
Supporting Information

Mechanistic Insights and Origin of Chemoselectivity for S–O bond Cleavage in Dinitrobenzenesulfonic Carbamates

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SP	ZPE	δG	E+ZPE	G	E/B2	imaginary frequencies
R1	0.101590	0.068867	-804.899658	-804.932381	-805.12221435	—
R2	0.353239	0.296742	-1783.178487	-1783.234985	-1783.94348798	—
CAT	0.343915	0.296782	-1112.698793	-1112.745925	-1113.23536709	—
TS1R	0.447531	0.389598	-1917.604598	-1917.662531	-1918.36395564	-134.3157
TS1S	0.447377	0.389088	-1917.604035	-1917.662323	-1918.36293410	-144.496
M1R	0.448684	0.391098	-1917.615469	-1917.673056	-1918.37919548	—
M1S	0.448569	0.390690	-1917.611605	-1917.669485	-1918.37436032	—
TS2R	0.799567	0.709745	-3700.770699	-3700.860522	-3702.29488415	-398.3965
TS2S	0.799580	0.709424	-3700.770660	-3700.860817	-3702.29532959	-343.9274
M2	0.802807	0.713071	-3700.777207	-3700.866943	-3702.30775792	—
M3R	0.682892	0.610402	-2511.459196	-2511.531686	-2512.60983056	—
M3S	0.683015	0.608560	-2511.465992	-2511.540447	-2512.61125718	—
TS3R	0.681224	0.605601	-2511.452308	-2511.527931	-2512.59904690	-164.6636
TS3S	0.681046	0.603900	-2511.449818	-2511.526964	-2512.59603292	-115.9068
P	0.336532	0.284007	-1398.753254	-1398.805779	-1399.36465379	—
R2^a	0.208798	0.162288	-1382.409044	-1382.455553	-1382.92482786	—
TS2^aR	0.654406	0.571673	-3299.989381	-3300.072114	-3301.26478971	-592.7806
TS2^aS	0.655225	0.574555	-3299.993823	-3300.074492	-3301.27005852	-382.3812
R2^b	0.233012	0.186988	-1217.259346	-1217.305371	-1217.74459323	—
TS2^bR	0.680016	0.602146	-3134.841526	-3134.919396	-3136.08675141	-639.3994
TS2^bS	0.679507	0.598060	-3134.839096	-3134.920543	-3136.08571100	-265.6143
TS2C	0.798158	0.710322	-3700.734864	-3700.822701	-3702.25750357	-879.6981
HCO₃⁻	0.026988	0.001242	-264.399343	-264.425089	-264.54006094	—
TS2R-B	0.471559	0.410122	-2182.029272	-2182.090709	-2182.91675827	-1152.7594
TS2S-B	0.472124	0.412394	-2182.023169	-2182.082900	-2182.90968509	-1200.9847
M2B	0.477617	0.414310	-2182.065678	-2182.128985	-2182.95477801	—
TS3-B	0.798316	0.708270	-3700.747834	-3700.837879	-3702.26982975	-1363.6921

Table S2. NBO charge analyses on TS2R/TS2S, M2 and TS2C

Charge/Substrate	TS2S	TS2R	M2	TS2C
M1A part	0.64e	0.60e	0.85e	-0.26e
R2 part	-0.64e	-0.60e	-0.85e	0.26e

Cartesian Coordinate for all stationary points

R1

C	-2.02872970	0.95787618	-0.03909904
C	-3.41509470	0.85228618	-0.03911304
C	-3.98578370	-0.41641082	-0.03911804
C	-3.21075470	-1.57634782	-0.03910804
C	-1.82960570	-1.45510982	-0.03909504
C	-1.23569670	-0.18987682	-0.03909204
H	-1.56202170	1.93932218	-0.03909904
H	-4.04553170	1.73370118	-0.03912004
H	-3.68996070	-2.54859282	-0.03911004
H	-1.19378670	-2.33430782	-0.03908904
C	0.23977530	-0.06425082	-0.03908204
H	0.62476830	0.97444818	-0.03907304
O	0.99724830	-1.01006082	-0.03908204
Cl	-5.72374070	-0.56282482	-0.03914004

R2

N	-0.88566828	0.42673107	0.00000000
O	-0.70179028	-0.18840593	1.25971500
C	-2.32315428	0.38290907	-0.39188100
C	-3.17746528	1.14778907	0.61477400
C	-2.79516928	-1.04816193	-0.58439700
C	-0.29788528	1.71121807	-0.07084300
O	-0.60672128	2.45743007	-0.97209500
O	0.59721172	1.92879707	0.88011500
C	1.24816872	3.25119407	0.95629600
C	0.19106372	4.33869207	1.12311600
C	2.12373972	3.45326607	-0.27348900
C	2.09904972	3.15828107	2.21592100
H	-2.32919428	0.89925407	-1.35306600
H	-4.22187628	1.14137807	0.29447900
H	-2.85249528	2.18915407	0.69502200
H	-3.11760928	0.67867907	1.60067600
H	-2.78934328	-1.59717793	0.36102600
H	-2.16842928	-1.58134593	-1.29958400
H	-3.82261128	-1.02560793	-0.95539400
H	0.69372372	5.28533107	1.33738400
H	-0.45948728	4.09750707	1.96874900
H	-0.41199628	4.45678507	0.22389900
H	2.72128672	4.35926407	-0.14186200
H	1.52287572	3.55292007	-1.17728100
H	2.80745472	2.60551507	-0.38623400
H	1.48920672	2.87320607	3.07646100

