721570530	1.87442268121104	0.94711838673041
H	4.97602661786216	1.29536908092305	1.86877366258627
H	4.21447060830921	1.64107638342584	0.32088018624649
H	5.96824507761676	1.52445055489494	0.43593513083985
C	-0.28798371741270	3.28544175095060	0.73464964367090
H	-1.23157940333398	2.85130280022699	0.41222906405020
H	-0.51212758021934	4.07674627724557	1.45765162900516

H	0.16858435000093	3.76705271988056	-0.13208375688339
C	0.21047930759020	1.03309346439001	1.79271539616703
H	0.98473608704211	0.40587905447863	2.21395402399869
C	-1.10516161774718	0.56001688473596	1.84787872322947
H	-1.87578298915784	1.25779492627465	1.55089034153012
C	-0.80106197533590	-1.81474412461887	2.48428693969169
C	-1.23325332515234	-3.02871098051111	3.26185974157633
C	-2.40716137950381	-2.76847798655671	4.19028611151098
C	-3.48093836493397	-2.03415855000720	3.40727250500495
C	-3.01680038187830	-0.64707825598587	2.92462325367235
C	-1.56365017743421	-0.67696357028166	2.40005341236417
H	-0.36879796237643	-3.40842303285656	3.81881569826675
H	-1.48904885611545	-3.82804203226055	2.55236573395578
H	-2.79358643106683	-3.70615991775978	4.59579009722241
H	-2.07857829529696	-2.16754227262587	5.04249963476920
H	-4.39033523585942	-1.90856091990949	3.99956166239459
H	-3.75640498753843	-2.64266896991297	2.53909002537389
C	0.51434342924676	-2.00794632564155	1.78337420236230
H	0.58014773450695	-3.03539938485095	1.41384752296364
H	0.65137507323861	-1.33354825684824	0.94213159934207
H	1.35979568094077	-1.87582461202326	2.46818179738710
C	-3.11179816370017	0.35886452026832	4.08674961501854
H	-2.81041103378380	1.35720775396275	3.76746949000854
H	-4.13703657648628	0.41644669927653	4.46029431121673
H	-2.46217898865801	0.07047783217125	4.91400012656842
C	-3.98823400845961	-0.21574429273189	1.81123495671987

H	-5.01441322118327	-0.32576885893915	2.17097463772830
H	-3.86015553521708	0.82512618944783	1.51286909528488
H	-3.86957037787725	-0.84135936278151	0.92511504312877

retinal_triplet_cis13.xyz

C	1.78353902318314	2.76325008704324	1.11444448089955
C	0.38058204595201	2.44055295480401	1.22756818817816
H	2.46882887070757	2.01962198848722	1.51340253783652
C	2.32793680278390	3.87639204742528	0.54889012103915
H	1.67510373611272	4.63026770548644	0.12702018530349
C	3.73636642320218	4.08494736012335	0.48532644298168
H	4.34512451971793	3.31607605837845	0.94463348434769
C	4.38016186546695	5.16748292864941	-0.10853915097666
C	5.77332212901287	5.30969380764379	-0.11463564696844
H	6.20284318062346	6.17092154153354	-0.61477723933742
C	6.74304402263405	4.43029460983130	0.48496411631125
O	7.95114471507658	4.62777016466246	0.44267383054986
H	6.36221250019291	3.53554505978034	1.01200816918613
C	3.56101234144967	6.24276306484914	-0.78016192555155
H	2.88565234441123	5.82071481708815	-1.52787189254101
H	2.94497188917386	6.78173532961051	-0.05526864478408
H	4.20453722163843	6.96736930711182	-1.27719974787143
C	-0.63013498788016	3.46260111048796	0.80026893792424
H	-1.64100119027836	3.19104071567667	1.09464165717853
H	-0.40162241893079	4.43603705967822	1.24193569579418

