

Supplementary material – structure coordinates from DFT computations

“Importance of the decoration in shaped cobalt nanoparticles in the acceptor-less secondary alcohol dehydrogenation”

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Unit cell parameters

Gas phase

1.0000000000000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000

Co(0001) and 0.44A-Co(0001)

2.4700000000000000
3.0000000000000000 0.0000000000000000 0.0000000000000000
-1.5000000000000000 2.5980769230999998 0.0000000000000000
0.0000000000000000 0.0000000000000000 10.0000000000000000

Co(11-20) and 0.75A-Co(11-20)

2.4700000000000000
3.4655869999999998 0.0000000000000000 0.0000000000000000
0.0000000000000000 3.2469629999999996 0.0000000000000000
0.0000000000000000 0.0000000000000000 9.0000000000000000

Structure coordinates

Gas phase

CH₃CHOHCH₃

C 9.05727660601130 9.83848202755766 9.14990568009756
C 9.88999836062234 9.86369458777389 10.42402443093607
C 11.37864831630566 9.93238304791078 10.13972189343974
O 9.58082901898763 11.02202026389804 11.22423306114328
H 7.98087804575459 9.78257009725453 9.37741512321324
H 9.31287360850106 8.96407077538498 8.53196576706025
H 9.24199996346701 10.74994491339453 8.56162566561125
H 8.61922543268804 11.03687377764047 11.37569991274660
H 9.67882963330154 8.94935989203773 11.01424977932254
H 11.70393118522313 9.05108600526347 9.56891312203027
H 11.60722099854013 10.83533131181667 9.55405438609617
H 11.94828783059748 9.97418430006746 11.07819217830325

CH₃COCH₃

C 8.85930336589311 9.94472813343407 9.39161408337085
C 9.76699069176661 9.98036259772917 10.60073268993406
C 11.25070449483118 10.06292464347808 10.32341817596659
O 9.32552624973042 9.94626583218817 11.74351028779483
H 7.81030058092256 9.88137942751408 9.70164538617652
H 9.11326298424669 9.08541315618038 8.75126787961463

H	9.01371295204655	10.84604038320137	8.77765024843427
H	11.57113666442143	9.20518280610906	9.71158996305363
H	11.47580588462858	10.96654619525907	9.73510582559499
H	11.81325713151310	10.08115682490640	11.26346646005956

H₂

H	10.12456982289507	10.00000000000000	10.00000000000000
H	10.87543017710487	10.00000000000000	10.00000000000000

Co(0001)

Slab

Co	1.234999999999998	0.713029720000001	0.000000000000000
Co	3.705000000000000	0.713029720000001	0.000000000000000
Co	6.175000000000002	0.713029720000001	0.000000000000000
Co	-0.000000000000003	2.852109000000001	0.000000000000000
Co	2.469999999999999	2.852109000000001	0.000000000000000
Co	4.940000000000001	2.852109000000001	0.000000000000000
Co	1.235000000000001	4.991178400000001	0.000000000000000
Co	3.704999999999997	4.991178400000001	0.000000000000000
Co	-1.235000000000001	4.991178400000001	0.000000000000000
Co	0.000000000000000	0.000000000000000	2.016750060000002
Co	2.470000000000002	0.000000000000000	2.016750060000002
Co	4.939999999999998	0.000000000000000	2.016750060000002
Co	1.235000000000001	2.139079280000001	2.016750060000002
Co	3.704999999999997	2.139079280000001	2.016750060000002
Co	6.174999999999999	2.139079280000001	2.016750060000002
Co	0.000000000000003	4.278163500000000	2.016750060000002
Co	2.469999999999999	4.278163500000000	2.016750060000002
Co	4.940000000000001	4.278163500000000	2.016750060000002
Co	1.23497682501879	0.71302694463138	4.05904646246965
Co	3.70500125662219	0.71328233253065	4.05942013061739
Co	6.17498505215958	0.71302581974189	4.05908069526933
Co	-0.00004516538345	2.85213443190213	4.05908619880554
Co	2.47011064096946	2.85202166301253	4.05927296867633
Co	4.93978809852492	2.85196618462428	4.05940313939318
Co	1.23492935514950	4.99119625849530	4.05906322210116
Co	3.70496914714544	4.99120197605712	4.05905397238262
Co	-1.23502654172234	4.99118997264621	4.05902118230701
Co	-3.70479436260314	6.41710060871723	5.99952723059638
Co	-1.23468968909384	6.41710205186396	5.99939030925380
Co	1.23522326695550	6.41718368340350	5.99946541994550
Co	1.23514554394988	2.13883971201992	5.99943504721747
Co	3.70489918713957	2.13920491435725	5.99804579631305

Co	6.17513531352026	2.13879997313417	5.99947751979111
Co	0.00018892633220	4.27797018206056	5.99941756607738
Co	2.47017740746237	4.27807867610093	5.99944871631207
Co	-2.46978478586227	4.27793587909056	5.99944044571696

CH₃CHOHCH₃

Co	1.23499999999998	0.71302972000001	0.00000000000000
Co	3.70500000000000	0.71302972000001	0.00000000000000
Co	6.17500000000002	0.71302972000001	0.00000000000000
Co	-0.00000000000003	2.85210900000001	0.00000000000000
Co	2.46999999999999	2.85210900000001	0.00000000000000
Co	4.94000000000001	2.85210900000001	0.00000000000000
Co	1.23500000000001	4.99117840000001	0.00000000000000
Co	3.70499999999997	4.99117840000001	0.00000000000000
Co	-1.23500000000001	4.99117840000001	0.00000000000000
Co	0.00000000000000	0.00000000000000	2.01675006000002
Co	2.47000000000002	0.00000000000000	2.01675006000002
Co	4.93999999999998	0.00000000000000	2.01675006000002
Co	1.23500000000001	2.13907928000001	2.01675006000002
Co	3.70499999999997	2.13907928000001	2.01675006000002
Co	6.17499999999999	2.13907928000001	2.01675006000002
Co	0.00000000000003	4.27816350000000	2.01675006000002
Co	2.46999999999999	4.27816350000000	2.01675006000002
Co	4.94000000000001	4.27816350000000	2.01675006000002
Co	1.21625552717948	0.71585596634796	4.07131033203157
Co	3.70118054275294	0.72359535791531	4.05308859848827
Co	6.18150314750090	0.71462519062409	4.07075263026711
Co	-0.00585391714093	2.86158334189579	4.05332743301245
Co	2.46941437231237	2.85992465560626	4.04722036211922
Co	4.93306068871030	2.85872324548729	4.05201014742165
Co	1.22858920317476	5.00150458121609	4.04916582758059
Co	3.70124250336344	5.01878160500807	4.07234675866082
Co	-1.23857422865447	4.99953725280528	4.05081961307722
Co	-0.00673131940865	0.02244923780507	6.08786334094086
Co	2.48024183469410	0.00640524027058	5.98059939679443
Co	4.92055540207792	0.00529052095047	5.98717903886270
Co	1.23722679475684	2.17087303775262	5.97892125709965
Co	3.70003073220782	2.15134893379685	5.99589460623397
Co	6.16126291320278	2.16269345714633	5.98600676512382
Co	-0.00554145154488	4.28987728693451	5.99649113494373
Co	2.45766258711141	4.27210369833026	5.97453301269036
Co	4.93821056555610	4.26950864428063	5.97951127993988
C	1.15633494394160	1.63486219011950	9.36525884704851
C	1.18948712657840	0.16598440066997	9.01912709873906

C	-2.44336570744238	5.66109023427553	10.21758391769631
O	3.67282599713821	6.29804109662666	8.26626470090761
H	-1.65375027397558	6.38136793127817	8.34462694661438
H	0.30353393799478	1.86251079653623	10.02132568929962
H	1.06211592832727	2.24622521028133	8.44960396317122
H	2.09039871808522	1.92438329848054	9.86687755056988
H	3.53895794032498	5.32333721378587	8.24810799957361
H	-2.42391853654083	4.60718549417850	9.89719202505834
H	-3.30865175524005	5.81875587920437	10.87889497071552
H	-1.52496678208430	5.85519132117158	10.78986796973806

TS OH

Co	1.23499999999998	0.71302972000001	0.00000000000000
Co	3.70500000000000	0.71302972000001	0.00000000000000
Co	6.17500000000002	0.71302972000001	0.00000000000000
Co	-0.00000000000003	2.85210900000001	0.00000000000000
Co	2.46999999999999	2.85210900000001	0.00000000000000
Co	4.94000000000001	2.85210900000001	0.00000000000000
Co	1.23500000000001	4.99117840000001	0.00000000000000
Co	3.70499999999997	4.99117840000001	0.00000000000000
Co	-1.23500000000001	4.99117840000001	0.00000000000000
Co	0.00000000000000	0.00000000000000	2.01675006000002
Co	2.47000000000002	0.00000000000000	2.01675006000002
Co	4.93999999999998	0.00000000000000	2.01675006000002
Co	1.23500000000001	2.13907928000001	2.01675006000002
Co	3.70499999999997	2.13907928000001	2.01675006000002
Co	6.17499999999999	2.13907928000001	2.01675006000002
Co	0.00000000000003	4.27816350000000	2.01675006000002
Co	2.46999999999999	4.27816350000000	2.01675006000002
Co	4.94000000000001	4.27816350000000	2.01675006000002
Co	1.23517845002606	0.71964800604744	4.05690152592494
Co	3.70118673631630	0.71452146932896	4.04411429091842
Co	6.17001769938837	0.71409827371732	4.05532687961131
Co	-0.00136859488835	2.85415061819885	4.06797097970228
Co	2.46634799635253	2.85953544347494	4.04547238699908
Co	4.93435120076364	2.86120048698470	4.04300426916679
Co	1.21852503595912	4.98595685391654	4.06739318650169
Co	3.70284629483341	5.00418541413332	4.04804402092854
Co	-1.22498633809216	4.98638563338447	4.06349619872338
Co	-0.00838448485800	0.02300021726409	6.01946821299783
Co	-1.23106933990336	6.40135797448335	5.98632029801011
Co	1.21978193467660	6.40543171492682	5.98865883849774
Co	1.29463701318622	2.13372020704217	6.00263201518554
Co	3.70295206713091	2.13104484389819	5.97327787022884

Co	6.10916043427712	2.12289010981615	5.98202109733257
Co	-0.00332948540359	4.26711749954264	6.06798785482619
Co	2.50087319730283	4.30316364876714	5.97797974802805
Co	4.91387139022636	4.29609155228575	5.98137107656318
C	1.40246980731443	4.12337934102604	9.28078124294465
C	0.57085195384287	2.87106416876983	9.09843533947217
C	1.31086905546183	1.60596722829819	9.48843110519790
O	0.17785684877345	2.79574178226156	7.69143828708568
H	0.85093942736033	5.01462485588928	8.94830832861852
H	2.32974041152118	4.04926293137340	8.68567975803266
H	1.67742018773771	4.24712649248921	10.33935129368256
H	-0.37277411703764	2.95396853394185	9.66467434256969
H	-0.00982511814968	1.61184268867875	7.22356535986478
H	2.22665568688247	1.50846267587491	8.88360231296528
H	1.58943072680457	1.64277441593969	10.55196157733817
H	0.69088307494681	0.71366087554243	9.31809449960881

CH₃CHOCH₃

Co	1.23499999999998	0.713029720000001	0.000000000000000
Co	3.705000000000000	0.713029720000001	0.000000000000000
Co	6.175000000000002	0.713029720000001	0.000000000000000
Co	-0.000000000000003	2.852109000000001	0.000000000000000
Co	2.469999999999999	2.852109000000001	0.000000000000000
Co	4.940000000000001	2.852109000000001	0.000000000000000
Co	1.235000000000001	4.991178400000001	0.000000000000000
Co	3.704999999999997	4.991178400000001	0.000000000000000
Co	-1.235000000000001	4.991178400000001	0.000000000000000
Co	0.000000000000000	0.000000000000000	2.016750060000002
Co	2.470000000000002	0.000000000000000	2.016750060000002
Co	4.939999999999998	0.000000000000000	2.016750060000002
Co	1.235000000000001	2.139079280000001	2.016750060000002
Co	3.704999999999997	2.139079280000001	2.016750060000002
Co	6.174999999999999	2.139079280000001	2.016750060000002
Co	0.000000000000003	4.278163500000000	2.016750060000002
Co	2.469999999999999	4.278163500000000	2.016750060000002
Co	4.940000000000001	4.278163500000000	2.016750060000002
Co	1.23006397464251	0.71924567816569	4.06080174798167
Co	3.69943129929166	0.71235486730755	4.05294406894747
Co	6.17129950293065	0.72001165733768	4.06185713107513
Co	-0.00614562492959	2.85063775487293	4.08001546849778
Co	2.45729862339479	2.84833366009734	4.05973055811982
Co	4.94216643911188	2.84927745816209	4.06119546491173
Co	1.22394593670957	4.98615487628488	4.06154980747004
Co	3.70061113244995	4.99091198020495	4.04326576060783

Co	-1.23268477071813	4.98704178278279	4.06197024585382
Co	3.70178413402015	6.38821213697214	5.98369052252931
Co	2.47166557207793	0.00130852356322	5.98838408302617
Co	4.93071953416333	0.00293443768242	5.98474919562724
Co	1.27084237765303	2.11416007693743	6.05709924347761
Co	3.70175119267929	2.13210110593110	5.98439808077579
Co	6.13323039907832	2.11777740203835	6.06390451059917
Co	-0.00167559120746	4.32188069259349	6.06283923882797
Co	2.49154020082878	4.29122817023397	5.98303944083703
Co	4.91302468608583	4.29155303122666	5.98399196016223
C	1.39155706573550	3.34226131079552	9.31905665052060
C	0.03868228155562	2.83732889278878	8.85638202237847
C	-0.27267518416636	1.43334752018173	9.33629444470093
O	0.00508582010027	2.85080299353353	7.40416975161204
H	1.59347437688537	4.34267255117452	8.90614253096733
H	2.18475801538702	2.65951053605855	8.97535355540556
H	1.42368218832120	3.39965871299249	10.41716141195748
H	-0.75640510850177	3.53257800620758	9.17707033952483
H	0.49342027120619	0.73275066245004	8.96623111044996
H	-0.28344736478199	1.39705408115807	10.43564682215985
H	6.15742191766029	1.10480855464242	8.95893708433601

H

Co	1.23499999999998	0.71302972000001	0.00000000000000
Co	3.70500000000000	0.71302972000001	0.00000000000000
Co	6.17500000000002	0.71302972000001	0.00000000000000
Co	-0.00000000000003	2.85210900000001	0.00000000000000
Co	2.46999999999999	2.85210900000001	0.00000000000000
Co	4.94000000000001	2.85210900000001	0.00000000000000
Co	1.23500000000001	4.99117840000001	0.00000000000000
Co	3.70499999999997	4.99117840000001	0.00000000000000
Co	-1.23500000000001	4.99117840000001	0.00000000000000
Co	0.00000000000000	0.00000000000000	2.01675006000002
Co	2.47000000000002	0.00000000000000	2.01675006000002
Co	4.93999999999998	0.00000000000000	2.01675006000002
Co	1.23500000000001	2.13907928000001	2.01675006000002
Co	3.70499999999997	2.13907928000001	2.01675006000002
Co	6.17499999999999	2.13907928000001	2.01675006000002
Co	0.00000000000003	4.27816350000000	2.01675006000002
Co	2.46999999999999	4.27816350000000	2.01675006000002
Co	4.94000000000001	4.27816350000000	2.01675006000002
Co	1.22822279737980	0.73297976959173	4.06429217747705
Co	3.69584512432660	0.73264127808241	4.06482976988869
Co	6.16844983032037	0.73047915374842	4.05611513854075

Co	-0.00483048833861	2.86965131475594	4.05874598546345
Co	2.46193224168898	2.86977673989484	4.06454797990832
Co	4.92991818529906	2.87011420206122	4.05952830419819
Co	1.22868657199416	5.01121877480357	4.05585673793252
Co	3.69578001832127	5.01161874275478	4.05604169870663
Co	-1.24268888577076	5.01274407682037	4.05912284669336
Co	7.39741991628162	0.02089004885711	5.99292354616610
Co	2.46232742086469	0.01913408949270	6.03085191086971
Co	4.93708172566192	0.02138111557463	5.99231835425041
Co	1.22310516545935	2.16448088740511	6.03074572840506
Co	3.70130548014714	2.16386839041844	6.03049175416637
Co	-1.24214013890502	2.16298546596579	5.99314074930364
Co	-0.00571129775347	4.30288948201923	5.99338760438967
Co	2.46336519686183	4.30569952213634	5.99217183928032
Co	-2.47766088850865	4.30239021456791	5.99316539737824
H	2.46167384837851	1.44794980628563	7.02645892862807