H	2.55629872	4.13067507	2.41239400
H	2.90731972	2.43300607	2.09051000
C	1.87389772	-0.83920693	0.74416000
C	2.28423872	-1.03846593	-0.56956700
C	3.56718172	-0.67505193	-0.97443400
C	4.42669272	-0.14808693	-0.02880800
C	4.05801572	0.05993107	1.29177100
C	2.76708472	-0.27304793	1.66036300
N	2.38000772	0.07650107	3.03868000
O	3.27720472	0.19349407	3.85194800
O	1.20454672	0.27674107	3.25267400
N	5.79727372	0.21793707	-0.43393300
O	6.10347672	0.02788107	-1.59403800
O	6.52611772	0.68369207	0.41937600
S	0.25266872	-1.51490693	1.14377500
O	-0.14065428	-2.29044193	-0.00949100
O	0.24065072	-2.10474193	2.45887100
H	1.59837172	-1.49471293	-1.27237400
H	3.89632172	-0.81412093	-1.99639900
H	4.74904372	0.48044307	2.01141200
Cat			
C	-2.35104671	0.89371979	0.00000000
C	-3.55341671	1.45822479	-0.25854300
C	-4.33806571	-0.47491521	0.90812800
C	-1.76520371	3.78194079	0.17722700
H	-1.79726371	3.34348979	1.18218400
H	-1.29919671	4.76551579	0.28759500
C	-3.19861071	3.97871179	-0.34471700
H	-3.21179271	4.78618979	-1.08498400
H	-3.84386071	4.30212679	0.47942800
C	-3.80371471	2.73308679	-1.01600000
H	-3.37970871	2.61851079	-2.01880700
H	-4.87814571	2.87773779	-1.15416600
C	-0.97166871	1.39848779	-0.32637200
H	-0.34949571	1.25158479	0.56503900
H	-0.52581471	0.77683279	-1.11186600
C	-0.90167571	2.88455679	-0.72189100
H	-1.19085071	3.01494179	-1.77059100
H	0.14740629	3.18771979	-0.65945300
S	-2.61672171	-0.59614421	0.87305500
N	-4.60820471	0.67559079	0.26410100
C	-5.97910271	1.11360679	0.16619700
C	-6.72181571	0.76600879	-0.96317300

C	-6.50761071	1.88395579	1.20479200
C	-8.04057671	1.21472279	-1.03790900
C	-7.82892171	2.31279079	1.08798700
C	-8.60914071	1.98625179	-0.02351000
H	-8.63591071	0.95534679	-1.91009500
H	-8.26001471	2.91544779	1.88424800
C	-5.66758171	2.21105879	2.41065600
H	-5.40263371	1.29556679	2.94881000
H	-4.72632671	2.69206679	2.12272900
H	-6.20377671	2.87540979	3.09020100
C	-6.09923371	-0.06352321	-2.05348800
H	-5.23973971	0.45056779	-2.49817000
H	-5.73107871	-1.01226921	-1.65179900
H	-6.82157771	-0.27143921	-2.84443400
C	-10.04526871	2.43597679	-0.10915200
H	-10.69766571	1.75307179	0.44477700
H	-10.17375471	3.43216479	0.32118200
H	-10.39185671	2.45895579	-1.14461000

TS1R

C	-1.75523350	0.36231884	0.00000000
C	-2.32203150	1.58062184	-0.18150100
C	-3.85521050	0.67709084	1.35364300
C	0.58525050	2.12999184	-0.33561600
H	0.48842750	1.83980584	0.71753500
H	1.58632550	2.55728584	-0.44335200
C	-0.44563250	3.22212284	-0.66841700
H	-0.07993750	3.83208884	-1.50134700
H	-0.55077450	3.89530984	0.18918100
C	-1.83017550	2.68518284	-1.07185000
H	-1.79200050	2.30327684	-2.09701600
H	-2.55430350	3.50420084	-1.07617700
C	-0.48336950	-0.18591316	-0.59109200
H	0.05714350	-0.69849916	0.21333900
H	-0.72438750	-0.95527116	-1.33375500
C	0.45368850	0.87066484	-1.20490600
H	0.11720950	1.14096384	-2.21172600
H	1.43175650	0.39832784	-1.33165900
S	-2.70954950	-0.57131416	1.12218600
N	-3.48963450	1.71248384	0.59671200
C	-4.29477450	2.91067184	0.61720200
C	-5.23028750	3.10512184	-0.40119300
C	-4.13287850	3.80439984	1.67810700
C	-6.02244550	4.25077784	-0.34027800