H	-0.62367243500305	3.59683392990977	-0.28632986846459
C	0.04652647344105	1.19252189194212	1.71071694790571
H	0.88312953284485	0.56391572913932	1.98718122425269
C	-1.24374484966938	0.68091641857626	1.93143154611455
H	-2.06138069756556	1.37787626472283	1.80825525583200
C	-0.81479537064976	-1.73068481426944	2.28131576745767
C	-1.10232623256317	-3.02795168578884	2.98590998885648
C	-2.12937484877379	-2.91335467003255	4.09923995690956
C	-3.31005989941618	-2.10471619813675	3.59228285913190
C	-2.92179930810482	-0.66150553067218	3.22100944545524
C	-1.59110082001339	-0.60764112854272	2.43705088508897
H	-0.15620082994700	-3.42781662046520	3.36993759367170
H	-1.43733018451686	-3.76250963946931	2.24016079359134
H	-2.45031747574580	-3.90364514584299	4.42976856791645
H	-1.68058689401867	-2.42370194922470	4.96745114868654
H	-4.11205937505350	-2.06937702406384	4.33423413858429
H	-3.72420009305077	-2.60184796400879	2.70863716992932
C	0.37782445747245	-1.81961673229975	1.37349763927511
H	0.40094119349058	-2.80464019610185	0.89837168291211
H	0.37774503412446	-1.06422317529836	0.59141083701445
H	1.31402170924331	-1.73072235320169	1.93692901623918
C	-2.76298349773774	0.17584743016477	4.50420801251047
H	-2.45850601733347	1.19644370213058	4.26763489578803
H	-3.70500945597826	0.21449830763094	5.05628058017865
H	-2.00016306185649	-0.24602302755785	5.16028162268629
C	-4.08495770736261	-0.09188173065450	2.38880292418926

H	-5.02187939383401	-0.25243023564804	2.92797422014165
H	-3.99737133450339	0.97890978882070	2.20246430607123
H	-4.15823058716916	-0.59961769210918	1.42574675357389

catalyst.xyz

Ir	0.17693909307973	0.00059234873043	0.00050263183573
C	-1.83134220300360	4.48317657073386	-0.29489861595087
C	-0.80705069630995	4.15836817814888	-1.17926287098350
C	-0.19733626526375	2.92539664300507	-1.04583661791628
C	-1.56937614942360	2.32366214193065	0.75415337886899
C	-2.21553995953614	3.56528743212475	0.66511181475897
C	-1.85741543752194	1.25297062005831	1.70393946392024
C	-1.29059328111817	-0.96674499407176	2.50614468079910
C	-2.19661968192115	-0.79823460849764	3.54015164703555
C	-2.97224870426008	0.34037987666103	3.68018971272477
C	-2.78830940486940	1.33870321377316	2.74824020536325
C	-2.51664276148792	-0.63102992980245	-1.22759261523072
C	-3.45316498203390	-0.73648370469580	-2.24006423936259
C	-3.04724211694233	-0.54186676368709	-3.55286474792449
C	-1.71275745543469	-0.27474583527114	-3.80922908232508
C	-0.80865483711756	-0.19612482339727	-2.75587051021697
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C	1.25378913478776	0.15638430926913	-4.17521188999726
C	2.62535796990406	0.34733738383979	-4.23558179276367
C	3.35222972261010	0.41369536007556	-3.05387878431341
C	2.67607565552368	0.29560325691007	-1.85170772192373

C	0.18293768895076	-3.03822748171641	-0.32924039494124
C	2.01870512939939	1.46211309798140	1.87352807670465
C	2.97927995215041	1.60589649632604	2.85128725079493
C	3.61475761108692	0.46471291071214	3.33919250791079
C	3.26403402968534	-0.76997102848720	2.83745561240868
C	2.27252913203202	-0.87461809816734	1.85273799450118
C	1.76454789678522	-2.09314390285562	1.24956497986249
C	2.16625777316543	-3.39648794476260	1.56914132191700
C	1.61608485385119	-4.51299200736844	0.97597356573948
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H	-3.01621543009423	3.80317780819306	1.34340494879166
H	-0.74144607839208	-1.89468377844526	2.45044029442672
H	-3.68529261791663	0.44965557485561	4.48383303165237
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H	-1.37780207685419	-0.12666864845764	-4.82439423308841
H	0.67717276598004	0.09131494782427	-5.08514347557548
H	3.12019420079654	0.44261916886411	-5.19247495376981
H	4.42320739154603	0.55972680332433	-3.05846881866633
H	3.19277355761344	0.34462135360759	-0.90368189114877
H	-0.60472309394434	-2.96063857644690	-1.06584699291444
H	1.49530803989952	2.31375368724329	1.46911463752023
H	4.37174307171831	0.54783172741063	4.10779728849410