TS OH-CH

Co	1.23499999999998	0.71302972000001	0.00000000000000
Co	3.70500000000000	0.71302972000001	0.00000000000000
Co	6.17500000000002	0.71302972000001	0.00000000000000
Co	-0.00000000000003	2.85210900000001	0.00000000000000
Co	2.46999999999999	2.85210900000001	0.00000000000000
Co	4.94000000000001	2.85210900000001	0.00000000000000
Co	1.23500000000001	4.99117840000001	0.00000000000000
Co	3.70499999999997	4.99117840000001	0.00000000000000
Co	-1.23500000000001	4.99117840000001	0.00000000000000
Co	0.00000000000000	0.00000000000000	2.01675006000002
Co	2.47000000000002	0.00000000000000	2.01675006000002
Co	4.93999999999998	0.00000000000000	2.01675006000002
Co	1.23500000000001	2.13907928000001	2.01675006000002
Co	3.70499999999997	2.13907928000001	2.01675006000002
Co	6.17499999999999	2.13907928000001	2.01675006000002
Co	0.00000000000003	4.27816350000000	2.01675006000002
Co	2.46999999999999	4.27816350000000	2.01675006000002
Co	4.94000000000001	4.27816350000000	2.01675006000002
Co	1.23553358153490	0.72575660800522	4.06369703586219
Co	3.70532152531669	0.71122115205264	4.04330412847910
Co	6.17172103136199	0.72704579258424	4.05777877782701
Co	-0.00076418617494	2.85096607276209	4.08074432733665
Co	2.45606994183055	2.84210446791947	4.06393800643500
Co	4.94180258471977	2.84821971360302	4.06645790302684
Co	1.22018608608523	4.98589875218691	4.05869426365057
Co	3.69941953306472	4.99252032938781	4.02870727718460

Co	-1.23106915817755	4.99014462606041	4.06701237437590
Co	3.69913022562590	6.38242316971309	5.96031540580675
Co	-1.22028959858151	6.41148194540611	5.99374691648711
Co	1.23485399870932	6.41639183318569	5.97315145159969
Co	1.26497524167193	2.11697422917281	6.11005910126638
Co	3.71430525831232	2.12653240407783	5.99257088274443
Co	6.13753303788870	2.11369957065601	6.05988178103784
Co	0.00437279300083	4.31999796585595	6.06195820745466
Co	2.49582698230584	4.29689760876517	5.96067730393961
Co	4.91377345847914	4.29283520906345	5.97412269003269
C	1.79496947657078	3.25504225475536	8.99892901481760
C	0.95589958965022	2.27859531352873	8.21171890981366
C	0.50569467938311	1.05974453061045	8.97987812820399
O	-0.08829682107416	2.89661132885024	7.53175900598681
H	2.07480170909209	4.12127943520548	8.37535068892532
H	2.71308289333360	2.77601888898802	9.36494459787260
H	1.21147854555494	3.62097561274970	9.86103252508835
H	2.10620526192091	1.60902032899085	7.35128713777466
H	1.36763450237655	0.48470662194924	9.34417302231705
H	-0.10557349230080	1.37914502168817	9.84104703918208
H	-0.11155576007777	0.40213327111146	8.34286814953806

CH₃COCH₃

Co	1.23499999999998	0.71302972000001	0.00000000000000
Co	3.70500000000000	0.71302972000001	0.00000000000000
Co	6.17500000000002	0.71302972000001	0.00000000000000
Co	-0.00000000000003	2.85210900000001	0.00000000000000
Co	2.46999999999999	2.85210900000001	0.00000000000000
Co	4.94000000000001	2.85210900000001	0.00000000000000
Co	1.23500000000001	4.99117840000001	0.00000000000000
Co	3.70499999999997	4.99117840000001	0.00000000000000
Co	-1.23500000000001	4.99117840000001	0.00000000000000
Co	0.00000000000000	0.00000000000000	2.01675006000002
Co	2.47000000000002	0.00000000000000	2.01675006000002
Co	4.93999999999998	0.00000000000000	2.01675006000002
Co	1.23500000000001	2.13907928000001	2.01675006000002
Co	3.70499999999997	2.13907928000001	2.01675006000002
Co	6.17499999999999	2.13907928000001	2.01675006000002
Co	0.00000000000003	4.27816350000000	2.01675006000002
Co	2.46999999999999	4.27816350000000	2.01675006000002
Co	4.94000000000001	4.27816350000000	2.01675006000002
Co	6.18107896421352	0.71211877852285	4.03084627244931
Co	1.25172163845660	0.70612100188637	4.05797657122373
Co	3.70280070447655	0.70097069259269	4.05701904949326

Co	0.01217740782666	2.86477000268732	4.06513186462863
Co	2.48272980633029	2.84630928590059	4.04296508426974
Co	4.94972847766002	2.86199213659964	4.05676932526623
Co	-1.22886067584671	4.98893812039328	4.07159432493342
Co	1.23190255291399	4.97696675698700	4.06389386607896
Co	3.72207340662232	4.98364371887771	4.05788308069851
Co	6.19257634633033	2.10473101554952	5.96764804468787
Co	1.26210500250890	2.13317482524016	5.97252289739564
Co	3.71605684467071	2.13298098221229	5.97130820195946
Co	0.05341949711938	4.24946030877704	6.10877087073196
Co	2.49149980203005	4.26007845486517	5.97179614598403
Co	4.91586574139870	4.24552256130380	6.05267157282827
Co	2.48612229961599	0.03720377337085	6.05289868308077
Co	4.97945246995325	0.00376195724902	5.96692482982322
Co	7.40105146893670	0.00739427637109	5.96436826621870
C	-0.19549282777268	4.38847728319682	8.08993058737676
C	0.74094433265360	5.31429482746197	8.82049933879469
C	-0.52643150683123	3.11597045262089	8.82390510174494
O	-1.28206965579165	5.01576888642979	7.50724665487148
H	0.32554192748805	5.55867118182301	9.81716027330977
H	1.72289060142728	4.84275032856769	8.95816095354854
H	0.87727486212049	6.26408882627544	8.27106579224134
H	-0.94270996691001	3.35588105652171	9.82140954708565
H	-1.28110602347284	2.51970642080340	8.27905874809633
H	0.37389708910045	2.50257102790805	8.96181879309110

TS CH

Co	1.23499999999998	0.71302972000001	0.00000000000000
Co	3.70500000000000	0.71302972000001	0.00000000000000
Co	6.17500000000002	0.71302972000001	0.00000000000000
Co	-0.00000000000003	2.85210900000001	0.00000000000000
Co	2.46999999999999	2.85210900000001	0.00000000000000
Co	4.94000000000001	2.85210900000001	0.00000000000000
Co	1.23500000000001	4.99117840000001	0.00000000000000
Co	3.70499999999997	4.99117840000001	0.00000000000000
Co	-1.23500000000001	4.99117840000001	0.00000000000000
Co	0.00000000000000	0.00000000000000	2.01675006000002
Co	2.47000000000002	0.00000000000000	2.01675006000002
Co	4.93999999999998	0.00000000000000	2.01675006000002
Co	1.23500000000001	2.13907928000001	2.01675006000002
Co	3.70499999999997	2.13907928000001	2.01675006000002
Co	6.17499999999999	2.13907928000001	2.01675006000002
Co	0.00000000000003	4.27816350000000	2.01675006000002
Co	2.46999999999999	4.27816350000000	2.01675006000002

Co	4.940000000000001	4.278163500000000	2.016750060000002
Co	1.23134193782698	0.73999269288360	4.05833212249426
Co	3.70497486586764	0.73916834485337	4.06024392157564
Co	6.17053440856737	0.72462102930565	4.04601445265494
Co	0.00608691717994	2.85458030892853	4.06368340812776
Co	2.47602725118367	2.85095656568127	4.08399369380104
Co	4.91980247825264	2.85339917607571	4.06323281069039
Co	1.23101733312935	5.00333136964384	4.05271842922256
Co	3.70724629068889	5.00211001747032	4.04497199570897
Co	-1.23672713622484	4.99393729203954	4.03982245633968
Co	7.40280592171992	0.00251556185451	5.96766582128711
Co	-1.23946777089255	6.37790710936540	5.95547107619976
Co	4.93866911451672	0.00170135554205	6.00149785903845
Co	1.22360314712571	2.15754844595448	6.06229326806875
Co	3.70221466398362	2.13998505586109	6.12894647443756
Co	6.16715230324052	2.13891598296990	5.98373452683864
Co	-0.00785991400484	4.28706076745993	5.98540649719327
Co	2.46999295808811	4.31862665026403	5.96867597775271
Co	-2.47041485877924	4.29221640770109	5.97195172468049
C	3.14972838125717	1.92413857400493	8.32464787536924
C	3.59881640912996	0.82634327267097	9.27550318870313
C	3.57453464442226	3.28267172429191	8.83526300987202
O	1.70791468504733	1.92876036246464	8.22843420347200
H	1.39425047725538	0.99342011779827	8.21468692644535
H	4.69718843829427	0.79889311551073	9.31814178436747
H	3.20577654020390	1.02705854985033	10.28698145609778
H	-0.44948603725576	6.25128839168983	8.94146121235181
H	3.72637605349567	0.97866726987151	7.17716949488341
H	4.66355498971106	3.40308220152296	8.75864781182228
H	3.27776283269330	3.37451475977000	9.89901313323326
H	3.09963604220963	4.10603464523987	8.27645304466687

CH₃COHCH₃

Co	1.234999999999998	0.713029720000001	0.000000000000000
Co	3.705000000000000	0.713029720000001	0.000000000000000
Co	6.175000000000002	0.713029720000001	0.000000000000000
Co	-0.000000000000003	2.852109000000001	0.000000000000000
Co	2.469999999999999	2.852109000000001	0.000000000000000
Co	4.940000000000001	2.852109000000001	0.000000000000000
Co	1.235000000000001	4.991178400000001	0.000000000000000
Co	3.704999999999997	4.991178400000001	0.000000000000000
Co	-1.235000000000001	4.991178400000001	0.000000000000000
Co	0.000000000000000	0.000000000000000	2.016750060000002
Co	2.470000000000002	0.000000000000000	2.016750060000002

Co	4.939999999999998	0.000000000000000	2.016750060000002
Co	1.235000000000001	2.139079280000001	2.016750060000002
Co	3.704999999999997	2.139079280000001	2.016750060000002
Co	6.174999999999999	2.139079280000001	2.016750060000002
Co	0.000000000000003	4.278163500000000	2.016750060000002
Co	2.469999999999999	4.278163500000000	2.016750060000002
Co	4.940000000000001	4.278163500000000	2.016750060000002
Co	1.21444528388911	0.71712827675737	4.08054861194428
Co	3.70619335029649	0.71002030019829	4.03883436760539
Co	6.18206798356611	0.70025873656850	4.06655983082670
Co	0.01053216456999	2.83644973663803	4.06446301366387
Co	2.45321387446750	2.83528103451247	4.05429086777958
Co	4.93364639307099	2.84426891893321	4.04392389876993
Co	1.23234311656108	4.98279668336545	4.05158971082836
Co	3.69746422875686	4.99939296412148	4.06460071843988
Co	-1.23908706352059	4.98043238115116	4.03944976731328
Co	3.69674978697830	6.40098653000103	6.07520607625189
Co	-1.21275784225659	6.39634915723977	5.94821297580849
Co	1.22247571840773	6.40582295690596	5.97920863467830
Co	1.21493829502657	2.12201923341896	6.12374634313401
Co	3.69173394305596	2.12724449110964	5.97413118733323
Co	6.14690356623231	2.15097913467951	5.97171786702485
Co	-0.00378304876466	4.27835363128573	5.98118869712009
Co	2.45345736723660	4.25240802500963	5.98236685015094
Co	4.93483803347573	4.26433724717401	5.96938896689445
C	0.89747074757716	1.71244392663449	8.07797155103406
C	2.17530015824209	1.78495374179030	8.89477251564594
C	-0.19188934004374	2.55805035925888	8.70945883970968
O	0.37155812333622	0.32758109606077	8.15108719618577
H	2.57618271604587	2.80767248524730	8.87638141238734
H	1.96710887319988	1.50553372216458	9.94661214885607
H	2.95774048839959	1.11716834144246	8.49632009411141
H	0.06666110631525	3.62501077655026	8.64608389281806
H	-0.32011150653194	2.27827698119396	9.77339498803792
H	-1.17502107304020	2.41531323964347	8.21682205610248
H	-2.56675376814852	6.13359551889745	8.23058529159936

TS CH-OH

Co	1.234999999999998	0.713029720000001	0.000000000000000
Co	3.705000000000000	0.713029720000001	0.000000000000000
Co	6.175000000000002	0.713029720000001	0.000000000000000
Co	-0.000000000000003	2.852109000000001	0.000000000000000
Co	2.469999999999999	2.852109000000001	0.000000000000000
Co	4.940000000000001	2.852109000000001	0.000000000000000

Co	1.235000000000001	4.991178400000001	0.000000000000000
Co	3.704999999999997	4.991178400000001	0.000000000000000
Co	-1.235000000000001	4.991178400000001	0.000000000000000
Co	0.000000000000000	0.000000000000000	2.016750060000002
Co	2.470000000000002	0.000000000000000	2.016750060000002
Co	4.939999999999998	0.000000000000000	2.016750060000002
Co	1.235000000000001	2.139079280000001	2.016750060000002
Co	3.704999999999997	2.139079280000001	2.016750060000002
Co	6.174999999999999	2.139079280000001	2.016750060000002
Co	0.000000000000003	4.278163500000000	2.016750060000002
Co	2.469999999999999	4.278163500000000	2.016750060000002
Co	4.940000000000001	4.278163500000000	2.016750060000002
Co	1.24462026248730	0.73023214465393	4.05909097265731
Co	3.70516600703851	0.72402043601929	4.05565240514025
Co	6.18238788073681	0.71711381388640	4.04423968767468
Co	0.02032493108368	2.84879179601159	4.04993752125610
Co	2.47297199931982	2.84358754916241	4.07971194459516
Co	4.93469708364158	2.84709281847809	4.06244954629697
Co	1.23400883640784	4.99467700990148	4.03863783831209
Co	3.71500231026827	4.99467243911248	4.04690696274764
Co	-1.23033139580091	4.98762392585965	4.05002194421265
Co	0.00546073058038	0.01743710810788	5.97783026823653
Co	-1.23565891605870	6.38302286153696	5.97417267350387
Co	4.95955943641855	0.00425526444660	5.96695498838627
Co	1.26776339969802	2.13476306432675	6.11441607200810
Co	3.72374044823676	2.11878421776163	6.05614342137054
Co	-1.19678091351132	2.14440843784552	5.97010034543704
Co	0.01597449120198	4.27625799254675	5.96956718709254
Co	2.48847574741856	4.32550809795113	5.97074993801199
Co	4.93351705257440	4.28140083071647	6.00140656343978
C	1.94546931825694	2.18161552466186	8.06616254055427
C	1.19845628986562	3.28857582602864	8.79367444972924
C	1.72376102474966	0.82187581412002	8.70770562971354
O	3.31961144667922	2.43331671248534	8.01592694252832
H	0.11405831617484	3.11152668229629	8.78951191166199
H	1.55054091227498	3.32432438126805	9.84274967058947
H	1.39655435471541	4.27558156933410	8.34092444092195
H	2.07661098631007	0.85568732455051	9.75642085411159
H	0.66232671892632	0.53755640838203	8.69990603609517
H	2.30744235186781	0.02325897772484	8.20529486418549
H	3.61654873848551	3.52463001113787	7.20216898495215

0.44A-Co(0001)