C	-4.95494350	4.93099384	1.70228100
C	-5.90375150	5.16833684	0.70503700
H	-6.76268450	4.41852184	-1.11909800
H	-4.84822250	5.64240284	2.51758500
C	-3.11763450	3.54092384	2.75877000
H	-3.40552450	2.67133284	3.35849300
H	-2.13223950	3.32327384	2.33358600
H	-3.02717850	4.40270684	3.42165800
C	-5.40117650	2.07861484	-1.48737400
H	-4.49819250	1.98920484	-2.10176100
H	-5.60176450	1.09419784	-1.04858300
H	-6.23656150	2.34207484	-2.13867700
C	-6.80303550	6.37575484	0.77391800
H	-7.71701150	6.14361584	1.33025900
H	-6.30983150	7.20705284	1.28256300
H	-7.09906050	6.70581684	-0.22422200
C	-5.41415450	-0.06323216	2.56390600
H	-5.30239850	0.76881984	3.28707800
O	-5.05937450	-1.21605116	2.84728800
C	-6.51052150	0.18619984	1.55636200
C	-7.14159450	1.42516284	1.47165700
C	-6.91168850	-0.85239916	0.71568500
C	-8.15551050	1.64017284	0.54232700
H	-6.82447650	2.24139284	2.11872900
C	-7.91801850	-0.65460516	-0.22300500
H	-6.41960750	-1.81498116	0.81466700
C	-8.52492850	0.59672084	-0.29855600
H	-8.64250650	2.60602484	0.46117200
H	-8.23311150	-1.45239316	-0.88665400
Cl	-9.78496850	0.86629784	-1.48420800
TS1S			
C	-1.94830325	0.24959742	-0.02550469
C	-2.51929425	1.44175342	-0.32480269
C	-4.14128525	0.63523242	1.17130731
C	0.38817275	2.02025642	-0.36092169
H	0.22784375	1.81592942	0.70473331
H	1.38985075	2.45212242	-0.44119669
C	-0.62992025	3.06606042	-0.84685969
H	-0.22296325	3.59812742	-1.71337669
H	-0.78323625	3.81658742	-0.06424969
C	-1.98788925	2.47955042	-1.27283169
H	-1.89210225	2.01484942	-2.25901869
H	-2.71832725	3.28469942	-1.38270869

C	-0.63832725	-0.32498558	-0.49349769
H	-0.14232525	-0.76277358	0.38101631
H	-0.82580925	-1.15448158	-1.18489669
C	0.32201975	0.69460842	-1.13276369
H	0.04273175	0.88048942	-2.17550869
H	1.31046275	0.22783142	-1.16435769
S	-2.96728925	-0.60286358	1.10633531
N	-3.73538925	1.61837142	0.36826231
C	-4.49965925	2.84238242	0.26351931
C	-5.44513125	2.95827142	-0.75708669
C	-4.24040525	3.86140142	1.18110631
C	-6.15827325	4.15245342	-0.84102569
C	-4.98405425	5.03575842	1.06110731
C	-5.94652725	5.19604042	0.06258831
H	-6.90509425	4.26465942	-1.62373069
H	-4.80436025	5.84434342	1.76530731
C	-3.21358125	3.67712142	2.26502331
H	-3.59006825	2.94855642	2.99026531
H	-2.26706125	3.30038542	1.86226231
H	-3.01931825	4.62182442	2.77601331
C	-5.69824025	1.81517542	-1.70155169
H	-4.78725525	1.53027842	-2.23965769
H	-6.04318425	0.93414242	-1.14811569
H	-6.46203325	2.08211942	-2.43417669
C	-6.76212925	6.46025442	-0.02846969
H	-6.94782925	6.73595742	-1.06948569
H	-7.73586025	6.32551342	0.45366031
H	-6.25897325	7.29339242	0.46664431
C	-5.66289325	0.76164642	2.55300831
C	-6.80554725	0.67504642	1.56412831
C	-7.53423425	1.82317442	1.26784731
C	-7.14883725	-0.53536358	0.96117131
C	-8.57978925	1.77944242	0.35015831
H	-7.25021225	2.75384042	1.75137831
C	-8.19693525	-0.60261258	0.04972531
H	-6.58115825	-1.43275958	1.19894531
C	-8.89463225	0.56526342	-0.24926069
H	-9.14005425	2.67299042	0.09625831
H	-8.46985725	-1.53759258	-0.42688369
Cl	-10.20220525	0.50203342	-1.41514469
O	-5.51528525	1.78091342	3.24916231
H	-5.37711825	-0.23750858	2.94442431

M1R

C	-2.67310790	1.50563605	0.00000000
C	-3.21763990	2.72725005	-0.23689200
C	-4.74174290	1.87886605	1.27003900
C	-0.31162990	3.24068205	-0.27510500
H	-0.47169490	2.97615705	0.77715300
H	0.69843610	3.65557305	-0.33494000
C	-1.30956890	4.33370005	-0.69328300
H	-0.89734790	4.90703605	-1.53024600
H	-1.44625490	5.03975305	0.13277600
C	-2.68031790	3.79656105	-1.14287000
H	-2.59818990	3.37319405	-2.14848500
H	-3.39631890	4.61935505	-1.21159500
C	-1.39453190	0.92991505	-0.54984500
H	-0.89732790	0.40095405	0.27140900
H	-1.62904690	0.16986105	-1.30372300
C	-0.40855790	1.96538605	-1.12503500
H	-0.68004490	2.22018105	-2.15509600
H	0.56848210	1.47826905	-1.18420500
S	-3.62963190	0.60597305	1.14295700
N	-4.39592990	2.91103805	0.50703300
C	-5.15846090	4.13832705	0.49954600
C	-6.06652890	4.35423205	-0.54154600
C	-4.95388690	5.04763105	1.53865700
C	-6.80633390	5.53298705	-0.50812400
C	-5.72941590	6.20866905	1.53238700
C	-6.66072890	6.46287605	0.52502300
H	-7.52635190	5.72230905	-1.30044100
H	-5.59334690	6.93429605	2.33009000
C	-3.94101190	4.78250405	2.62206700
H	-4.30992390	4.03605005	3.33379900
H	-3.00248690	4.40031205	2.20797100
H	-3.72631490	5.69751605	3.17585700
C	-6.26460990	3.32700605	-1.62239700
H	-5.33043590	3.11317105	-2.15282100
H	-6.62554490	2.38518805	-1.19305700
H	-6.99879290	3.67562205	-2.35026600
C	-7.50859890	7.70790805	0.55268300
H	-8.51703090	7.47650205	0.91023100
H	-7.08343090	8.46227505	1.21753800
H	-7.60634290	8.13963005	-0.44626300
C	-5.91527590	1.59344105	2.24928600
H	-5.92699290	2.48978605	2.92665900
O	-5.68582790	0.41421605	2.80496100
C	-7.21156590	1.68435605	1.41682600