H	3.73929736517995	-1.66110590835122	3.20846108542801
H	1.94481949840242	-5.50510608750023	1.24716944141581
N	-0.55915308172110	2.04113318414177	-0.11564094508087
C	-1.11029828064673	0.04718525881669	1.57073569067635
N	-1.22845491300960	-0.35212745526220	-1.47303822715288
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N	1.67768913562781	0.26306565171247	1.38314043808159
C	0.73745103638638	-1.91904940524574	0.28268663828308
F	-3.55224236562291	2.44123992965554	2.88023742140435
F	-2.33109300324209	-1.77396181280262	4.44839671393104
F	3.11919543425048	-3.60316567124616	2.50174941491891
F	0.07289577892481	-5.36886477374417	-0.56603187694474
C	-0.32581210397985	5.10287412542123	-2.24802112843211
C	3.29652690548573	2.95789420481500	3.42876808450558
F	2.86350344619778	3.04828784730749	4.70092522188175
F	4.62181833050597	3.18948494398581	3.44012476998397
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F	-1.26017175662336	6.00394946557781	-2.58195432795045
F	0.77256940728511	5.77724174417127	-1.85276841215560
F	0.01293880637601	4.42759763418917	-3.37128134058888

complex_catalyst_acetate.xyz

Ir	-0.01753701572929	2.80005526581563	-0.20910262759467
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C	2.21971148438782	4.67867031313438	-1.29062025478504

C	0.65320856634079	5.68705563340270	0.13032705625611
C	1.10522192482886	6.94887491598816	-0.26631281644665
C	-0.42397250267414	5.39699186561507	1.07522304521534
C	-1.83587004052628	3.70125589032498	2.09262030275253
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C	-2.00029778535850	6.01101757126070	2.83928257607882
C	-1.02856264209820	6.33901624263758	1.91612903197164
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C	-2.72305653898078	4.86311069732518	-2.90206483226772
C	-2.31281866863023	4.41409421958843	-4.14834010357779
C	-1.23992184603505	3.54166455719474	-4.22475303472708
C	-0.59222104805650	3.13619773882551	-3.06316710919073
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C	1.21257077981200	1.79627212159028	-4.21014833268103
C	2.27667281042441	0.91360594637100	-4.10455739163803
C	2.66538784565430	0.47404529156116	-2.84709475200779
C	1.98465073318752	0.94550186455737	-1.73641559219227
C	-2.55413815650688	1.12085442152184	-0.59376856889718
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C	2.73238811406438	1.36762413574430	2.80752213426277
C	2.12963726211955	0.18741789346099	3.22878522680775
C	0.92355940799933	-0.18749504461804	2.67805019223409
C	0.31596394316378	0.61498168302423	1.70877708753685
C	-0.95367949459759	0.35730030894519	1.05703707205388
C	-1.82209248086683	-0.70001969703230	1.35532152254461
C	-3.03681179325903	-0.86898628704197	0.72691087633097

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H	-2.43990870520125	6.76252778361601	3.47820890860939
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H	-3.55579077968091	5.54284628322041	-2.79226702539835
H	-2.82106234988110	4.73370588038601	-5.04759762907664
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H	2.79669408908287	0.57915809534571	-4.99169412204079
H	3.48829873100224	-0.21453733896126	-2.72036888082296
H	2.27386347110214	0.66183769213152	-0.73556999877183
H	-2.90080750291541	1.80115567878029	-1.35826203968943
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H	2.59762100190150	-0.42357348953791	3.98781887429165
H	0.44083792027774	-1.09389206617559	2.99696947824536
H	-3.69196369026235	-1.68778831580256	0.98451744542039
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C	-0.86660227069751	4.04431056843745	1.15344541255880
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C	-1.33733503206426	1.29349061215553	0.06158777061629
F	-0.66322675211309	7.63703199858915	1.85274398926758