Slab

Co	1.234999999999998	0.713029720000001	0.000000000000000
Co	3.705000000000000	0.713029720000001	0.000000000000000
Co	6.175000000000002	0.713029720000001	0.000000000000000
Co	-0.000000000000003	2.852109000000001	0.000000000000000
Co	2.469999999999999	2.852109000000001	0.000000000000000
Co	4.940000000000001	2.852109000000001	0.000000000000000
Co	1.235000000000001	4.991178400000001	0.000000000000000
Co	3.704999999999997	4.991178400000001	0.000000000000000
Co	-1.235000000000001	4.991178400000001	0.000000000000000
Co	0.000000000000000	0.000000000000000	2.016750060000002
Co	2.470000000000002	0.000000000000000	2.016750060000002
Co	4.939999999999998	0.000000000000000	2.016750060000002
Co	1.235000000000001	2.139079280000001	2.016750060000002
Co	3.704999999999997	2.139079280000001	2.016750060000002
Co	6.174999999999999	2.139079280000001	2.016750060000002
Co	0.000000000000003	4.278163500000000	2.016750060000002
Co	2.469999999999999	4.278163500000000	2.016750060000002
Co	4.940000000000001	4.278163500000000	2.016750060000002
Co	1.24904882582550	0.73261286173992	4.09003713044129
Co	3.68423529152051	0.70890678692203	4.04876596353762
Co	6.16815601248806	0.73596756716001	4.04918445747177
Co	-0.00985438308153	2.83512579002977	4.07304982671870
Co	2.44304731251214	2.85595166184536	4.04855735722493
Co	4.95350442241349	2.87270830255026	4.07173152134491
Co	1.22406564280015	4.99764107450544	4.03114020736984
Co	3.71190340120918	4.99418457285658	4.04779908164513
Co	-1.26134101266045	5.00850818891894	4.07285557947830
Co	7.39704999106457	0.00485763304218	5.94674456023402
Co	2.48803877915044	0.00577095211687	6.08277333074451
Co	1.23156530963715	6.40793113561021	5.95303759842274
Co	1.23629592531959	2.16772309304670	6.08236109269454
Co	3.69095040992859	2.14829030695666	5.92378046713566
Co	6.15119981191665	2.12399451200027	6.07654076125773
Co	-0.00436334089202	4.28794680583374	5.95136531405432
Co	2.44627682089472	4.30388137622418	5.95284797019215
Co	4.90213198714756	4.28485061612398	6.07258880119717
C	1.97720541679419	1.17053471126402	10.14854944259912
C	2.00260630498956	1.17312242697734	8.64507260877506
C	5.32838226682497	3.09362073149348	8.63326336799113
C	5.34663550810510	3.11973574614994	10.13588475185530
O	2.55514923358994	0.18505432180854	8.05472353948145

O	1.43959491575834	2.15212660871837	8.04907533107372
O	4.74869116911550	4.06247446806562	8.03514942172281
O	5.91515816326606	2.12518696666530	8.04388015794086
H	1.01000617001285	0.75307687912278	10.46993608846884
H	2.04786997210255	2.19457641298096	10.53495752521633
H	2.78052144635885	0.54303832031735	10.55045319135629
H	4.40017204430898	3.51720769592304	10.52229436111032
H	5.54892998788669	2.12219420126221	10.54138022034904
H	-1.25775329007217	3.80149328274886	10.45058503312716

CH₃CHOHCH₃

Co	1.23499999999999	0.71302972000001	0.00000000000000
Co	3.70500000000000	0.71302972000001	0.00000000000000
Co	6.17500000000002	0.71302972000001	0.00000000000000
Co	-0.00000000000003	2.85210900000001	0.00000000000000
Co	2.46999999999999	2.85210900000001	0.00000000000000
Co	4.94000000000001	2.85210900000001	0.00000000000000
Co	1.23500000000001	4.99117840000001	0.00000000000000
Co	3.70499999999997	4.99117840000001	0.00000000000000
Co	-1.23500000000001	4.99117840000001	0.00000000000000
Co	0.00000000000000	0.00000000000000	2.01675006000002
Co	2.47000000000002	0.00000000000000	2.01675006000002
Co	4.93999999999998	0.00000000000000	2.01675006000002
Co	1.23500000000001	2.13907928000001	2.01675006000002
Co	3.70499999999997	2.13907928000001	2.01675006000002
Co	6.17499999999999	2.13907928000001	2.01675006000002
Co	0.00000000000003	4.27816350000000	2.01675006000002
Co	2.46999999999999	4.27816350000000	2.01675006000002
Co	4.94000000000001	4.27816350000000	2.01675006000002
Co	1.20688426059589	0.72294944067506	4.06404932877023
Co	3.71629021600280	0.72512013002619	4.06793962325577
Co	6.17402839569523	0.71253446098809	4.11832972351652
Co	-0.01156778537450	2.83577444058867	4.05536317465665
Co	2.46753678684523	2.83569382353474	4.05701829963288
Co	4.92769081630526	2.83008225315008	4.06682588946893
Co	1.23518596236861	5.01316582822728	4.03537844192920
Co	3.69901038370580	5.00858930742707	4.05231354788280
Co	-1.24543135469068	4.99488582641752	4.01740058057814
Co	-3.67864070730561	6.39484910993694	6.08828785894538
Co	-1.25866734683631	6.41504627162510	5.93035532376959
Co	1.20350971943032	6.40202951805167	6.04949499034810
Co	1.21860167382919	2.18002983196914	6.02857330427666
Co	3.67579310193189	2.13053476593972	6.06283706365756
Co	-1.24525536573019	2.17966404268238	6.05161433255159

Co	-0.01560659683108	4.31288207937629	5.91151849684967
Co	2.47558390621847	4.28626157574778	5.93789220129944
Co	4.93661212987133	4.28093171475016	5.94081222445323
C	1.21912151738261	0.29736155910771	10.14463046101566
C	-2.99979097105095	5.66038035730344	9.18285604523909
C	3.55699548769303	4.61918992533025	9.87510520782608
C	4.45204290460158	1.13813754212591	10.16051909172736
C	4.24967905943303	1.01919156592434	8.67607354093274
C	0.00069323655429	3.64970284680513	9.89002051716667
C	-0.02503473897800	3.03075927213505	8.52178574484859
O	3.64040350011382	6.32526839560447	8.15443937218784
O	4.79415685918042	0.00039723849542	8.09946677687404
O	3.58992318842818	1.89980560061249	8.06154450242809
O	1.08583617836552	2.98597655337655	7.88702492134587
O	-1.13596909468762	2.64031496834693	8.03994710588836
H	-2.15917464369644	5.17717358498643	8.65531428912807
H	0.37487887719639	0.74236721061613	10.69385918330554
H	1.74018562035236	1.09078778648301	9.59623341555161
H	-1.80258980309827	6.26781478694229	10.88089686867851
H	2.65773132163342	6.28949148071511	8.35509584858863
H	3.19457395185519	3.85977675902503	9.17117127804815
H	2.69699736455388	5.10859476468718	10.35854995300802
H	4.14272270306723	4.12435424786684	10.66292337616809
H	4.30871314729298	0.17088578662485	10.65732316397033
H	3.78260993185030	1.88621625254773	10.59257304323438
H	5.49383153364091	1.44885893128316	10.32457458301051
H	0.81568249697319	3.22495267813866	10.48829621589763
H	0.21661372265996	4.71848140635150	9.74928194930455
H	-0.96039095863257	3.53371849081481	10.40132117392118

TS OH

Co	1.23499999999998	0.71302972000001	0.00000000000000
Co	3.70500000000000	0.71302972000001	0.00000000000000
Co	6.17500000000002	0.71302972000001	0.00000000000000
Co	-0.00000000000003	2.85210900000001	0.00000000000000
Co	2.46999999999999	2.85210900000001	0.00000000000000
Co	4.94000000000001	2.85210900000001	0.00000000000000
Co	1.23500000000001	4.99117840000001	0.00000000000000
Co	3.70499999999997	4.99117840000001	0.00000000000000
Co	-1.23500000000001	4.99117840000001	0.00000000000000
Co	0.00000000000000	0.00000000000000	2.01675006000002
Co	2.47000000000002	0.00000000000000	2.01675006000002
Co	4.93999999999998	0.00000000000000	2.01675006000002
Co	1.23500000000001	2.13907928000001	2.01675006000002

Co	3.704999999999997	2.139079280000001	2.016750060000002
Co	6.174999999999999	2.139079280000001	2.016750060000002
Co	0.000000000000003	4.278163500000000	2.016750060000002
Co	2.469999999999999	4.278163500000000	2.016750060000002
Co	4.940000000000001	4.278163500000000	2.016750060000002
Co	1.24226585667942	0.67725317999680	4.06929077039708
Co	3.71845189744219	0.67318726528735	4.07674047774573
Co	6.18407922334707	0.68016720818514	4.09337020610005
Co	0.00689751204370	2.83909899601169	4.01759920084257
Co	2.48388259047058	2.84804697506736	4.02128330908631
Co	4.95193670909658	2.83747156379538	4.05044590836462
Co	1.26656313276253	4.99146357357225	4.07200634746125
Co	3.71621180321855	4.98101241793513	4.08515189734169
Co	-1.23804776045238	4.98969274022703	4.05789950077952
Co	-3.68874276863607	6.39761020742458	6.08061574168208
Co	-1.25038563772738	6.40706365535529	6.06844714298625
Co	1.23782469834500	6.38514438331719	6.13355228455014
Co	1.23272343310850	2.13076859010205	5.91351808030554
Co	3.68812804176721	2.10763455205922	5.93805831671710
Co	-1.17852574027959	2.13277127913821	5.96939725015094
Co	0.00248884098097	4.27449864766850	5.92811086470459
Co	2.46559038128196	4.21365683629022	6.01190481392864
Co	4.95733309361708	4.23394460861151	6.02634167237487
C	-0.98917836820091	3.67095289966811	9.39869150187579
C	5.06688025019419	3.09126644389708	9.07649591872177
C	4.78494043085802	1.83769312377780	9.86877952215898
C	1.28567403086647	0.63386845742020	10.13177357184981
C	1.23091657250074	0.38823971382982	8.64696440222652
C	1.82910599263079	4.86291402297081	10.11941376460327
C	1.75470349090616	4.91193088846241	8.61771834451316
O	5.00637469873684	2.82405318266749	7.63719374500237
O	0.10444908113439	0.16812139186736	8.09825559449693
O	2.33861694266400	0.41805692053218	8.01812523332688
O	2.32541759887240	3.96422125397822	7.97843953417563
O	1.14405607353585	5.87985454376099	8.07059034325761
H	-0.81388914949335	4.60917932041685	8.85866706211621
H	-0.20602341914418	2.94896748782860	9.12548851431471
H	-0.91563866972204	3.86496091090800	10.47987505801705
H	4.26953885103349	3.83029553685607	9.23611359411830
H	4.97312697107509	1.60288114508808	7.17851014175360
H	5.62376970152639	1.13984045637732	9.76211569057848
H	4.66569249666351	2.09811144675376	10.93182848102566
H	3.88379603950075	1.33523529752042	9.50265370705664
H	1.78098148395390	1.59625231739389	10.31745433561404

H	-1.80424367790280	6.27345305828825	10.60660465280745
H	0.28523505805059	0.64590764006803	10.57538649122628
H	1.03627385792166	5.46525814717889	10.57332614445033
H	2.80156111134994	5.27478939999064	10.42419911007327
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Co	3.70500000000000	0.71302972000001	0.00000000000000
Co	6.17500000000002	0.71302972000001	0.00000000000000
Co	-0.00000000000003	2.85210900000001	0.00000000000000
Co	2.46999999999999	2.85210900000001	0.00000000000000
Co	4.94000000000001	2.85210900000001	0.00000000000000
Co	1.23500000000001	4.99117840000001	0.00000000000000
Co	3.70499999999997	4.99117840000001	0.00000000000000
Co	-1.23500000000001	4.99117840000001	0.00000000000000
Co	0.00000000000000	0.00000000000000	2.01675006000002
Co	2.47000000000002	0.00000000000000	2.01675006000002
Co	4.93999999999998	0.00000000000000	2.01675006000002
Co	1.23500000000001	2.13907928000001	2.01675006000002
Co	3.70499999999997	2.13907928000001	2.01675006000002
Co	6.17499999999999	2.13907928000001	2.01675006000002
Co	0.00000000000003	4.27816350000000	2.01675006000002
Co	2.46999999999999	4.27816350000000	2.01675006000002
Co	4.94000000000001	4.27816350000000	2.01675006000002
Co	1.22637863586837	0.70531407348267	4.08499620758047
Co	3.67848713359649	0.72232347630003	4.05415426714574
Co	6.18487885560425	0.72364814835254	4.04206814378372
Co	-0.00566385882735	2.84923520218311	4.05610091698360
Co	2.47042903036776	2.83594982860222	4.05381094705841
Co	4.92617996751554	2.85915612092062	4.06669665426382
Co	1.22369998973534	4.98408060300004	4.01410594644234
Co	3.71135933218468	5.00543675018957	4.05065208413042
Co	-1.25302205078922	4.99825599875373	4.06606693810972
Co	3.66150526018207	6.40810964946662	6.03078172798090
Co	-1.21290528632090	6.41405917956577	6.05179272743554
Co	1.23912994421814	6.39721997354528	5.89963940263841
Co	1.26083450217308	2.13575511738855	6.03234305800906
Co	3.72345028848617	2.11438143830842	6.04706640697325
Co	6.16622557918331	2.14214596522747	6.01841270930272
Co	0.01354668768468	4.30266164229659	5.98097997153976
Co	2.46841622435337	4.27000658689399	5.91671902971054
Co	4.90185445907434	4.28628820257347	6.02044011384333
C	1.31772778616897	4.02489042301378	9.10457882995597

C	0.00335634614025	3.35234418575111	8.79680850421703
C	-0.27040502186037	2.18484874171668	9.71399435228018
C	3.55347120120571	0.83860059680154	10.12563835320632
C	3.42892423339491	0.87964676802107	8.62561053625969
C	4.11245483545419	5.21730614838612	10.07350576965676
C	4.08888734464549	5.26802818925719	8.57192158101956
O	0.01002170922488	2.92565176352376	7.40310159809531
O	2.69424678520068	0.00932040882144	8.05793462041950
O	4.04374335178390	1.80614905898235	8.00621669103053
O	4.68242990174906	4.32952989489951	7.95662173164007
O	3.48315149072996	6.23012454260812	7.99252140247552
H	1.44103700533866	4.93457312054489	8.49962744499801
H	2.15880531423973	3.34769751682136	8.89264484953044
H	1.35794071310785	4.30914418844755	10.16642121397002
H	-0.81861781334831	4.07541456765563	8.87051280572386
H	0.57142256842859	1.48282985236933	9.71216582636439
H	-0.42166177597583	2.56180934107682	10.73754179704110
H	6.24612383061169	1.64763515538213	9.38333576868710
H	2.71011542689667	1.39606742625663	10.56223203125608
H	4.48319794753549	1.31802916764948	10.44906821943421
H	-0.19477720166325	6.22295402517266	10.49021796385868
H	4.08450002506154	4.17435669756816	10.41004343003458
H	3.28403986082456	5.78872912259402	10.50354394520513
H	-2.35172561525941	5.66093180059816	10.41374469974830