C	-7.98718190	2.83869605	1.34535300
C	-7.61777190	0.54553305	0.72063700
C	-9.13561390	2.87854505	0.55627900
H	-7.68808790	3.72765405	1.89811400
C	-8.75735590	0.56431105	-0.07594000
H	-7.02473190	-0.35711995	0.83584700
C	-9.49892690	1.74063005	-0.15343700
H	-9.73789290	3.77858005	0.49292700
H	-9.07405590	-0.31477295	-0.62668100
Cl	-10.93433890	1.78133005	-1.15800900

M1S

C	-2.39935589	1.28019322	0.00000000
C	-2.93294289	2.49491122	-0.28470500
C	-4.50926689	1.74111522	1.23236200
C	-0.00459389	2.95574322	-0.39011000
H	-0.14859789	2.75981122	0.67949000
H	1.01072111	3.34849422	-0.49315600
C	-0.99160089	4.03787922	-0.85799200
H	-0.58539489	4.54881522	-1.73716500
H	-1.09995189	4.79800822	-0.07752800
C	-2.37963489	3.50247522	-1.25251100
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H	-3.07943889	4.33406322	-1.35832900
C	-1.12697989	0.65238022	-0.50287900
H	-0.63123689	0.18813422	0.35763000
H	-1.36955189	-0.16289578	-1.19368500
C	-0.13799989	1.63315422	-1.15881900
H	-0.42565289	1.82827922	-2.19742400
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C	-6.10348389	6.43365622	0.07317100
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H	-2.52032489	4.40128122	1.87204900
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C	0.40709240	-0.54831695	-1.24375100
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O	2.04619140	1.72846705	0.50414300
O	1.07018540	3.20461405	-0.91393600
C	2.32079240	3.93509305	-1.13167200
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H	0.51790840	-1.63375095	-1.17516500
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H	-1.66575560	-0.22939195	1.52702600
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H	1.96931940	5.09846705	0.64638500
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H	2.83219540	5.52859505	-2.48336300
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C	-2.51978289	-1.38844968	-0.11104200
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C	-2.37000889	1.53963232	0.49773400

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H	0.10592011	-1.37268468	-1.04434500
H	-0.11969689	-0.15653368	-2.30171600
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O	-3.68887170	0.85354892	2.42918900
C	-5.84572270	0.84402292	0.68210200
O	-6.98681470	0.99348192	1.07174400
O	-5.24003670	-0.30193008	0.37992500
C	-5.84541570	-1.57825408	0.75844000
C	-4.76605370	-2.58064708	0.37060600
H	-4.55481670	-2.51884808	-0.70009700
H	-5.09937570	-3.59455508	0.60470900
H	-3.84482270	-2.37569708	0.92328000
C	-7.11801670	-1.80642808	-0.04847700
H	-7.88925170	-1.08794808	0.22928500
H	-7.48800370	-2.81781408	0.14180200
H	-6.90634070	-1.71254108	-1.11728800
C	-6.09277170	-1.61017208	2.26260100
H	-6.87707470	-0.90867908	2.54798200
H	-5.17299170	-1.35485808	2.79559200
H	-6.39879070	-2.61922808	2.55186700

R2^a

S	-1.40096619	1.37681157	0.00000000
O	-1.99948619	2.33773957	-0.89276200
O	-0.64821919	1.81463257	1.15622900
O	-0.39001919	0.48874957	-0.95004800
C	-2.59481119	0.17623757	0.57066500
C	-3.66707219	-0.31399743	-0.18264300
C	-4.59662719	-1.17494343	0.37481200
C	-4.44594819	-1.58335843	1.69877500
C	-3.38199519	-1.11197043	2.45485200
C	-2.46491019	-0.22112243	1.89616900
H	-5.41945119	-1.52366743	-0.23720000
H	-3.26133319	-1.42320243	3.48602200
H	-1.64829619	0.17777557	2.48602400
N	0.32812081	-0.43117843	-0.16824000
C	1.71825781	-0.02249043	-0.00828400
H	1.73205981	0.91545157	0.54488700
H	2.21757381	-0.80026243	0.56566400
H	2.20528481	0.09830857	-0.97993300
C	0.04240181	-1.76520043	-0.46337600
O	-1.15269819	-1.90420043	-1.02581100
O	0.79007881	-2.66419243	-0.15555200
C	-1.57425819	-3.25960843	-1.21766800
H	-1.68440819	-3.75741943	-0.25250500
H	-2.53362319	-3.19301243	-1.72706500
H	-0.85010219	-3.79903443	-1.82905800
H	-5.16551919	-2.26961943	2.13005900
N	-3.84557019	-0.00615743	-1.61029000
O	-2.84884119	0.14936457	-2.28400800
O	-4.98903119	0.03069557	-2.02811700