F	-3.30637089099323	4.32804152712221	3.81294722952099
F	-1.48707991261039	-1.61166852736242	2.29195091644020
F	-4.54744252615529	-0.08654125789460	-0.87968691710647
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F	5.09819712406265	1.27382622819336	2.74615646042998
F	4.62693021304001	6.95044847028417	-2.59386067253158
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F	3.20093315380594	6.15402272701718	-4.01548071208043
C	2.94552082461220	9.61924287298821	0.91914537225818
C	1.90081704734097	10.30239679434442	1.46425779158920
H	3.16682036715841	9.79406104152410	-0.13115402465726
C	3.70652002617281	8.58883915473066	1.55910648660378
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H	4.84231496870605	7.97900260954533	-0.10790311310180
C	5.15698383001019	6.57209331180988	1.49651575349884
C	5.87642219953687	5.75472637136761	0.70611687640771
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C	6.44142714705847	4.42269436427042	1.08529796126921
O	6.64771197762965	3.61474638651038	-0.10306254808461
H	7.44010129801466	4.49365315128342	1.51966981127950
C	4.87814994486776	6.26097583271817	2.94246752762832
H	5.20399312610355	7.08812508353621	3.57638147257872

H	3.80859252757338	6.12136719412247	3.11984941354407
H	5.39268060367576	5.36737884888846	3.28176313764350
C	1.57709591739259	10.24828503593909	2.93047324699471
H	1.51719004700796	11.26135745202863	3.33438491180422
H	0.61014249317165	9.77115883369982	3.10832811146620
H	2.33007537690729	9.71616261044221	3.50376046905622
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H	1.29061158957384	11.05896640096221	-0.44830726565158
C	-0.12855138818667	11.63712060295540	1.01339619488382
H	-0.29678417219404	11.61879569509087	2.08137702969698
C	-2.02682994137285	13.12390754530155	0.92871123567480
C	-3.16944276682292	13.85658484926720	0.27830263843590
C	-3.15362149441891	13.81363701825919	-1.23858352904088
C	-2.81350742565853	12.40090837671810	-1.67857697390458
C	-1.40482444534864	11.96043993102912	-1.22982762472761
C	-1.19907421742207	12.28042482520759	0.26087749888507
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H	-4.10099746704990	13.40885869827379	0.65392088189855
H	-4.11938211805415	14.12847109895275	-1.63920984002902
H	-2.41451536062610	14.51939841415683	-1.62307664173723
H	-2.88655354958040	12.29256229136848	-2.76432347477263
H	-3.54742724486893	11.71409578768908	-1.24243436602785
C	-1.88835302349093	13.43946252035511	2.39702174815342
H	-2.79272573733507	13.92316880231773	2.76608572328703
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H	-1.05728071650608	14.12713147545756	2.57914096096307

C	-0.35373208351386	12.67658599334201	-2.09816027776330
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H	-0.48502471075125	12.40708341159547	-3.14961990014019
H	-0.44401137515128	13.75955683050110	-2.01034845318695
C	-1.33771904776854	10.44159734186207	-1.48068613471328
H	-1.67871736236259	10.22990101825550	-2.49793226974085
H	-0.33608943700177	10.03269396959351	-1.37395441546355
H	-1.99113386713505	9.90815568758772	-0.78706799842034
H	5.79215868125747	3.88177132471562	1.76754955057691
C	5.60592398510074	2.94787553790882	-0.60110919566155
O	4.50646158770447	2.91122705459644	-0.08979736135954
C	5.97524268586572	2.22796223014242	-1.86819861998117
H	6.52292181226873	1.31785963775550	-1.61438307550884
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