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Co	1.23499999999998	0.71302972000001	0.00000000000000
Co	3.70500000000000	0.71302972000001	0.00000000000000
Co	6.17500000000002	0.71302972000001	0.00000000000000
Co	-0.00000000000003	2.85210900000001	0.00000000000000
Co	2.46999999999999	2.85210900000001	0.00000000000000
Co	4.94000000000001	2.85210900000001	0.00000000000000
Co	1.23500000000001	4.99117840000001	0.00000000000000
Co	3.70499999999997	4.99117840000001	0.00000000000000
Co	-1.23500000000001	4.99117840000001	0.00000000000000
Co	0.00000000000000	0.00000000000000	2.01675006000002
Co	2.47000000000002	0.00000000000000	2.01675006000002
Co	4.93999999999998	0.00000000000000	2.01675006000002
Co	1.23500000000001	2.13907928000001	2.01675006000002
Co	3.70499999999997	2.13907928000001	2.01675006000002
Co	6.17499999999999	2.13907928000001	2.01675006000002
Co	0.00000000000003	4.27816350000000	2.01675006000002
Co	2.46999999999999	4.27816350000000	2.01675006000002
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Co	1.23485273216388	0.70691637018677	4.03781408697422
Co	3.70525047252371	0.71265563402134	4.03619381099470
Co	6.18023421834880	0.72469952549210	4.04664256687857
Co	-0.01168179142873	2.85774320416037	4.07723101594401
Co	2.47505437008790	2.85531567403424	4.03812389395575
Co	4.96167848707001	2.85434827680157	4.07597956754064
Co	1.22856631752627	4.97940146412686	4.04714926234615
Co	3.72260460943326	4.98061314821525	4.05621565220369
Co	-1.22625045384857	4.97125484254647	4.07465668785460
Co	3.69661178763469	6.41024375320989	5.96926724537774
Co	2.47248128647753	0.00753335724590	5.98332478738937
Co	4.91209097127754	0.01556417464556	5.94109961265935
Co	1.26047684500664	2.12485094034174	5.96667715664715
Co	3.69953526265937	2.13414707214857	5.98441676013367
Co	6.18554015424643	2.11628613666008	6.05202461675878
Co	0.02415774892311	4.27676344669747	6.05035306845841
Co	2.47370899836800	4.29042220945640	5.97278038328918
Co	-2.46601783535883	4.27748346659369	6.05345712558414
C	-0.35285993563197	3.04583100728395	10.10409333631817
C	-0.39872372808463	3.08288709594232	8.60156294465844
C	3.38850953678357	5.16476970395904	9.95271373695855
C	3.66854476833482	5.01625569935748	8.49106669205252
O	-0.96944967383450	2.10389841849726	8.01269550957431
O	0.16134620537364	4.06515813843399	8.01012439934843
O	4.70738011129016	4.42655318126031	8.08555191909407
O	2.78054787956644	5.50780750515414	7.67839952924813
H	2.47812658740236	1.42151708230208	6.99226549779417
H	-1.34937239730978	2.79988309543027	10.49301964389636
H	-0.01250091370785	4.00621610213155	10.50592534384635
H	0.33757961724785	2.25051004715819	10.42433582416960
H	3.02050215872809	6.18020941645110	10.14952650985070
H	4.27843082767581	4.94088588814759	10.55048956638568
H	2.57989228837751	4.46650228302447	10.21760769733841

TS OH-CH

Co	1.23499999999998	0.71302972000001	0.00000000000000
Co	3.70500000000000	0.71302972000001	0.00000000000000
Co	6.17500000000002	0.71302972000001	0.00000000000000
Co	-0.00000000000003	2.85210900000001	0.00000000000000
Co	2.46999999999999	2.85210900000001	0.00000000000000
Co	4.94000000000001	2.85210900000001	0.00000000000000
Co	1.23500000000001	4.99117840000001	0.00000000000000
Co	3.70499999999997	4.99117840000001	0.00000000000000
Co	-1.23500000000001	4.99117840000001	0.00000000000000

Co	0.000000000000000	0.000000000000000	2.016750060000002
Co	2.470000000000002	0.000000000000000	2.016750060000002
Co	4.939999999999998	0.000000000000000	2.016750060000002
Co	1.235000000000001	2.139079280000001	2.016750060000002
Co	3.704999999999997	2.139079280000001	2.016750060000002
Co	6.174999999999999	2.139079280000001	2.016750060000002
Co	0.000000000000003	4.278163500000000	2.016750060000002
Co	2.469999999999999	4.278163500000000	2.016750060000002
Co	4.940000000000001	4.278163500000000	2.016750060000002
Co	1.28146814929476	0.72759674378743	4.06719627783987
Co	3.73420492408091	0.71962820418973	4.09125459706158
Co	6.18166104141825	0.72600369562275	4.02741312046739
Co	0.02279410342501	2.84958598826478	4.05522337398839
Co	2.49577225988534	2.82819922312582	4.07072472545817
Co	4.95408983769146	2.86948578319796	4.07661369354532
Co	1.24523962880471	4.99827433474371	4.02224803962884
Co	3.73078840240416	4.99585800428924	4.00783112309719
Co	-1.22213060532365	5.01039268482995	4.06889936321728
Co	0.04104524548810	0.00332494748514	5.90185948013768
Co	-1.16252022614767	6.41221694271557	6.08639920098356
Co	1.32094050274698	6.36466503922590	5.98839922775114
Co	1.26386018691934	2.13397227813912	6.09703555626781
Co	3.77051312321944	2.14175538985008	6.08114888235227
Co	6.17659975282510	2.12488733271566	5.98609060568946
Co	0.02849683378768	4.28807003810173	5.96353557714410
Co	2.50501420604753	4.27387659769478	5.90368509964259
Co	4.90928929524245	4.32975340819617	6.00132066645293
C	1.66814019707539	3.06158149899344	9.11797809779950
C	0.84376381017997	2.22931324749200	8.17582641061220
C	0.30267605023742	0.99100057380206	8.82944552596588
C	4.96911721178667	3.36862907016792	10.05854323118967
C	4.63958890550780	3.30851151374478	8.59355074962028
C	0.42056393408792	6.09482618889780	10.10400857140899
C	0.34447930447766	6.07751691684293	8.60191581350480
O	-0.11992818137845	2.94959466951804	7.49379035002612
O	4.36985429725275	2.18554981595738	8.06131639385955
O	4.67412853085973	4.40644015685174	7.95508422596349
O	1.42995011277863	5.96652195581259	7.93722890553371
O	-0.80239367985112	6.16577853212103	8.07698663348589
H	2.13403403862763	3.92531344623776	8.63331841705272
H	2.43388129134203	2.43039072279217	9.57869635686134
H	1.00427519756794	3.42995817141800	9.91734935450732
H	2.14118435067338	1.64806152161149	7.27322627201017
H	1.11475297738555	0.33406084910402	9.15184173794874

H	-0.30419315944345	1.29980704567914	9.69974700940990
H	7.04120863012979	0.42488144884219	8.16974131282640
H	4.46805269209663	4.22758129868312	10.52275746163090
H	-1.35565024295694	3.52335161432827	10.14724125634920
H	4.70700926338368	2.44114580906233	10.57640825316276
H	-0.20598526118232	5.29633004786771	10.52188293476223
H	3.70706793644736	0.62815176918196	10.46021122429049
H	1.45279052529164	5.98718699207259	10.45315414323774

CH₃COCH₃

Co	1.23499999999998	0.713029720000001	0.000000000000000
Co	3.70500000000000	0.713029720000001	0.000000000000000
Co	6.175000000000002	0.713029720000001	0.000000000000000
Co	-0.000000000000003	2.852109000000001	0.000000000000000
Co	2.46999999999999	2.852109000000001	0.000000000000000
Co	4.940000000000001	2.852109000000001	0.000000000000000
Co	1.235000000000001	4.991178400000001	0.000000000000000
Co	3.70499999999997	4.991178400000001	0.000000000000000
Co	-1.235000000000001	4.991178400000001	0.000000000000000
Co	0.000000000000000	0.000000000000000	2.016750060000002
Co	2.470000000000002	0.000000000000000	2.016750060000002
Co	4.93999999999998	0.000000000000000	2.016750060000002
Co	1.235000000000001	2.139079280000001	2.016750060000002
Co	3.70499999999997	2.139079280000001	2.016750060000002
Co	6.17499999999999	2.139079280000001	2.016750060000002
Co	0.000000000000003	4.278163500000000	2.016750060000002
Co	2.46999999999999	4.278163500000000	2.016750060000002
Co	4.940000000000001	4.278163500000000	2.016750060000002
Co	1.232485540000001	0.682769750000001	4.067200800000005
Co	3.701171500000000	0.690137759999998	4.052899500000000
Co	6.187473500000001	0.686030150000001	4.052701899999997
Co	0.006196933600002	2.865323499999999	4.047737200000005
Co	2.473013399999999	2.848478099999999	4.015800099999995
Co	4.953486199999997	2.863471000000002	4.031904500000000
Co	1.218979579999999	4.993722499999999	4.068065299999997
Co	3.732911000000000	4.991252499999998	4.076018700000007
Co	-1.224838420000002	4.981100800000000	4.120206999999995
Co	3.691093899999999	6.395472199999998	6.070914200000006
Co	2.468972480000001	0.033347717000000	6.052833800000008
Co	4.939431899999999	0.051919894000001	6.014697000000001
Co	1.244240270000000	2.134159040000001	5.934446699999992
Co	3.706012700000000	2.166926060000000	5.910314799999995
Co	-1.201701929999999	2.142448360000001	5.926962600000003
Co	0.037480273999998	4.251314600000001	6.094675599999992

Co	2.46719161000000	4.27201320000000	5.93405150000004
Co	4.941037400000002	4.23906339999999	6.064442800000008
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C	3.673013500000002	0.897202800000001	8.519030000000006
C	-2.94759919999999	5.32546819999999	10.13445940000003
C	4.260181900000003	5.19327379999998	8.64579039999997
C	0.45571006000000	3.80622060000002	9.13368950000001
C	1.10441109999999	4.47568940000000	10.30619849999993
C	-0.07070868999999	2.43269312000002	9.28287749999997
O	2.573863500000002	0.45863454000000	8.05652249999998
O	4.77191649999998	0.915750030000001	7.86297330000004
O	4.812745600000002	4.19606069999998	8.07289860000005
O	3.58387120000000	6.09134110000000	8.05215059999996
O	0.42676660000000	4.41868179999998	8.04916189999996
H	3.96405359999999	2.556672300000001	9.773962900000004
H	4.49295469999998	1.03520663999999	10.50246470000003
H	2.732388100000001	1.39908456999998	10.39842829999997
H	3.826030000000001	6.11112580000000	10.55379129999996
H	-1.89467772000000	5.59511809999999	10.29545400000003
H	4.278534000000001	4.37530860000000	10.65185030000003
H	0.342729790000001	4.71819399999998	11.06577289999992
H	1.81442741999998	3.78487979999999	10.78708279999995
H	1.620401510000001	5.38595849999999	9.98294959999996
H	-0.19817279299999	2.15334352999998	10.33766629999999
H	-1.01323352000002	2.30523865000001	8.73431520000006
H	0.647018970000002	1.726369450000001	8.82533469999999

TS CH

Co	1.23499999999998	0.713029720000001	0.00000000000000
Co	3.70500000000000	0.713029720000001	0.00000000000000
Co	6.175000000000002	0.713029720000001	0.00000000000000
Co	-0.000000000000003	2.852109000000001	0.00000000000000
Co	2.46999999999999	2.852109000000001	0.00000000000000
Co	4.940000000000001	2.852109000000001	0.00000000000000
Co	1.235000000000001	4.991178400000001	0.00000000000000
Co	3.70499999999997	4.991178400000001	0.00000000000000
Co	-1.235000000000001	4.991178400000001	0.00000000000000
Co	0.00000000000000	0.00000000000000	2.01675006000002
Co	2.470000000000002	0.00000000000000	2.01675006000002
Co	4.93999999999998	0.00000000000000	2.01675006000002
Co	1.235000000000001	2.139079280000001	2.01675006000002
Co	3.70499999999997	2.139079280000001	2.01675006000002
Co	6.17499999999999	2.139079280000001	2.01675006000002
Co	0.000000000000003	4.27816350000000	2.01675006000002

Co	2.469999999999999	4.278163500000000	2.016750060000002
Co	4.940000000000001	4.278163500000000	2.016750060000002
Co	1.22401994904934	0.71542700084467	4.03137681733080
Co	3.73916366671336	0.70971153040908	4.06109803676980
Co	6.17960599620684	0.70642792399376	4.10819227322627
Co	-0.00644018605785	2.84590397553509	4.08244154787203
Co	2.48057629523135	2.82457020404668	4.04873076514271
Co	4.93539328091933	2.81529187067597	4.06373311342589
Co	1.21926902506823	4.99411066452113	4.06113688383751
Co	3.70279991746920	4.99761388560474	4.01281614680093
Co	-1.22527740418893	4.96660663469427	4.01673761664684
Co	-3.64410878753854	6.37611860008190	5.99508861322274
Co	-1.20084840186929	6.37966229018507	5.89191167961746
Co	1.28492343812269	6.37800107262228	6.11446190566711
Co	1.24940076809806	2.13073298010777	5.98460374856124
Co	3.67402981534019	2.11207240880695	6.10056759784306
Co	6.15963823068179	2.14919890426558	6.07770962514271
Co	-0.02867624560931	4.28190768811869	6.02589406839241
Co	2.48066472317123	4.25516258963979	5.90327328293855
Co	4.91965988561470	4.25638545449547	5.89971700321122
C	2.94424345308408	1.97607726745440	8.26573780947299
C	3.25938547359220	0.98063930173502	9.35781630335086
C	3.29515356849524	3.37073890715939	8.68489700655142
C	-0.61872364166433	3.44823306791466	10.13892842226843
C	-0.69827537426695	3.37325643831411	8.63695241130606
C	2.87850238865976	6.22158988596883	10.15975251155328
C	2.82889162756523	6.22146113069592	8.65863025423197
O	1.54551150181250	1.97805846748697	8.01650840559611
O	-1.18512299144280	2.32417031511795	8.10459468036220
O	-0.26595602489923	4.37255395185104	7.98276508069960
O	1.72003509323529	6.12168170241406	8.07814273371608
O	-3.45761659569779	6.27148329713937	8.02156781643535
H	1.12099765572009	1.07030909958179	8.20400467891516
H	4.30233767255376	1.09320158235308	9.66364534075097
H	2.60895938150135	1.22754732694174	10.21865509338076
H	-0.60456857478968	6.35658516196123	9.05528274088175
H	3.63143884815925	0.91708235111645	7.12332191221602
H	4.35102278342788	3.61121668086159	8.56893620992608
H	3.01278622384355	3.50627572920574	9.74879495970316
H	2.68455826948253	4.07195512363839	8.10208498685536
H	-1.54618176953767	3.07967277463783	10.59771914915833
H	-0.41753444202722	4.47520380200491	10.46371172935068
H	0.21093335886501	2.80643953849104	10.47238712724925
H	2.05860459660963	5.61556690498377	10.56244726608844

H	3.84519138550878	5.84688779338866	10.51641951303613
H	6.45386768818315	0.83481444402275	10.51657754120496

CH₃COHCH₃

Co	1.23499999999998	0.71302972000001	0.00000000000000
Co	3.70500000000000	0.71302972000001	0.00000000000000
Co	6.17500000000002	0.71302972000001	0.00000000000000
Co	-0.00000000000003	2.85210900000001	0.00000000000000
Co	2.46999999999999	2.85210900000001	0.00000000000000
Co	4.94000000000001	2.85210900000001	0.00000000000000
Co	1.23500000000001	4.99117840000001	0.00000000000000
Co	3.70499999999997	4.99117840000001	0.00000000000000
Co	-1.23500000000001	4.99117840000001	0.00000000000000
Co	0.00000000000000	0.00000000000000	2.01675006000002
Co	2.47000000000002	0.00000000000000	2.01675006000002
Co	4.93999999999998	0.00000000000000	2.01675006000002
Co	1.23500000000001	2.13907928000001	2.01675006000002
Co	3.70499999999997	2.13907928000001	2.01675006000002
Co	6.17499999999999	2.13907928000001	2.01675006000002
Co	0.00000000000003	4.27816350000000	2.01675006000002
Co	2.46999999999999	4.27816350000000	2.01675006000002
Co	4.94000000000001	4.27816350000000	2.01675006000002
Co	1.21685372118889	0.73089926081319	4.06147446932070
Co	3.72065713914325	0.70584257585096	4.01159051508365
Co	6.18069300188981	0.70166548611213	4.10062254579060
Co	-0.00092019944478	2.81729479862193	4.06988513017857
Co	2.44716037905203	2.84879083969127	4.05568525488917
Co	4.96173925708124	2.85563429247955	4.05645239232232
Co	1.25013196596918	4.99104090659747	4.03211525916478
Co	3.71760334042392	4.99378973132368	4.07943922703122
Co	-1.24567056847792	4.98444728909365	4.02328742746940
Co	0.04159110042253	0.01796843125287	6.07680122058364
Co	2.47087381409374	0.03089187285893	5.90199326206037
Co	1.18412668545631	6.37785015198004	5.99446348407687
Co	1.23288597074321	2.20848592044366	6.16321724355872
Co	3.68930008252375	2.13258074680116	5.90905606166514
Co	6.14304213933221	2.10079148809442	6.08174755955354
Co	-0.02120057467500	4.25330630233675	5.90409668271020
Co	2.47790677008791	4.26534666485490	5.97823624566967
Co	-2.42853274077083	4.28747402530660	6.02108850819768
C	1.60002060825822	2.87357510672680	8.11734170774213
C	0.51477929839953	3.10771857576129	9.13765208622601
C	2.63207122883722	1.92123481354972	8.65367740251436
C	5.30593000380079	0.85002524046875	10.12612486637247