TS2^aR

S	-1.38486313	0.82930756	0.00000000
O	-1.75547713	-0.58114344	-0.21696400
O	-1.55740913	1.89955256	-1.00385200
O	0.32095987	0.40030656	-0.40776100
C	-0.80858213	1.56330256	1.56891800
C	-0.49944713	0.90427756	2.75242600
C	-0.04503413	1.57754056	3.87765600
C	0.06714287	2.96186356	3.83842100
C	-0.25792013	3.64440656	2.67051300
C	-0.68934413	2.95095756	1.54196900
H	0.19724587	1.00965056	4.76827700
H	-0.16853813	4.72456256	2.62635800
H	-0.92458413	3.47653356	0.62317900

N	1. 17652687	1. 48146256	-0. 42059700
C	1. 41458087	2. 03925456	-1. 74188900
H	0. 46850687	2. 41279856	-2. 12960300
H	2. 13134587	2. 85186056	-1. 63980200
H	1. 81623187	1. 27380656	-2. 41477800
C	2. 20085387	1. 46515556	0. 49300300
O	2. 00984287	0. 55643656	1. 46003800
O	3. 15189087	2. 22639456	0. 45338700
C	2. 94504787	0. 62662756	2. 53542300
H	2. 95476687	1. 63017456	2. 96703400
H	2. 59203287	-0. 09905444	3. 26640800
H	3. 94898587	0. 37456556	2. 18790900
H	0. 40529987	3. 50078656	4. 71631300
N	-0. 64461913	-0. 54539844	2. 88536900
O	-1. 65288013	-1. 05426144	2. 43679600
O	0. 23482387	-1. 14750244	3. 48019400
C	-6. 11418813	-1. 57596344	0. 88798100
C	-6. 91465213	-0. 53540144	1. 25247200
C	-4. 85090213	0. 48480556	1. 30922800
C	-8. 61288313	-2. 12124444	-0. 61002700
H	-7. 84969013	-1. 76244544	-1. 31149800
H	-9. 41074213	-2. 54834744	-1. 22357000
C	-9. 19216913	-0. 93319844	0. 17595700
H	-10. 21243013	-1. 16610044	0. 49685500
H	-9. 26300413	-0. 06541944	-0. 48644400
C	-8. 40398713	-0. 55512344	1. 44311100
H	-8. 62344813	-1. 27120144	2. 24101300
H	-8. 73612013	0. 42010856	1. 80786800
C	-6. 49148713	-2. 98795644	0. 52485700
H	-5. 94790213	-3. 24865644	-0. 39048200
H	-6. 12752213	-3. 66690044	1. 30366300
C	-7. 99258013	-3. 20769544	0. 27908700
H	-8. 52874613	-3. 27377144	1. 23156300
H	-8. 09595813	-4. 18712444	-0. 19487700
S	-4. 45226413	-1. 08821444	0. 83635300
N	-6. 16633213	0. 61999956	1. 48715300
C	-6. 73554413	1. 88011356	1. 92872700
C	-6. 69961313	2. 16378656	3. 29690900
C	-7. 24060913	2. 76347356	0. 97105900
C	-7. 11982813	3. 43336156	3. 69099400
C	-7. 64025213	4. 02081556	1. 41938500
C	-7. 56276813	4. 38033256	2. 76577800
H	-7. 09400313	3. 68789056	4. 74730700
H	-8. 01302813	4. 73999256	0. 69360800

C	-7.38674613	2.39150956	-0.48112400
H	-6.76248313	1.54123056	-0.76631500
H	-8.42850913	2.13030356	-0.69459000
H	-7.12097013	3.23760756	-1.11812200
C	-6.24634213	1.13407456	4.29801700
H	-5.18515613	0.90061156	4.17093900
H	-6.40146513	1.50199856	5.31316400
H	-6.81179713	0.20315156	4.18260900
C	-7.93738013	5.77186056	3.20185400
H	-8.82058313	6.12894756	2.66700400
H	-8.13826613	5.81306056	4.27408700
H	-7.11891813	6.46666856	2.98545200
C	-3.85599913	1.57385756	1.73805400
O	-3.38426713	1.43970956	2.87003700
C	-4.00230513	2.92088956	1.09441000
C	-4.23274113	3.07189256	-0.27271200
C	-3.91537413	4.04115356	1.92110000
C	-4.41608513	4.33880856	-0.81224200
H	-4.24411713	2.20050256	-0.92185400
C	-4.10052613	5.31398756	1.39457800
H	-3.71968313	3.89585456	2.97843400
C	-4.36003213	5.44324656	0.03351200
H	-4.59437613	4.47326556	-1.87304500
H	-4.05389113	6.19405456	2.02611100
Cl	-4.61601013	7.03672256	-0.63466300
H	-2.74770813	1.10849756	0.66271300
TS2 ^a S			
C	-1.06280194	0.99033815	0.00000000
C	-0.51060194	2.23670415	0.00726900
C	-2.60562894	2.70818815	0.82831900
C	1.75781706	0.43734615	0.64744800
H	1.14103106	0.30398415	1.54467700
H	2.72424606	-0.02131185	0.87299900
C	1.98286306	1.93725615	0.39105000
H	2.91834406	2.08111615	-0.15868200
H	2.09894706	2.45684015	1.34764700
C	0.87316806	2.61756415	-0.43092000
H	0.97230906	2.35078715	-1.48723100
H	0.98711206	3.70286815	-0.37338400
C	-0.44597894	-0.31689385	-0.42101100
H	-0.73197794	-1.06921585	0.32263400
H	-0.89036694	-0.63573685	-1.37008500
C	1.08922206	-0.29387885	-0.52528400

H	1.40042606	0.14949715	-1.47682800
H	1.41854606	-1.33553885	-0.55596500
S	-2.69106794	1.03836015	0.58726900
N	-1.40846894	3.18721315	0.49342400
C	-1.08429994	4.58646515	0.70031300
C	-1.18061494	5.46204215	-0.38583600
C	-0.76384794	4.99376415	1.99713800
C	-1.03038894	6.81909315	-0.11621800
C	-0.60413194	6.36404015	2.20628300
C	-0.76491594	7.28759315	1.17326800
H	-1.13001994	7.52961015	-0.93312800
H	-0.36009294	6.71513615	3.20550900
C	-0.60407794	4.00300415	3.12114500
H	-1.57687394	3.63890415	3.46601600
H	-0.01853494	3.13277615	2.80698100
H	-0.09338094	4.47101615	3.96385100
C	-1.40877994	4.96794115	-1.78936300
H	-0.45184894	4.72394515	-2.26477500
H	-2.03036794	4.07008515	-1.81965200
H	-1.89393094	5.73898015	-2.39064400
C	-0.67459494	8.76710015	1.43660900
H	-1.67897994	9.20109115	1.48485900
H	-0.17357094	8.97348315	2.38425300
H	-0.13499594	9.27916215	0.63647700
C	-3.66625194	3.54251215	1.55573700
C	-4.09128394	4.82660915	0.90786600
C	-4.23641794	5.94674715	1.72463100
C	-4.36291194	4.90942715	-0.45976200
C	-4.63269394	7.16160115	1.17683900
H	-4.03426894	5.85405915	2.78670100
C	-4.76824494	6.11669415	-1.01586100
H	-4.32052894	4.01607815	-1.07976200
C	-4.89310694	7.22993115	-0.18842400
H	-4.74627194	8.04342815	1.79762400
H	-5.01050894	6.18889015	-2.07051400
Cl	-5.41095094	8.74644315	-0.88039300
O	-3.76629594	3.34842115	2.76665300
H	-4.86052594	2.70371715	0.81466800
S	-6.05000294	1.94824515	0.30510000
O	-5.46158394	1.91096615	-1.04958600
O	-5.85616994	0.85717515	1.29263100
O	-7.62408794	1.38723315	-0.34736900
C	-6.88659394	3.37669515	1.14204000
C	-7.43444094	4.54946615	0.61307100

C	-7.87332094	5.58669015	1.42934600
C	-7.78059394	5.46438615	2.80912400
C	-7.24855594	4.30281315	3.35651700
C	-6.79823294	3.27590415	2.53067200
H	-8.28330294	6.47409315	0.96417600
H	-7.17562394	4.18723415	4.43263900
H	-6.36928494	2.37747115	2.95737800
N	-8.53657594	1.10638615	0.65036100
C	-8.61755094	-0.30743685	0.98936300
H	-7.63639794	-0.62420685	1.33501600
H	-9.35564694	-0.42549885	1.78006800
H	-8.91601694	-0.89500485	0.11417100
C	-9.69744694	1.84052515	0.65204800
O	-9.62011294	2.94036615	-0.11250700
O	-10.67590894	1.54595015	1.31516100
C	-10.72371594	3.83610815	0.02919100
H	-10.83711594	4.13767415	1.07312600
H	-10.47676494	4.69733015	-0.59038700
H	-11.64737094	3.36602415	-0.31265500
H	-8.12182594	6.27215415	3.44650900
N	-7.60421994	4.74871115	-0.83026800
O	-7.14016294	3.91819015	-1.57927600
O	-8.19492094	5.75425515	-1.20249900
R2 ^b			
S	-0.46698873	0.86151367	0.00000000
O	-0.43357273	-0.54483733	0.34536600
O	0.18315527	1.35587467	-1.19976800
O	0.24766027	1.68347367	1.29135500
C	-2.10791473	1.47870967	0.11666300
C	-3.05732473	0.75741667	0.83415100
C	-4.34788873	1.26645067	0.91474100
C	-4.68757073	2.47316167	0.29435300
C	-3.70602073	3.16865067	-0.42315800
C	-2.41005473	2.68162267	-0.52013600
H	-2.79091573	-0.18316933	1.30385500
H	-5.10573673	0.71564067	1.46309700
H	-3.96440673	4.09996467	-0.91765100
H	-1.64332773	3.21681467	-1.07189200
C	-6.08102773	3.02816567	0.41376600
H	-6.35220273	3.60758567	-0.47095300
H	-6.81398273	2.23062967	0.54937000
H	-6.14888173	3.69374467	1.28036800
N	1.50131727	2.21512067	1.00757800