C	5.30103033324583	0.86639752658902	8.62542396676819
C	-2.68585855079036	5.30750121376703	10.12319851344852
C	-2.78839137145164	5.37653549155055	8.62364774868631
O	2.32678898104467	4.11933830671206	7.97459631541972
O	1.06261481614755	6.27878493777837	8.01500510022130
O	5.76383488541575	1.86542024839235	8.01712151469982
O	-2.17563218090615	4.47999053976250	7.96201975549627
O	-3.47306421392110	6.31104331412471	8.09772623124985
H	1.73380398006847	4.91405059785463	8.18596574078009
H	0.09790248665935	2.15048758935409	9.45463572857600
H	0.99851875506287	3.58566798485990	10.01369632153412
H	-0.30751473010809	3.73931289108329	8.78616483053827
H	2.35710652418466	0.87097181725328	8.55443858916102
H	2.82027361670571	2.14197161064917	9.72447349669903
H	3.57630222559608	2.11251111032131	8.12722906788044
H	4.52866542626660	0.17839722422643	10.50902993000027
H	5.16216725868396	1.86589027967497	10.51263039488069
H	6.28471865870590	0.48934843232186	10.47052201691177
H	3.82696228431964	4.79659399333637	10.50620259695299
H	-2.64391293837142	6.31410985527937	10.55931728148073
H	-1.80349232778169	4.72752675269240	10.41833016340806

TS CH-OH

Co	1.23499999999998	0.71302972000001	0.00000000000000
Co	3.70500000000000	0.71302972000001	0.00000000000000
Co	6.17500000000002	0.71302972000001	0.00000000000000
Co	-0.00000000000003	2.85210900000001	0.00000000000000
Co	2.46999999999999	2.85210900000001	0.00000000000000
Co	4.94000000000001	2.85210900000001	0.00000000000000
Co	1.23500000000001	4.99117840000001	0.00000000000000
Co	3.70499999999997	4.99117840000001	0.00000000000000
Co	-1.23500000000001	4.99117840000001	0.00000000000000
Co	0.00000000000000	0.00000000000000	2.01675006000002
Co	2.47000000000002	0.00000000000000	2.01675006000002
Co	4.93999999999998	0.00000000000000	2.01675006000002
Co	1.23500000000001	2.13907928000001	2.01675006000002
Co	3.70499999999997	2.13907928000001	2.01675006000002
Co	6.17499999999999	2.13907928000001	2.01675006000002
Co	0.00000000000003	4.27816350000000	2.01675006000002
Co	2.46999999999999	4.27816350000000	2.01675006000002
Co	4.94000000000001	4.27816350000000	2.01675006000002
Co	1.24552714000002	0.69064163999999	4.08713369999992
Co	3.70159140000000	0.67898571000001	4.04860169999997
Co	6.19236410000004	0.67362827999998	4.05729609999996

Co	0.025930554000002	2.806932699999999	4.029459200000004
Co	2.462444270000001	2.823605200000002	4.055221299999993
Co	4.944989400000002	2.832274900000000	4.026890400000003
Co	1.245808719999997	4.981471300000001	4.034769699999997
Co	3.712829900000003	4.969071899999999	4.057543100000003
Co	-1.252882800000001	4.983521400000000	4.040648300000004
Co	-3.668221700000001	6.401029699999999	6.046955200000000
Co	-1.213276349999999	6.386283800000000	6.043225499999994
Co	4.945606900000001	0.012946430900002	6.016302500000000
Co	1.286677340000001	2.148262740000001	6.131058700000002
Co	3.704827099999999	2.121712709999999	5.937805900000004
Co	-1.191577399999997	2.099334509999999	5.932668300000002
Co	-0.011199671599998	4.244373899999998	5.891122899999996
Co	2.470123499999997	4.252129700000002	5.978783199999995
Co	4.974629399999998	4.212486199999999	5.984093700000006
C	1.815857550000001	2.810020199999999	8.091744700000003
C	0.747323200000000	2.423136689999999	9.083449699999996
C	3.164761599999999	2.364733540000001	8.593253499999993
C	-1.541200959999998	4.926538499999998	10.039389099999998
C	-1.507944879999999	5.012173399999998	8.542643199999994
C	6.216347799999998	0.113867000000001	8.570529499999991
C	6.056835199999998	0.029046953000001	10.060655799999999
O	1.901467749999999	4.185168000000002	7.914942099999994
O	-1.111546930000000	6.076249400000000	7.991586200000001
O	-1.877824910000001	3.973661900000000	7.887920300000006
O	5.199473499999999	0.521538030000000	7.914966800000005
O	3.623144199999998	6.253175500000000	8.028883200000009
H	1.111830980000002	4.881337499999999	7.006056199999993
H	0.859322880000002	1.368076190000001	9.337415100000005
H	0.934141649999998	3.022884800000002	9.994953800000002
H	-0.271867960000001	2.618397600000000	8.732808500000000
H	3.448811599999999	3.029257399999999	9.429447300000006
H	3.176938699999999	1.325402000000000	8.907709199999999
H	3.991445899999998	2.518757800000002	7.871470100000000
H	-0.890225049999997	4.110598699999998	10.378100200000004
H	-2.563934100000000	4.674524400000001	10.349250600000005
H	-1.231319699999998	5.871758099999999	10.498018700000002
H	1.403952940000002	5.945709899999999	10.292440599999992
H	6.014622899999999	1.048324810000000	10.472157800000003
H	3.186793999999999	5.910734700000001	10.521582500000003

Co(11-20)

Slab

Co	4.279991300000002	4.009995600000002	0.000000000000000
Co	5.707009099999999	6.014993400000000	0.000000000000000
Co	4.279991300000002	0.000000000000000	0.000000000000000
Co	5.707009099999999	2.005000270000003	0.000000000000000
Co	0.000000000000000	4.009995600000002	0.000000000000000
Co	1.427000510000001	6.014993400000000	0.000000000000000
Co	0.000000000000000	0.000000000000000	0.000000000000000
Co	1.427000510000001	2.005000270000003	0.000000000000000
Co	6.419999300000000	4.009995600000002	1.235000000000003
Co	7.846992400000003	6.014993400000000	1.235000000000003
Co	6.419999300000000	0.000000000000000	1.235000000000003
Co	7.846992400000003	2.005000270000003	1.235000000000003
Co	2.140000590000000	4.009995600000002	1.235000000000003
Co	3.567001100000001	6.014993400000000	1.235000000000003
Co	2.140000590000000	0.000000000000000	1.235000000000003
Co	3.567001100000001	2.005000270000003	1.235000000000003
Co	4.28959843703569	4.009995600000002	2.50914303278145
Co	5.69740196296432	6.014993400000000	2.50914303278145
Co	4.28959843703569	0.000000000000000	2.50914303278145
Co	5.69740196296432	2.005000270000003	2.50914303278145
Co	0.00959742993569	4.009995600000002	2.50914303278145
Co	1.41740325296432	6.014993400000000	2.50914303278145
Co	0.00959742993569	0.000000000000000	2.50914303278145
Co	1.41740325296432	2.005000270000003	2.50914303278145
Co	6.47047863669346	4.009995600000002	3.62823510933390
Co	7.79651306330651	6.014993400000000	3.62823510933390
Co	6.47047863669346	0.000000000000000	3.62823510933390
Co	7.79651306330651	2.005000270000003	3.62823510933390
Co	2.19048980669350	4.009995600000002	3.62823510933390
Co	3.51652176330655	6.014993400000000	3.62823510933390
Co	2.19048980669350	0.000000000000000	3.62823510933390
Co	3.51652176330655	2.005000270000003	3.62823510933390

CH₃CHOHCH₃

Co	4.279991300000002	4.009995600000002	0.000000000000000
Co	5.707009099999999	6.014993400000000	0.000000000000000
Co	4.279991300000002	0.000000000000000	0.000000000000000
Co	5.707009099999999	2.005000270000003	0.000000000000000
Co	0.000000000000000	4.009995600000002	0.000000000000000
Co	1.427000510000001	6.014993400000000	0.000000000000000
Co	0.000000000000000	0.000000000000000	0.000000000000000

Co	1.42700051000001	2.00500027000003	0.000000000000000
Co	6.419999300000000	4.009995600000002	1.235000000000003
Co	7.84699240000003	6.014993400000000	1.235000000000003
Co	6.419999300000000	0.000000000000000	1.235000000000003
Co	7.84699240000003	2.00500027000003	1.235000000000003
Co	2.140000590000000	4.009995600000002	1.235000000000003
Co	3.567001100000001	6.014993400000000	1.235000000000003
Co	2.140000590000000	0.000000000000000	1.235000000000003
Co	3.567001100000001	2.00500027000003	1.235000000000003
Co	4.29509132538887	3.99655129779574	2.50398766077952
Co	5.68845077107328	6.01245059793127	2.50144871089846
Co	4.30114869298670	0.01171373777087	2.49989288769483
Co	5.70488756696888	2.00718261153397	2.49798302310675
Co	0.00968680543003	4.00703336308123	2.50107847331490
Co	1.41281982317658	6.01456449030248	2.50445315657276
Co	0.01248235623341	0.00720554809617	2.49095462107956
Co	1.40862564112298	2.00503000979703	2.49953479007786
Co	6.45805118846317	4.02318436497987	3.61912396608841
Co	7.79481606953796	6.01652991521664	3.61260232264960
Co	6.45621339675660	8.00735698827576	3.60419207077063
Co	7.76480109350897	2.02145798950663	3.69276096453835
Co	2.21014489593198	4.01634651106308	3.61913564142359
Co	3.52708845205835	6.01269969805356	3.62874603595092
Co	2.22650356727397	8.00749426282458	3.60876359079558
Co	3.49071830916235	2.00242991488839	3.63227766741983
C	7.19275878265690	0.64946900426150	6.90940101792978
C	0.03128101564666	0.66597517009376	6.34050914021145
C	1.13966510250488	0.64646785400986	7.37012672857998
O	0.13938712619320	1.89032059432007	5.54559119168714
H	6.44982787689255	0.70036726821119	6.09231993357515
H	7.02999004974080	1.51108505230381	7.57291061810716
H	7.01953187464270	7.74076614105199	7.46931612927983
H	0.15329556504614	7.83332253542915	5.64137653963256
H	1.06518334061212	1.95502759975126	5.17885568251766
H	1.06625146232191	1.51415088376888	8.04136326570328
H	1.08056583708565	7.74562989421609	7.96826849350351
H	2.12303982101157	0.66389588264342	6.87283065520721

TS OH

Co	4.279991300000002	4.009995600000002	0.000000000000000
Co	5.707009099999999	6.014993400000000	0.000000000000000
Co	4.279991300000002	0.000000000000000	0.000000000000000
Co	5.707009099999999	2.005000270000003	0.000000000000000
Co	0.000000000000000	4.009995600000002	0.000000000000000

Co	1.42700051000001	6.01499340000000	0.00000000000000
Co	0.00000000000000	0.00000000000000	0.00000000000000
Co	1.42700051000001	2.00500027000003	0.00000000000000
Co	6.41999930000000	4.00999560000002	1.23500000000003
Co	7.84699240000003	6.01499340000000	1.23500000000003
Co	6.41999930000000	0.00000000000000	1.23500000000003
Co	7.84699240000003	2.00500027000003	1.23500000000003
Co	2.14000059000000	4.00999560000002	1.23500000000003
Co	3.56700110000001	6.01499340000000	1.23500000000003
Co	2.14000059000000	0.00000000000000	1.23500000000003
Co	3.56700110000001	2.00500027000003	1.23500000000003
Co	4.29510201913506	4.00167262342127	2.49850474274123
Co	5.70197965217125	6.00985771920779	2.49647852972521
Co	4.29636851471267	8.00096028809573	2.46323708856237
Co	5.68314654863781	2.00025433798043	2.49998859900278
Co	0.01905726127752	4.01066748922011	2.51492325780733
Co	1.42161241678074	6.02584478182654	2.50161952659889
Co	0.00906857523438	0.00523385709120	2.48269360539749
Co	1.42903793182941	2.01465889362354	2.47898706745480
Co	6.47968624837007	4.00720183650791	3.62392718490071
Co	7.80629436366101	6.01842735187292	3.62967153540385
Co	6.47564466438740	8.01397420511364	3.62614855220482
Co	7.79001704467969	1.99641811600936	3.61691967380276
Co	2.20024709921260	4.02118037836296	3.61641732438880
Co	3.54409867342485	6.04204603709215	3.62271711959551
Co	2.08129780734171	8.00596910794251	3.65779322146178
Co	3.53780790052028	2.05489189134713	3.68899138403371
C	1.62284114349699	1.49376198733040	6.72246063981244
C	2.95814115038081	0.79393113819296	6.57298189227780
C	4.09751091120156	1.49723858666659	7.28474197017598
O	3.30461761110014	0.72293077699989	5.15942186107286
H	1.32421219575658	1.53696591414450	7.78018428208424
H	0.83946390993161	0.96564024176149	6.15605995619072
H	1.68887447606634	2.52221890667438	6.33190727529209
H	2.87672505471612	7.76723558667660	6.91292744730547
H	3.70306730639819	7.65532714199097	4.57411076655880
H	5.04573781532367	0.97032994209391	7.10958179805703
H	3.91001154194416	1.54088976128928	8.36738791109711
H	4.19668558598864	2.52464814218253	6.90218064488647

CH₃CHOCH₃

Co	4.27999130000002	4.00999560000002	0.00000000000000
Co	5.70700909999999	6.01499340000000	0.00000000000000
Co	4.27999130000002	0.00000000000000	0.00000000000000

Co	5.707009099999999	2.00500027000003	0.000000000000000
Co	0.000000000000000	4.009995600000002	0.000000000000000
Co	1.42700051000001	6.01499340000000	0.000000000000000
Co	0.000000000000000	0.000000000000000	0.000000000000000
Co	1.42700051000001	2.00500027000003	0.000000000000000
Co	6.419999300000000	4.009995600000002	1.235000000000003
Co	7.846992400000003	6.01499340000000	1.235000000000003
Co	6.419999300000000	0.000000000000000	1.235000000000003
Co	7.846992400000003	2.005000270000003	1.235000000000003
Co	2.140000590000000	4.009995600000002	1.235000000000003
Co	3.567001100000001	6.01499340000000	1.235000000000003
Co	2.140000590000000	0.000000000000000	1.235000000000003
Co	3.567001100000001	2.005000270000003	1.235000000000003
Co	4.29403993190251	3.99682655876622	2.49258508205452
Co	5.69458281091035	6.01534320277544	2.50252578726769
Co	4.28875669445234	8.01240277800700	2.44137356713216
Co	5.67141710555202	2.00005175523714	2.49270986430799
Co	0.01503046908774	4.00879822960397	2.50407280691420
Co	1.41009304612180	6.03451658081693	2.50060717088659
Co	0.03214970675088	0.00365776695015	2.50108027217399
Co	1.42486842886926	2.00639456903489	2.45805035059072
Co	6.47036473854085	4.00701333020212	3.62199715011800
Co	7.79271038831620	6.01382588271683	3.62480616906513
Co	6.48573352416010	8.01742796755833	3.61208315597796
Co	7.78161623422526	2.00550052196908	3.61050914073894
Co	2.18887815838596	4.01164041443769	3.60420029001882
Co	3.51654165535097	5.99905365753483	3.59494069720251
Co	2.16761151280910	8.00107223859957	3.69987972665386
Co	3.53961400847757	2.02742337185872	3.69464867063416
C	3.31795331957558	7.30750698370630	6.90834649329249
C	3.96470697880869	0.39564120147582	6.09843564553398
C	4.49575730197298	1.54030499422802	6.94147668101965
O	3.00184982238686	0.91752320709852	5.16987179195184
H	2.95718038097105	6.50784604818991	6.23690097681744
H	2.45459965490211	7.69868585750892	7.46734771264230
H	4.03667195301706	6.86879194261251	7.61545459624307
H	4.80797341492270	7.98019106952623	5.50702415035535
H	3.67525189475908	2.01121793521421	7.50270485872419
H	5.25422533489922	1.17991351346927	7.65137546608033
H	4.95979736669709	2.29908120525761	6.29238742915543
H			
Co	4.279991300000002	4.009995600000002	0.000000000000000
Co	5.707009099999999	6.01499340000000	0.000000000000000

Co	4.27999130000002	0.00000000000000	0.00000000000000
Co	5.70700909999999	2.00500027000003	0.00000000000000
Co	0.00000000000000	4.00999560000002	0.00000000000000
Co	1.42700051000001	6.01499340000000	0.00000000000000
Co	0.00000000000000	0.00000000000000	0.00000000000000
Co	1.42700051000001	2.00500027000003	0.00000000000000
Co	6.41999930000000	4.00999560000002	1.23500000000003
Co	7.84699240000003	6.01499340000000	1.23500000000003
Co	6.41999930000000	0.00000000000000	1.23500000000003
Co	7.84699240000003	2.00500027000003	1.23500000000003
Co	2.14000059000000	4.00999560000002	1.23500000000003
Co	3.56700110000001	6.01499340000000	1.23500000000003
Co	2.14000059000000	0.00000000000000	1.23500000000003
Co	3.56700110000001	2.00500027000003	1.23500000000003
Co	1.41224977509001	1.99873369817055	2.48210490249475
Co	0.01262792316616	8.01880764739387	2.50486271141629
Co	1.42108277900471	6.00516070045284	2.50496645637688
Co	0.02758546095599	4.00948354564275	2.49963909159761
Co	5.67828583913966	2.00241001192533	2.50117091959327
Co	4.28659494283208	0.00731270542174	2.50488421587699
Co	5.69487371919247	6.01504938061508	2.50498258376331
Co	4.29410565924138	4.01285638276309	2.48403592273401
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Co	2.19569356190094	8.01834387486918	3.62315668260981
Co	3.51175413899422	6.01163780782626	3.62290652870625
Co	2.19258512518903	3.98376133527811	3.67323386039231
Co	7.78477881644661	2.00303208240079	3.61608334551059
Co	6.46803607226483	8.01882025545005	3.62376236199020
Co	7.80111751049616	6.01347749204154	3.62316588009701
Co	6.48118863746136	4.01054363074107	3.61583277182420
H	2.83667613482824	2.99320081199582	4.85561812366090

TS OH-CH

Co	4.27999130000002	4.00999560000002	0.00000000000000
Co	5.70700909999999	6.01499340000000	0.00000000000000
Co	4.27999130000002	0.00000000000000	0.00000000000000
Co	5.70700909999999	2.00500027000003	0.00000000000000
Co	0.00000000000000	4.00999560000002	0.00000000000000
Co	1.42700051000001	6.01499340000000	0.00000000000000
Co	0.00000000000000	0.00000000000000	0.00000000000000
Co	1.42700051000001	2.00500027000003	0.00000000000000
Co	6.41999930000000	4.00999560000002	1.23500000000003
Co	7.84699240000003	6.01499340000000	1.23500000000003
Co	6.41999930000000	0.00000000000000	1.23500000000003

Co	7.84699240000003	2.00500027000003	1.23500000000003
Co	2.14000059000000	4.00999560000002	1.23500000000003
Co	3.56700110000001	6.01499340000000	1.23500000000003
Co	2.14000059000000	0.00000000000000	1.23500000000003
Co	3.56700110000001	2.00500027000003	1.23500000000003
Co	4.30514808220165	4.01433118224963	2.48039415383642
Co	5.66730968401222	6.02238627936446	2.48355960814891
Co	4.25029810996461	8.00326384170476	2.48792272903008
Co	5.68905286660078	1.99519315136760	2.49875153430028
Co	0.03591947673000	4.01793655095925	2.49585967899776
Co	1.43635549500011	6.03252812704432	2.46814581434993
Co	0.03350579856710	8.01627290689718	2.48583149345194
Co	1.42237991841270	1.99635203987600	2.48457185252647
Co	6.48252526869600	4.01137974609561	3.61126999063107
Co	7.77819257553775	6.01390948738174	3.60315370725204
Co	6.48213578041925	8.01786315543966	3.59529966621597
Co	7.79440233887203	2.00545490523889	3.61140701842276
Co	2.20162979171025	4.00391653163459	3.61319225589218
Co	3.54654759237642	5.96731846477176	3.74116228608617
Co	2.14777250339381	0.03789430795534	3.74143980101164
Co	3.54127011159345	2.00636927488223	3.60739786166522
C	2.08528019571505	5.58426299984871	6.84980002915890
C	2.90078941274462	6.42018570935292	5.87792876432322
C	4.34498242319580	6.62606057788446	6.29768661034625
O	2.24438388244314	7.52055109296404	5.48783723393608
H	1.09459630811740	5.36923346814861	6.42807243784025
H	1.95406837248170	6.16869699695816	7.77607721136112
H	2.59098543339121	4.63971438850987	7.09045114987755
H	2.80081506503833	5.11832488486698	4.87099232723468
H	4.34376359620254	7.10667569999552	7.29374753971269
H	4.89106893845704	5.67590775883872	6.36651940744884
H	4.87294220290985	7.29560160380193	5.60007453417255

CH₃COCH₃

Co	4.27999130000002	4.00999560000002	0.00000000000000
Co	5.70700909999999	6.01499340000000	0.00000000000000
Co	4.27999130000002	0.00000000000000	0.00000000000000
Co	5.70700909999999	2.00500027000003	0.00000000000000
Co	0.00000000000000	4.00999560000002	0.00000000000000
Co	1.42700051000001	6.01499340000000	0.00000000000000
Co	0.00000000000000	0.00000000000000	0.00000000000000
Co	1.42700051000001	2.00500027000003	0.00000000000000
Co	6.41999930000000	4.00999560000002	1.23500000000003
Co	7.84699240000003	6.01499340000000	1.23500000000003

Co	6.419999300000000	0.000000000000000	1.235000000000003
Co	7.846992400000003	2.005000270000003	1.235000000000003
Co	2.140000590000000	4.009995600000002	1.235000000000003
Co	3.567001100000001	6.014993400000000	1.235000000000003
Co	2.140000590000000	0.000000000000000	1.235000000000003
Co	3.567001100000001	2.005000270000003	1.235000000000003
Co	4.28037867233397	4.01105101415485	2.45948481846710
Co	5.69491990761846	6.01233937715724	2.50483753374282
Co	4.29271360359535	0.01275163297394	2.49346922103536
Co	5.66070936387707	2.00978934341905	2.49045256677799
Co	0.03492590728636	4.00908980072362	2.50234893196463
Co	1.42155393422982	6.00438547455597	2.50351355365939
Co	0.02922617362635	8.01763344369962	2.49119094816269
Co	1.42189568367534	2.00523329573786	2.43989781176001
Co	6.47521867615892	4.00981297334619	3.61087290436927
Co	7.80457142369223	6.01601757086344	3.62209946618501
Co	6.48092419692370	0.00017908710485	3.60953646081565
Co	7.77302885454432	2.00414360527780	3.59334509121855
Co	2.14838131087199	4.02347088759530	3.70509076808855
Co	3.52931375295780	6.02020957437159	3.60039243931964
Co	2.19774168724091	8.01443075098106	3.62868621932834
Co	3.52056050433571	1.97185880090298	3.71750385383032
C	3.80351781912025	1.12712591596873	6.48393123325032
C	2.74678323949093	1.75973731161107	5.60739155454908
C	1.32478288796599	1.46682998080188	6.02793470364333
O	3.01872554260452	3.04699110607221	5.25431525481542
H	3.72912640272884	1.54484508133576	7.50541901294676
H	4.81221888704883	1.32950498625087	6.09739720442302
H	3.65616001875425	0.03973815345182	6.53891180644747
H	0.61277721275494	2.07370659177899	5.44102310733845
H	1.21169425897722	1.74573281244779	7.09306515655982
H	1.05208828890194	0.40430220909232	5.93346503930347

TS CH

Co	4.279991300000002	4.009995600000002	0.000000000000000
Co	5.707009099999999	6.014993400000000	0.000000000000000
Co	4.279991300000002	0.000000000000000	0.000000000000000
Co	5.707009099999999	2.005000270000003	0.000000000000000
Co	0.000000000000000	4.009995600000002	0.000000000000000
Co	1.427000510000001	6.014993400000000	0.000000000000000
Co	0.000000000000000	0.000000000000000	0.000000000000000
Co	1.427000510000001	2.005000270000003	0.000000000000000
Co	6.419999300000000	4.009995600000002	1.235000000000003
Co	7.846992400000003	6.014993400000000	1.235000000000003

Co	6.41999930000000	0.00000000000000	1.23500000000003
Co	7.84699240000003	2.00500027000003	1.23500000000003
Co	2.14000059000000	4.00999560000002	1.23500000000003
Co	3.56700110000001	6.01499340000000	1.23500000000003
Co	2.14000059000000	0.00000000000000	1.23500000000003
Co	3.56700110000001	2.00500027000003	1.23500000000003
Co	4.29150740138698	4.01149868823352	2.48452597727514
Co	5.68634927144144	6.02575958547492	2.50181345972267
Co	4.27723558756331	0.01414125196924	2.48998489894846
Co	5.68613938876217	1.99564258518628	2.50806096338202
Co	0.01203240952726	4.00145546519823	2.50175689194905
Co	1.39459449111464	6.01927554265077	2.47422027213173
Co	0.04783288265712	0.00763418802767	2.48703365862540
Co	1.43568768538829	1.99798430816172	2.48605922978591
Co	6.47108690617875	4.01368293266519	3.61975894762088
Co	7.80046505498322	6.01588898020115	3.62502047945161
Co	6.49700953273729	8.00927746923435	3.60167116672417
Co	7.78297485931331	1.99757865942711	3.61648570926920
Co	2.16657213668324	4.02988172209953	3.60894967452218
Co	3.50588830177930	6.01396109728103	3.59356337690211
Co	2.14715800376397	7.99548191657191	3.75410095939697
Co	3.53136923336570	2.08849472256291	3.67437779629067
C	1.41713255011099	1.00940350390240	6.25751562338848
C	2.70316739477842	0.34263226477900	5.81578164844001
C	3.21738610815495	7.39996243497284	6.87546949685739
O	3.70283387856938	1.38036457615285	5.61644714094643
H	1.53145861584853	1.37316771078686	7.29627056575919
H	0.58715525930462	0.29100459259242	6.22550946379507
H	1.16230364874799	1.86019992085476	5.60879310354263
H	2.84367258744750	7.14407539529893	4.84189587938503
H	4.58107335995138	0.94450294862801	5.49457592699121
H	3.37136078029126	7.94167970391521	7.82345747816236
H	4.16531930258900	6.93211808565940	6.56646652566685
H	2.48366826044458	6.59800679601507	7.03708143791507

CH₃COHCH₃

Co	4.27999130000002	4.00999560000002	0.00000000000000
Co	5.70700909999999	6.01499340000000	0.00000000000000
Co	4.27999130000002	0.00000000000000	0.00000000000000
Co	5.70700909999999	2.00500027000003	0.00000000000000
Co	0.00000000000000	4.00999560000002	0.00000000000000
Co	1.42700051000001	6.01499340000000	0.00000000000000
Co	0.00000000000000	0.00000000000000	0.00000000000000
Co	1.42700051000001	2.00500027000003	0.00000000000000

Co	6.419999300000000	4.009995600000002	1.235000000000003
Co	7.846992400000003	6.014993400000000	1.235000000000003
Co	6.419999300000000	0.000000000000000	1.235000000000003
Co	7.846992400000003	2.005000270000003	1.235000000000003
Co	2.140000590000000	4.009995600000002	1.235000000000003
Co	3.567001100000001	6.014993400000000	1.235000000000003
Co	2.140000590000000	0.000000000000000	1.235000000000003
Co	3.567001100000001	2.005000270000003	1.235000000000003
Co	4.28307018489483	4.00551128460284	2.49887113535072
Co	5.68814763350857	6.01984165577412	2.50316207265866
Co	4.27695882172912	0.01121580850602	2.47871150207544
Co	5.67918020587998	2.00015096797682	2.50535790500137
Co	0.01693276127930	4.00107510959884	2.50456364829227
Co	1.40707270324375	6.02785997171574	2.50123828993433
Co	0.04122948028987	0.00719803106045	2.50043160812383
Co	1.44184821605575	1.98621721662264	2.49936729425978
Co	6.47181164790425	4.01174515611253	3.62266090573404
Co	7.79429061037310	6.01323848617181	3.62459845367064
Co	6.49764563438214	8.01352840766437	3.59770435315377
Co	7.77789607491509	2.00317282544208	3.61814207169335
Co	2.17037506233281	4.01912761328039	3.61204831874525
Co	3.50436429581150	6.01498109297744	3.61391250448911
Co	2.18170537710112	7.99041581556453	3.71300982799848
Co	3.52214501652437	2.05162054051535	3.70457453423575
C	1.51672826243189	0.60692794350918	6.34025423232498
C	2.78032772376500	0.20160821024273	5.60227264098230
C	3.49237989452992	7.07237511944720	6.28444334155835
O	3.67314123944624	1.38980793073451	5.65199163676662
H	0.76743018205417	7.82630262837378	6.27064245690892
H	1.07873140619985	1.52050836823897	5.91367114261833
H	1.74703871793951	0.79014920258118	7.40724653336475
H	4.60334849623600	1.07178420491863	5.61628017347141
H	4.43410039460378	6.80459529298074	5.76774000743333
H	3.74505373230828	7.33508326511347	7.33162294749552
H	2.84576696158664	6.18244923586628	6.30487011920456

TS CH-OH

Co	4.279991300000002	4.009995600000002	0.000000000000000
Co	5.707009099999999	6.014993400000000	0.000000000000000
Co	4.279991300000002	0.000000000000000	0.000000000000000
Co	5.707009099999999	2.005000270000003	0.000000000000000
Co	0.000000000000000	4.009995600000002	0.000000000000000
Co	1.427000510000001	6.014993400000000	0.000000000000000
Co	0.000000000000000	0.000000000000000	0.000000000000000

Co	1.42700051000001	2.00500027000003	0.000000000000000
Co	6.419999300000000	4.009995600000002	1.235000000000003
Co	7.84699240000003	6.014993400000000	1.235000000000003
Co	6.419999300000000	0.000000000000000	1.235000000000003
Co	7.84699240000003	2.00500027000003	1.235000000000003
Co	2.140000590000000	4.009995600000002	1.235000000000003
Co	3.567001100000001	6.014993400000000	1.235000000000003
Co	2.140000590000000	0.000000000000000	1.235000000000003
Co	3.567001100000001	2.005000270000003	1.235000000000003
Co	4.28601244947093	4.00155500711092	2.48881787115175
Co	5.69268961313596	6.01500978701293	2.49418457436878
Co	4.31027324555168	0.00313881850070	2.49143665758793
Co	5.69518296818786	2.00189247784862	2.49216962263708
Co	0.01475603167446	4.00655078193532	2.50392262312888
Co	1.41008772001197	6.02945776808582	2.48969931348327
Co	0.02576150703659	0.00274528303594	2.47199784160432
Co	1.42906538325729	1.98681548835887	2.48429273606186
Co	6.48224729730659	4.01147178644538	3.61496323695132
Co	7.79987193102856	6.02462437267754	3.62376541756107
Co	6.48164938044601	8.01444922655174	3.61395566684322
Co	7.79797497894960	1.99600829623142	3.61784744745687
Co	2.16476168223928	4.00245230168770	3.60521238069199
Co	3.48540758438937	5.98973045178818	3.62515150261349
Co	2.13011464855462	7.98929900755753	3.67270909889924
Co	3.50244066854933	2.04191147870224	3.69357894056156
C	1.84410475783297	0.53487934299673	6.30330454829107
C	3.01163641425301	0.02366687003213	5.47389701371697
C	3.61382292525772	6.76966996015982	6.03062985713688
O	3.99263036232285	1.01356076675343	5.30400983683609
H	1.04005429930997	7.80728823508385	6.35398622839853
H	1.43245571259704	1.46665586631711	5.88775744691684
H	2.19550571831343	0.74136411274920	7.33207066745100
H	4.77460691214004	0.53643892865016	4.27690885396843
H	4.44045205120667	6.36469774745619	5.39270839197997
H	4.11503910226738	6.98160018857459	6.99491180217877
H	2.84955988912593	5.99830493574433	6.19908259383603

0.75A-Co(11-20)

Slab

Co	4.279991300000002	4.009995600000002	0.000000000000000
Co	5.707009099999999	6.014993400000000	0.000000000000000
Co	4.279991300000002	0.000000000000000	0.000000000000000
Co	5.707009099999999	2.005000270000003	0.000000000000000