C	2.55284127	1.21923067	0.85198400
H	2.47944327	0.70387367	-0.11095000
H	3.50838927	1.73714267	0.91266900
H	2.46176127	0.51229167	1.67576700
C	1.50719127	3.33026667	0.16804500
O	0.42389927	4.11888067	0.23363700
O	2.45152627	3.58776867	-0.53520200
C	-0.21672573	4.36947167	1.49815100
H	-0.44356373	5.43491467	1.51162300
H	-1.13583373	3.78813667	1.57473800
H	0.44805027	4.11685767	2.32516000
TS2 ^b R			
S	-1.75523350	1.02254427	0.00000000
O	-1.32480950	0.92952727	-1.41032200
O	-1.14878950	1.90810027	1.02826400
O	-0.87108650	-0.46909173	0.55652000
C	-3.26815650	0.17241827	0.44351800
C	-4.21746150	-0.04654073	-0.54703300
C	-5.46463650	-0.53665673	-0.17481500
C	-5.77414050	-0.77473573	1.16841700
C	-4.79161750	-0.54412873	2.13801000
C	-3.53143850	-0.07077673	1.78609400
H	-3.98911850	0.19158727	-1.58238200
H	-6.21928650	-0.71162473	-0.93626700
H	-5.01987150	-0.73184173	3.18380800
H	-2.76444350	0.13203727	2.52964400
C	-7.15671550	-1.21626273	1.57036900
H	-7.78227250	-0.34333273	1.78865300
H	-7.64262250	-1.77911373	0.77055400
H	-7.13095950	-1.83776273	2.46828500
N	0.39909750	-0.22091973	1.03038000
C	1.33963450	0.29699527	0.05009100
H	1.16769350	1.36268627	-0.14465600
H	2.35027350	0.15846927	0.43329300
H	1.20072750	-0.27123073	-0.86860300
C	0.48859050	0.27074627	2.31379300
O	-0.45549850	-0.16409273	3.18193600
O	1.39091850	0.99092927	2.68548000
C	-0.79133850	-1.55808673	3.15859200
H	-1.34346250	-1.74071273	4.08073700
H	-1.40523150	-1.80377973	2.29209400
H	0.11818150	-2.16444973	3.15411200
C	0.09297950	4.96361027	-0.18778800

C	-0.75408850	5.32706927	0.81511900
C	-2.19574950	4.15685227	-0.53930100
C	1.84465050	4.87695327	2.17533700
H	1.57244750	3.85808927	1.87300700
H	2.67779850	4.77259727	2.87585200
C	0.66868450	5.52468827	2.92160300
H	1.04096250	6.32053327	3.57540000
H	0.20435650	4.77580227	3.56802000
C	-0.39704750	6.16532927	2.00923400
H	-0.02672550	7.12460327	1.63471200
H	-1.29413750	6.39321227	2.58819400
C	1.56676850	5.23360327	-0.34342200
H	2.02893350	4.30459927	-0.69650800
H	1.71501450	5.97297827	-1.13846800
C	2.28770550	5.67389827	0.94171300
H	2.14102450	6.74581027	1.11286000
H	3.35824950	5.53902627	0.76665700
S	-0.74033050	4.06514927	-1.40237500
N	-2.05882550	4.86557427	0.58191800
C	-3.19637750	5.30323427	1.36876900
C	-4.08690250	6.19862127	0.75874100
C	-3.37728050	4.82065527	2.66551600
C	-5.21765950	6.56891127	1.48040000
C	-4.52055450	5.23762327	3.34902800
C	-5.45895250	6.08772827	2.76978000
H	-5.92977950	7.25191327	1.02397500
H	-4.68800750	4.85907027	4.35478800
C	-2.43567450	3.84432827	3.32095000
H	-1.69895350	3.43045127	2.62956800
H	-1.91708250	4.32245827	4.15790500
H	-3.00506350	3.00614727	3.73570800
C	-3.85581750	6.73093927	-0.63227000
H	-2.80468550	6.98295727	-0.80132900
H	-4.14879950	6.00030527	-1.39595200
H	-4.45381950	7.62904127	-0.79355300
C	-6.72589750	6.45263027	3.49638400
H	-7.54185450	5.79288227	3.18212900
H	-6.60858050	6.34798627	4.57685200
H	-7.02800950	7.47880227	3.27480500
C	-3.35472550	3.37614227	-1.14826000
H	-2.74384550	2.15522027	-0.37907200
O	-3.25493150	3.20508527	-2.37078000
C	-4.69982950	3.27554627	-0.47581800
C	-4.86871250	2.86805827	0.84742000

C	-5.82036250	3.53352927	-1.26530700
C	-6.13740650	2.75305827	1.39667100
H	-4.00147350	2.60765427	1.44545300
C	-7.10029150	3.42845127	-0.72952700
H	-5.67849450	3.81299727	-2.30402700
C	-7.24082350	3.04266727	0.59858200
H	-6.27037250	2.42625427	2.42242000
H	-7.97625450	3.63777827	-1.33284100
Cl	-8.84343450	2.89963527	1.28219600