Co	0.0000000000000000	4.009995600000002	0.0000000000000000
Co	1.427000510000001	6.014993400000000	0.0000000000000000
Co	0.0000000000000000	0.0000000000000000	0.0000000000000000
Co	1.427000510000001	2.005000270000003	0.0000000000000000
Co	6.419999300000000	4.009995600000002	1.235000000000003
Co	7.846992400000003	6.014993400000000	1.235000000000003
Co	6.419999300000000	0.0000000000000000	1.235000000000003
Co	7.846992400000003	2.005000270000003	1.235000000000003
Co	2.140000590000000	4.009995600000002	1.235000000000003
Co	3.567001100000001	6.014993400000000	1.235000000000003
Co	2.140000590000000	0.0000000000000000	1.235000000000003
Co	3.567001100000001	2.005000270000003	1.235000000000003
Co	4.23490318298893	4.00196475672465	2.47339906555706
Co	5.69182080256962	6.00226012247115	2.45148602104875
Co	4.23234847104778	0.00538518576931	2.48486152542871
Co	5.72311555083230	2.02558138097380	2.46110232866338
Co	8.53708733259773	3.98424647250804	2.47360252142020
Co	1.47431546446202	6.00968006519792	2.48868080786551
Co	0.01663119819368	0.01396320319094	2.45126367276099
Co	1.47121712378294	2.01409548592496	2.47685868293758
Co	6.39080533606354	4.04912247824716	3.71254026360972
Co	7.83149818298476	6.02896005987066	3.58088785537058
Co	6.43533513426737	8.00101957986081	3.58304062541281
Co	7.88485164152126	1.97390106863127	3.70109635212307
Co	2.06322764096508	4.00353981122048	3.72118101224955
Co	3.63954612097371	6.02098755621118	3.71504815016783
Co	2.06371398903547	8.01695279415723	3.71400586770687
Co	3.64638600142197	2.00902071445528	3.72211338688878
C	2.84498637014492	0.99659568062149	7.73544636443124
C	2.84847615323356	0.99828365554652	6.23303372905139
C	2.86499680177303	5.00919776066307	6.23162447560887
C	2.91525033765919	4.99134939103866	7.73242651319168
C	6.88088867917574	2.81298278859930	6.20726060071065
C	6.61764873626112	2.65359229808114	7.67732215912865
O	2.03343887533447	0.22795479504871	5.62871411048389
O	3.68579083285103	1.76361846055752	5.64315515160881
O	3.65568110413121	5.80686968779343	5.62763153956441
O	2.05018747782908	4.22274174360273	5.64110157118860
O	7.57985017772328	1.92239461741612	5.61373443640351
O	6.36632905455424	3.82584852599253	5.62483075961425
H	2.89157754778921	2.02692054688585	8.11071119289412
H	3.74308542760834	0.46722408251253	8.08995729442901
H	1.95219364902915	0.49123645781646	8.11999603671356
H	2.86300180936087	6.01796996919107	8.11791287849304

H	3.88315416077445	4.56901652801163	8.04221796644613
H	2.09838269872512	4.38933277074267	8.14529643969452
H	6.83574093255845	3.59349586435838	8.20227813001189
H	7.20938104381326	1.83253790778848	8.09625532292967
H	5.54608708262346	2.43757263379538	7.80538888598337

CH₃CHOHCH₃

Co	4.27999130000002	4.00999560000002	0.00000000000000
Co	5.70700909999999	6.01499340000000	0.00000000000000
Co	4.27999130000002	0.00000000000000	0.00000000000000
Co	5.70700909999999	2.00500027000003	0.00000000000000
Co	0.00000000000000	4.00999560000002	0.00000000000000
Co	1.42700051000001	6.01499340000000	0.00000000000000
Co	0.00000000000000	0.00000000000000	0.00000000000000
Co	1.42700051000001	2.00500027000003	0.00000000000000
Co	6.41999930000000	4.00999560000002	1.23500000000003
Co	7.84699240000003	6.01499340000000	1.23500000000003
Co	6.41999930000000	0.00000000000000	1.23500000000003
Co	7.84699240000003	2.00500027000003	1.23500000000003
Co	2.14000059000000	4.00999560000002	1.23500000000003
Co	3.56700110000001	6.01499340000000	1.23500000000003
Co	2.14000059000000	0.00000000000000	1.23500000000003
Co	3.56700110000001	2.00500027000003	1.23500000000003
Co	4.24019085278007	4.00155538535976	2.47131089087488
Co	5.73973557465082	6.01174471847947	2.46059010890115
Co	4.29666556764522	0.00669439139746	2.44683682570158
Co	5.74548571785770	2.01963794817736	2.47307206793956
Co	8.51050906464332	4.00592324416639	2.46734877984992
Co	1.44257420747548	5.99319557269911	2.45664507339900
Co	8.52021798642611	0.00425794485474	2.47941493045935
Co	1.44639774900489	2.02443660603126	2.45937483048121
Co	6.33034050844188	4.01528012490085	3.71092138137101
Co	7.91089147449899	6.03402915827741	3.68294667231740
Co	6.36587460834989	0.00284754766174	3.70035379980543
Co	7.92298898684469	2.02548632589994	3.70780316206253
Co	2.05817543713076	4.00973084302900	3.70491544437957
Co	3.56647512369480	6.03670286060324	3.67094809700421
Co	2.14677217468181	8.01974108223031	3.56059957499638
Co	3.61319279511465	1.97478230152337	3.70386789379240
C	4.32743824413349	6.53129019095361	7.95730257102358
C	3.70848984537523	6.95342012669328	6.64047723320567
C	2.20724889430384	7.10335977380117	6.71277389101266
C	2.67511671612618	2.87456006367045	7.72985936022926
C	2.72820059183659	2.92290952882914	6.22668116241248

C	7.21674171959438	0.95992749479877	6.23249666329561
C	7.25821775876601	0.88228829135110	7.73365347403829
C	7.29176817475334	4.94610137231328	6.21815097527040
C	7.58652360312652	4.65606930823644	7.66031534022986
O	3.98370953214555	5.92716891995209	5.63856034531612
O	1.98659504402151	3.76516927252668	5.62837685824942
O	3.50598089488004	2.09619197164676	5.63926723382544
O	7.97149698131037	1.80218045398358	5.64510420250570
O	6.42724123750246	0.15752039845833	5.63185530081007
O	8.06120504636432	5.73958581488458	5.60192958538753
O	6.29305558244470	4.34149715416507	5.66858815317757
H	5.41778256190163	6.44131930370815	7.86012376937503
H	3.91538914763092	5.56969425327625	8.29630597075094
H	4.11966215816627	7.29002929257027	8.72570138265311
H	4.16862014431783	7.88920947014704	6.29492641037355
H	4.86849429425236	5.50121384058895	5.76564096925316
H	1.72083539831767	6.15207876155349	6.96319627361029
H	1.93780313932708	7.87478815126726	7.44649618380000
H	1.78817980298753	7.41788198769177	5.73645673691530
H	3.66715215298667	2.64371185284737	8.13860817341629
H	1.98661639947128	2.07051460377360	8.03296411822117
H	2.30303592357562	3.82296323942842	8.13455142904897
H	6.24011874052973	0.98684398894050	8.13410969531178
H	7.63070285567268	7.91035388240208	8.02828347191968
H	7.90747497150566	1.65788974719180	8.15265049357933
H	7.95376269101511	5.55413616517051	8.17282991800439
H	6.71159483541538	4.24035278480465	8.17202542790066
H	8.39474484630022	3.90878249592550	7.66513991126998

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Co	4.279991300000002	4.009995600000002	0.000000000000000
Co	5.707009099999999	6.014993400000000	0.000000000000000
Co	4.279991300000002	0.000000000000000	0.000000000000000
Co	5.707009099999999	2.005000270000003	0.000000000000000
Co	0.000000000000000	4.009995600000002	0.000000000000000
Co	1.427000510000001	6.014993400000000	0.000000000000000
Co	0.000000000000000	0.000000000000000	0.000000000000000
Co	1.427000510000001	2.005000270000003	0.000000000000000
Co	6.419999300000000	4.009995600000002	1.235000000000003
Co	7.846992400000003	6.014993400000000	1.235000000000003
Co	6.419999300000000	0.000000000000000	1.235000000000003
Co	7.846992400000003	2.005000270000003	1.235000000000003
Co	2.140000590000000	4.009995600000002	1.235000000000003
Co	3.567001100000001	6.014993400000000	1.235000000000003

Co	2.14000059000000	0.00000000000000	1.235000000000003
Co	3.567001100000001	2.005000270000003	1.235000000000003
Co	4.25898954983026	4.02001986359433	2.45226947290209
Co	5.76245618619313	6.00665091370168	2.46838149004579
Co	4.29251229281884	7.98768563554702	2.46408825134754
Co	5.74174654422662	2.00570542953401	2.47938032220648
Co	8.51294274031891	4.02220258377824	2.46887478916656
Co	1.46674535020787	6.02084330640433	2.46740572393374
Co	8.52130451054212	8.01699903308123	2.47588639196836
Co	1.41795993530882	2.01396415690090	2.43594031717136
Co	6.34039950227709	4.02632552390855	3.71074487827805
Co	7.96442009967731	6.00818249356854	3.72329855957315
Co	6.34017728974066	7.99839227631850	3.71130107088915
Co	7.89967687968218	1.98822117223915	3.69940575019835
Co	2.05226156523638	3.98531157904207	3.68869876372600
Co	3.64705109117994	5.99717850615492	3.70485217826046
Co	2.06308542982171	0.01582212166031	3.64216224160629
Co	3.56528842124017	2.08844422376097	3.65299575903634
C	1.96620378652273	0.77664082177068	7.04984954780443
C	3.39060672254268	0.66276871060281	6.54796689710792
C	4.31347421920757	1.74736359538103	7.05829159137201
C	2.69177342441923	5.03835988186863	7.72176871926456
C	2.76385893785313	4.95467113830645	6.22293227827452
C	7.24120823729435	7.09147604959545	7.73931520016947
C	7.24449686830967	7.03283932591810	6.23773642698413
C	7.50832803954159	3.32614878791323	7.68392032524678
C	7.27912929379878	3.14985401534748	6.21130790185374
O	3.35396560896463	0.71000931410012	5.08854148618286
O	2.04246175945447	4.08841200051869	5.62660693704664
O	3.53988045719079	5.77143061514521	5.62587426853666
O	6.38585025519688	7.75121867507419	5.62965190182733
O	8.10277477947530	6.29416034257319	5.64975928846685
O	6.44682335056591	3.92585527368725	5.63522779220642
O	7.95517765554032	2.25152932184689	5.60914334530623
H	1.94824806728647	0.70398938320493	8.14925117231197
H	1.34906794255435	7.98538163979620	6.63652759589119
H	1.52203497681916	1.73344941243245	6.74467513226309
H	3.80620839690161	7.69403877396561	6.78811615481840
H	4.16225023397870	0.01714017686461	4.26851353362555
H	5.33175294469883	1.55782502975509	6.70341148198032
H	4.31574904170317	1.75025203975440	8.15941379118164
H	3.98807390144847	2.73308752379832	6.70432394749435
H	2.09168729026038	5.92077947164594	7.99253917984861
H	3.69874554777189	5.17554586636657	8.13677119272881

H	2.22751992913784	4.13921016531920	8.14123216120772
H	6.21655704358342	6.94791568801138	8.10862149180330
H	7.57068952580664	0.07291904024412	8.05227822352011
H	7.90915812322527	6.33788229643785	8.16859560824531
H	6.64718095473853	3.81129913624066	8.15635316077258
H	8.39213198945081	3.97123865529475	7.80162309770468
H	7.72467369867051	2.36359938694137	8.16234657072349

CH₃CHOCH₃

Co	4.279991300000002	4.009995600000002	0.000000000000000
Co	5.707009099999999	6.014993400000000	0.000000000000000
Co	4.279991300000002	0.000000000000000	0.000000000000000
Co	5.707009099999999	2.005000270000003	0.000000000000000
Co	0.000000000000000	4.009995600000002	0.000000000000000
Co	1.427000510000001	6.014993400000000	0.000000000000000
Co	0.000000000000000	0.000000000000000	0.000000000000000
Co	1.427000510000001	2.005000270000003	0.000000000000000
Co	6.419999300000000	4.009995600000002	1.235000000000003
Co	7.846992400000003	6.014993400000000	1.235000000000003
Co	6.419999300000000	0.000000000000000	1.235000000000003
Co	7.846992400000003	2.005000270000003	1.235000000000003
Co	2.140000590000000	4.009995600000002	1.235000000000003
Co	3.567001100000001	6.014993400000000	1.235000000000003
Co	2.140000590000000	0.000000000000000	1.235000000000003
Co	3.567001100000001	2.005000270000003	1.235000000000003
Co	4.25479831375935	3.99741973755865	2.45680990689730
Co	5.74964904005043	6.00477842948760	2.45876313451976
Co	4.28508870308731	8.00434277755621	2.41467634017287
Co	5.74238952793217	2.01205169550496	2.48091445925673
Co	8.51618471105802	4.01005372278538	2.47248272405901
Co	1.44815434856815	6.02152900849156	2.45689916672014
Co	8.52981979444336	8.01490402563713	2.47545948966477
Co	1.42071727479199	2.02540262821033	2.42547507678079
Co	6.34059522982698	4.01694722979488	3.70866031157598
Co	7.93223054278313	6.01559163994777	3.71138964621684
Co	6.34662473679499	7.98940578668424	3.68112691401107
Co	7.90813330680578	2.00728737895931	3.71483552988003
Co	2.07164146788528	3.99821244349099	3.69905036066732
Co	3.62851396341030	6.02405052882532	3.66069065342265
Co	2.11256534884208	8.00591035457124	3.67515047938996
Co	3.60675162367074	2.01705645817173	3.67684254994402
C	1.93603857247022	0.36220266997932	7.18700638767734
C	3.22796904787192	0.70125215577361	6.46626139559930
C	3.90174550974131	1.90299358313343	7.09318787765557

C	2.93309779666673	5.09439070327915	7.70260766250449
C	2.86773517162912	5.04141174629635	6.20238733690470
C	7.12175789410364	0.90065247160166	6.21145730444122
C	7.16055885912128	0.79100543111750	7.70789030666778
C	7.24232278633089	4.93224515831635	6.22365735539496
C	7.40583190070841	4.76865447336567	7.70645297322392
O	2.88608024077184	0.99501744673001	5.10258772323676
O	3.61504512267521	5.85790855201878	5.56690014192747
O	2.10895626153277	4.18741500446862	5.63672913394968
O	7.90903744396649	1.72337197143731	5.63644124953371
O	6.31297734183473	0.13354432849729	5.58973521414299
O	7.98941386225498	5.77956250629337	5.63156422980020
O	6.39711596074654	4.18236117011273	5.63077936500392
H	1.43610969192027	7.51888484512057	6.72279256947708
H	1.26246225416021	1.22617095783913	7.11847229218914
H	2.12497692133035	0.13958556033818	8.24890268020976
H	3.91509594179950	7.86288847027603	6.45558562502460
H	3.16856326721656	2.70733718862065	7.18221102796247
H	4.26797593940638	1.64776715831835	8.09884543799298
H	4.74836419354317	2.25752854171611	6.48898096972341
H	3.87529556012476	4.62745036158860	8.02448332618898
H	2.09513140390190	4.55440381120054	8.15578782995286
H	2.94562851551014	6.13657374400063	8.03858942495018
H	7.38021748416096	1.76272584245547	8.16488876433819
H	6.21369536025127	0.38872912411391	8.08250964266383
H	7.96932731656305	0.09673598445067	7.97715630165180
H	7.64919085566775	5.72641187822585	8.18101455596532
H	6.50555646274552	4.32937001233832	8.15153109227270
H	8.24952408321788	4.07929031410028	7.86619569650559

H

Co	4.279991300000002	4.009995600000002	0.000000000000000
Co	5.707009099999999	6.014993400000000	0.000000000000000
Co	4.279991300000002	0.000000000000000	0.000000000000000
Co	5.707009099999999	2.005000270000003	0.000000000000000
Co	0.000000000000000	4.009995600000002	0.000000000000000
Co	1.427000510000001	6.014993400000000	0.000000000000000
Co	0.000000000000000	0.000000000000000	0.000000000000000
Co	1.427000510000001	2.005000270000003	0.000000000000000
Co	6.419999300000000	4.009995600000002	1.235000000000003
Co	7.846992400000003	6.014993400000000	1.235000000000003
Co	6.419999300000000	0.000000000000000	1.235000000000003
Co	7.846992400000003	2.005000270000003	1.235000000000003
Co	2.140000590000000	4.009995600000002	1.235000000000003

Co	3.567001100000001	6.014993400000000	1.235000000000003
Co	2.140000590000000	0.000000000000000	1.235000000000003
Co	3.567001100000001	2.005000270000003	1.235000000000003
Co	1.41107717503058	1.98815262172293	2.43886729558805
Co	8.51711039406785	8.00920710159324	2.47153776375601
Co	1.45692671233462	6.02172537023235	2.46387512554330
Co	8.52780549579761	4.01671549293383	2.47528446878058
Co	5.74237384121097	1.99717491010636	2.47807141221670
Co	4.25167452886007	8.01372864971677	2.46364643536357
Co	5.75139094663235	6.02622422879633	2.47140162110689
Co	4.29810054701800	4.02496178615419	2.43776404953924
Co	3.55561065426531	2.04159191243419	3.62932730405591
Co	2.09524699359359	0.02803077356431	3.70123322221872
Co	3.61405439762360	5.98369585999029	3.69911944620374
Co	2.15453045272725	3.97156780952919	3.62859826885123
Co	7.90716608240977	2.00977482014208	3.70297130561943
Co	6.33059405911364	8.01069036013622	3.71426755873174
Co	7.93773156993622	6.02298060802582	3.71043849119346
Co	6.35844168819714	4.00622070280136	3.70558224198412
C	7.05003841831560	5.10703727587199	7.71163658928701
C	7.13590661743658	5.03483519046859	6.21574908969500
C	2.87706195605817	7.02600940632029	6.21466158830794
C	2.92614987203093	7.03848663428605	7.71478930895891
C	7.16893830810956	0.96002517626938	6.21660383622309
C	7.24426850124773	0.92936186588745	7.71501535150266
O	6.34642501365291	4.23492107761328	5.61414940435574
O	7.97279051986642	5.79712320450817	5.62328665140986
O	3.55128105398295	6.12360593751521	5.61329474502423
O	2.18489215952100	7.91803185177871	5.62027945905031
O	7.95148060874120	1.75943335673616	5.60562250904749
O	6.32181412316829	0.20170015855055	5.63382677112240
H	2.85405208066583	3.00779309296041	4.79598249397060
H	6.13926605357901	5.66876550547018	7.96979763553952
H	7.92395370197288	5.61999074493363	8.12717895249147
H	6.95237952935768	4.10115008042948	8.13713756169735
H	3.93706972588765	7.34192012416367	8.02702834965673
H	2.74698433342874	6.02589797896915	8.09992525334486
H	2.19469071336690	7.74344839179406	8.12335426399527
H	6.73986838693364	1.82275932911222	8.11245244713348
H	8.29484146529915	0.96511526372373	8.02989713561019
H	6.75233715461237	0.03591136788235	8.11224619636801

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Co	3.567001100000001	2.005000270000003	1.235000000000003
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Co	4.22641423834331	4.02528115626430	2.47089993379088
Co	5.71874513712416	6.01836503298051	2.46165208023564
Co	1.45457628556666	2.00265441606806	2.42746022140297
Co	8.53501023823226	8.00815871049827	2.44684102248584
Co	4.25933408528621	8.01483952909725	2.44326010762181
Co	8.52659776395248	4.01358377603500	2.44506458384392
Co	5.74601434392264	2.00696377540895	2.44389480908634
Co	6.41389245680768	0.02311034644074	3.67266797223898
Co	7.88313139941171	5.99161795281421	3.70884652609326
Co	3.70022071416082	1.98272880171087	3.67795481086334
Co	6.31359202661330	3.97106778944042	3.68255479551593
Co	7.95684514761306	2.04468085338388	3.68336071790324
Co	2.06996929765694	3.95328289356376	3.73809301301379
Co	3.56375613764484	6.01403128875842	3.79622217376103
Co	2.06181946955441	0.08833188773319	3.67711991210715
C	2.69566396776134	6.62306296175477	5.85574104482578
C	7.05876700077832	4.87325543115497	6.21097516797537
C	7.35553564807334	0.98472798356659	6.19229783571588
C	2.69255958231458	2.53307208725648	6.17481014620284
C	4.17564471902605	6.78014117605087	5.87392117347948
C	2.13118016808250	5.84505975169472	7.01551591041588
C	7.11492395704193	4.80975408172779	7.71176923777094
C	7.46267849723357	0.84768834019340	7.68371445305940
C	2.43282182533313	2.17299625124022	7.60879895040719
O	1.95168458806815	7.64748628753131	5.47403631351474
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O	7.85525995073309	5.67480402405346	5.61899258088267
O	1.88968982706247	3.32176623998935	5.58955361279743

O	8.06293538629019	1.86093303303393	5.60498160006579
O	6.57151686612507	0.18441754726991	5.58441689205571
O	3.70223591330495	1.99111698774955	5.60301787187058
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H	4.66131804433767	6.01780531374722	6.48910414480622
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H	2.74772509047717	4.97618100714139	7.25945981464260
H	4.43386400841055	7.80064035865831	6.18548139612228
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H	3.37750980617105	2.05241160106139	8.15412951990558
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Co	7.846992400000003	6.014993400000000	1.235000000000003
Co	6.419999300000000	0.000000000000000	1.235000000000003
Co	7.846992400000003	2.005000270000003	1.235000000000003
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Co	5.74527248445854	6.01819738696936	2.44858308497450
Co	4.22549211114236	0.02451606348579	2.48018154818381
Co	5.70633219500872	1.98968569178284	2.47007102563663
Co	8.53589830828641	3.99236054467789	2.47669953948734
Co	1.45864431911614	6.02631288770886	2.44983401416700
Co	8.52430911560752	8.00916163023095	2.46368508613937

Co	1.43815713796067	1.98892524340565	2.47058161518814
Co	6.36476139100913	4.01431232614294	3.67639928360594
Co	7.97303240258069	6.00032686638225	3.71337515805646
Co	6.33000676253163	7.95285534287565	3.67265992726454
Co	7.84655718620175	1.98587992468328	3.68483539481525
Co	2.13405083760198	4.07016556196924	3.61052579827579
Co	3.67130144723264	6.05029553403864	3.70155934765313
Co	2.05944359823106	0.00547279407472	3.72175405690542
Co	3.52823550403983	2.02225871453085	3.74443202250812
C	4.31103419796855	1.90370838750216	6.64402623195120
C	3.17959463777910	2.48319402443133	5.85466276199899
C	1.83810990797658	2.53681300794548	6.49662243369032
C	7.18209724976381	0.72745752441941	6.18691485745434
C	7.37381049233443	0.60049032009517	7.66949879000229
C	7.27717487463085	4.88058477434695	6.20162073906392
C	7.33585942272194	4.73750726744846	7.69604672246779
C	2.61844436745376	6.81429104710477	6.20853521889221
C	2.37908329921019	6.57197501987074	7.67123398694867
O	3.48168967393171	3.47172873197066	5.01801367977864
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O	6.45462839442017	7.88536157429637	5.59650423173173
O	8.15920130120500	5.60095513148605	5.62642021690488
O	6.36687163678784	4.23856694291745	5.58463224399046
O	1.86915902822440	7.65971237727253	5.61481292573037
O	3.53262922685851	6.14340954437312	5.63014663262639
H	4.24959170033816	2.26782611803183	7.68737831685287
H	5.26356034427060	2.23070294062089	6.21720255322883
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H	1.09683198403268	3.00033170275955	5.83658871507186
H	1.93537414874158	3.15971078930283	7.40715858425635
H	1.47839171057300	1.54451802931735	6.78189056158828
H	7.45243647425109	1.59099908182529	8.13308153733315
H	6.55404720196191	0.02741503024465	8.11720308598295
H	8.31849755333121	0.06234861421837	7.84050215666971
H	7.63953851525973	5.68140803001837	8.16392656932528
H	6.36662332388110	4.40762262276901	8.08679181790507
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H	2.14301177240277	7.51143829205473	8.18797202904127
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Co	7.846992400000003	6.014993400000000	1.235000000000003
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Co	5.72437099295642	2.01222284537608	2.46790578542619
Co	8.51420692826973	4.00670959701786	2.48146622996788
Co	1.40013302247128	6.00557031456538	2.43479921593765
Co	0.00733405809068	0.02263298346903	2.47496834997085
Co	1.46116375413024	1.98802643294926	2.48398338561279
Co	6.31492031136665	4.04161556341839	3.70389833662792
Co	7.92882614208587	6.02284188453581	3.71363132516860
Co	6.40444092750672	0.00194297030397	3.63850949210200
Co	7.87104425870365	2.01622885736585	3.70420698389814
Co	2.07748201394781	4.01946271861746	3.65383062097021
Co	3.57133744926741	5.97998358346858	3.54378789077558
Co	2.18402490568405	7.95905999067186	3.76452268624356
Co	3.63651789468637	2.03279173169742	3.80266310094715
C	1.61433536109733	0.73949351209584	6.33969028380213
C	2.83875135709659	0.04131413957857	5.82285723653733
C	3.29408815706722	6.96349604262622	6.76158570806317
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C	7.04945223894001	3.10118712549557	6.23005776617081
C	7.22583243043074	3.18640984465970	7.71483821831742
C	7.00125072131896	6.99218037160515	6.22105672707459
C	6.88747212364714	6.93690763855701	7.71331940539278
O	3.89335193720541	0.97746854302625	5.62123841947794
O	3.08732783648928	3.60510259250667	5.25186955561523
O	1.44123002367947	4.20945643429195	6.66015044568060
O	7.71280238427442	2.20281109036864	5.61289519609759
O	6.28670801279850	3.94020608150495	5.64354355671478

O	7.87977626187422	6.28943834101365	5.64327805018713
O	6.18986732447974	7.75474304645206	5.57283796860097
H	1.78843192049907	1.05454227121495	7.38669697586052
H	0.76279804364279	0.05346733875749	6.32354836353236
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H	2.56358346781132	6.81007185224815	4.73704573599364
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H	4.37619231349864	4.23570228537966	7.50360562709896
H	3.06151412271261	3.59061147409196	8.55218474210259
H	4.00537645140687	2.51396638578889	7.44519732934241
H	6.39084625786059	3.70828078447138	8.19256031821833
H	7.35462876143284	2.18586715048101	8.14550719972964
H	8.16048985822461	3.74603237257467	7.88014984571002
H	6.01794696332243	6.31502044985944	7.97496405725001
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Co	7.846992400000003	6.014993400000000	1.235000000000003
Co	6.419999300000000	0.000000000000000	1.235000000000003
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Co	3.567001100000001	2.005000270000003	1.235000000000003
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Co	5.72577039871822	2.01910864897715	2.44900871686131
Co	8.51972619801974	4.02188933304191	2.47116439874183
Co	1.44592983370128	6.03386662017971	2.46648411535607
Co	0.00753104106020	0.01041028785870	2.47524651441042

Co	1.44628417574055	1.98592500382577	2.46618964058278
Co	6.33702755639006	4.06535774930567	3.68885505017506
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Co	6.37835810887834	0.00207412100804	3.62369348944543
Co	7.84026428372607	2.01210655439307	3.67772757329709
Co	2.05150753406221	3.99059402079617	3.65531541800181
Co	3.59073586200291	6.02243896661524	3.69181810358942
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Co	3.63013181372281	2.00559560210193	3.67093303825573
C	1.52530778012262	1.17138820388040	6.14386746923402
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O	6.34386141961519	3.97564778247985	5.62993888837141
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H	1.25394109472103	1.95487463905243	5.43773337435431
H	1.66402244426292	1.65751098444307	7.13049132227035
H	4.71097256972820	0.87144348853390	5.66818169972680
H	4.08121627056894	7.01370399176986	6.75108891424174
H	3.15609589969428	0.09765029245448	7.81517379919753
H	2.33517738041703	6.76207337344664	7.00180245969312
H	4.46658466610701	4.72547487034698	7.83820233494741
H	2.71524272412186	4.46041162660984	8.15584993356091
H	3.71666100794324	3.11692032079003	7.56462585489287
H	7.87326195025945	2.43957447460731	8.06245245214623
H	7.01998011844072	4.02499180206552	8.11274670064387
H	6.08909116344681	2.51150952870609	8.08001201961357
H	7.78696518319826	6.79634376188084	8.15064006861002
H	6.46060901150343	8.01616005509523	8.06464201953203
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Co	5.707009099999999	6.014993400000000	0.000000000000000
Co	4.279991300000002	0.000000000000000	0.000000000000000
Co	5.707009099999999	2.005000270000003	0.000000000000000
Co	0.000000000000000	4.009995600000002	0.000000000000000
Co	1.427000510000001	6.014993400000000	0.000000000000000
Co	0.000000000000000	0.000000000000000	0.000000000000000
Co	1.427000510000001	2.005000270000003	0.000000000000000
Co	6.419999300000000	4.009995600000002	1.235000000000003
Co	7.846992400000003	6.014993400000000	1.235000000000003
Co	6.419999300000000	0.000000000000000	1.235000000000003
Co	7.846992400000003	2.005000270000003	1.235000000000003
Co	2.140000590000000	4.009995600000002	1.235000000000003
Co	3.567001100000001	6.014993400000000	1.235000000000003
Co	2.140000590000000	0.000000000000000	1.235000000000003
Co	3.567001100000001	2.005000270000003	1.235000000000003
Co	4.26896531003030	4.01889281328726	2.41520373113837
Co	5.74979357782298	6.02106526804777	2.45414336584363
Co	4.28304695854182	8.00387097170219	2.52241191066088
Co	5.74080860041805	1.98578292301286	2.47786879496645
Co	8.51653339254745	4.01120325476696	2.44348295104435
Co	1.46528972529305	6.03842981776614	2.45400494080327
Co	8.54285599007123	8.01533537833678	2.46179547369101
Co	1.41607802490251	1.99086196926618	2.43022225114345
Co	6.33643069327667	4.04845553474486	3.69888625264192
Co	7.96910234013263	5.97140535244466	3.70055727818960
Co	6.39002952409106	7.97371395333972	3.72614270982150
Co	7.86700201972181	2.01525259431452	3.67551111407521
Co	1.99667145505736	4.00317634464141	3.66083721467590
Co	3.59637253586104	5.98106963335164	3.71346828629861
Co	2.15023890038521	7.93899293233002	3.80471995440566
Co	3.52510185947978	2.11715243861859	3.58664031748250
C	1.64712055117367	0.80462467666722	5.78384245930768
C	3.04272084542083	0.33377984241740	5.67077040951914
C	3.52704822983749	7.56427474957191	6.85324069980764
C	3.58082363274141	4.04929663767778	7.49899879627442
C	3.20298969338454	4.44017107588381	6.10192221508824
C	7.05278338272687	3.00208993380885	6.20789076348335
C	7.03591742060877	2.92042540643197	7.70749169844911
C	7.29972208122680	6.91026208236087	6.23629892697341
C	7.30567412518486	6.89908989250512	7.74050383346194
O	3.97863388551658	1.28129643233763	5.28567207784708
O	3.93476584104610	5.26543965503493	5.47350875569743
O	2.16545985869929	3.89220247841976	5.59020052397424
O	6.29176073384207	3.83925119479464	5.62801077448910

O	7.82023265333346	2.19662211148351	5.58898376513987
O	6.48626310565979	7.70154408224437	5.65794967239727
O	8.10736977015763	6.13729287716729	5.62273570424330
H	1.07974132598036	0.21376159473762	6.50937673210524
H	0.98358526570196	0.73364160583896	4.82179338219080
H	1.57899855165693	1.88382486419669	5.97119519261474
H	4.72143752773987	0.72864408805815	4.31432424957189
H	4.50912760554194	7.12362338044625	6.68177571396266
H	3.60840938830167	0.26908163299916	7.68677451355195
H	2.80450537142697	6.79492755272459	7.14459438040767
H	4.31303996452434	4.74749647616170	7.91707510156142
H	2.68754363095240	3.99058368839936	8.13472702550109
H	4.03141497691995	3.04649051060420	7.44600469760916
H	8.03701289421966	2.67179722215161	8.08153736450291
H	6.68048172993739	3.85775449653204	8.14831559390991
H	6.34979874344911	2.10977031901303	7.99865903945184
H	8.04861303161031	6.19125230144098	8.12367787617056
H	7.51937781010610	7.91049738274264	8.11417693065746
H	6.30501819787055	6.62249444466210	8.10353818329751