TS2^{bs}

S	-1.70692432	1.89210947	0.00000000
O	-1.55066232	1.67903247	-1.46241200
O	-1.40728832	0.88973647	1.05116800
O	-3.52316232	1.53736847	-0.01127300
C	-2.21792232	3.53207747	0.50664200
C	-2.52895032	4.46900447	-0.47412500
C	-2.74881732	5.78654847	-0.09281400
C	-2.66779032	6.17362447	1.25009400
C	-2.36789632	5.20585747	2.20985200
C	-2.13026732	3.87999547	1.84826100
H	-2.56948432	4.16725047	-1.51610300
H	-2.97271832	6.53329547	-0.85100900
H	-2.30040932	5.49293947	3.25554100
H	-1.87219032	3.13017147	2.58960800
C	-2.88494332	7.61466147	1.63221600
H	-3.91914332	7.91928347	1.44440300
H	-2.66843632	7.78345947	2.68898200
H	-2.24040532	8.27138847	1.03927600
N	-3.84535132	0.20486247	0.11873700
C	-3.44971632	-0.64681353	-0.99034400
H	-2.38470432	-0.90059053	-0.94525500
H	-4.03958732	-1.56284553	-0.95605000
H	-3.65177132	-0.09696453	-1.90833100
C	-3.77590732	-0.34086353	1.38022400
O	-4.07770132	0.46062747	2.41907200
O	-3.53725132	-1.51781453	1.57255300
C	-4.96446832	1.57032347	2.26172500
H	-5.50947432	1.64673347	3.20409000
H	-4.40985032	2.48794947	2.06666800
H	-5.66341232	1.39654847	1.44116500
C	3.15635768	0.28607047	-0.79364800
C	3.97602068	1.23517647	-0.26000500
C	1.92288368	2.16334547	0.18811400

C	5.44226868	-1.29919553	0.20015900
H	4.58289168	-1.43375353	0.86858300
H	6.15109668	-2.09152453	0.45515100
C	6.11141468	0.05626047	0.47990900
H	7.16236468	0.01734647	0.17630500
H	6.10634468	0.25184247	1.55691000
C	5.47740668	1.24484047	-0.26562400
H	5.79891268	1.23999147	-1.31126200
H	5.83510668	2.18438247	0.16161900
C	3.51601268	-1.01217753	-1.46629600
H	2.85152068	-1.78457353	-1.06324800
H	3.29149868	-0.93807853	-2.53583900
C	4.97181468	-1.46062153	-1.25264600
H	5.64043668	-0.91845653	-1.92971500
H	5.02508568	-2.51047153	-1.55173900
S	1.49341168	0.73186147	-0.59515200
N	3.24238868	2.28426247	0.29867800
C	3.84390568	3.38813447	1.02549100
C	4.17972768	4.55768847	0.34764500
C	4.04526168	3.20463847	2.40115200
C	4.73050368	5.59382047	1.10879100
C	4.60223868	4.26401747	3.10613600
C	4.94726868	5.46656647	2.47717100
H	4.99409368	6.52159847	0.60702500
H	4.76655068	4.15383647	4.17500100
C	3.64286768	1.92263747	3.07912100
H	2.55402068	1.81366347	3.05423200
H	4.07694468	1.04797647	2.58285400
H	3.97053468	1.92188547	4.11930600
C	3.98642768	4.73782847	-1.13511500
H	3.51104868	3.87608647	-1.60737700
H	3.35896268	5.61322147	-1.32919100
H	4.95230968	4.90408447	-1.62056500
C	5.56031368	6.58744247	3.27461000
H	6.59135168	6.34354847	3.54888400
H	5.57351968	7.51839347	2.70504100
H	5.00691168	6.75534547	4.20203900
C	0.99375668	3.21223447	0.80824800
C	0.78432968	4.45223247	-0.00526000
C	0.72968468	5.66917447	0.67153900
C	0.63182568	4.41054347	-1.39384800
C	0.53530968	6.85084447	-0.03424300
H	0.84210268	5.67746947	1.75072100
C	0.43121968	5.58363947	-2.10907100

H	0.61768168	3.45543747	-1.91409000
C	0.38498968	6.79114047	-1.41611000
H	0.49333468	7.80580247	0.47766400
H	0.29565768	5.56559447	-3.18424400
Cl	0.11049268	8.27007447	-2.30292400
O	0.85227268	3.18049647	2.02421100
H	-0.33984932	2.46941747	0.10062100
TS2C			
C	-1.67471820	0.66827696	0.00000000
C	-1.16305220	0.02782896	1.06562900
C	0.84682680	0.74836996	0.08209000
C	-3.68730120	1.21468796	2.10682500
H	-3.09977120	2.12364996	1.92647800
H	-4.55883720	1.52541196	2.69108400
C	-2.86607820	0.22140896	2.94867900
H	-3.54411020	-0.41872004	3.52404200
H	-2.26268620	0.77266696	3.67975400
C	-1.95559720	-0.69819904	2.11977000
H	-2.56393220	-1.45802604	1.62003100
H	-1.28049720	-1.24016304	2.78637100
C	-3.11237720	0.89866996	-0.37300700
H	-3.19781120	1.94983996	-0.68137200
H	-3.37735420	0.30701796	-1.25852400
C	-4.13594120	0.65017696	0.75084300
H	-4.35227520	-0.41986704	0.84334600
H	-5.07490520	1.12042396	0.44362500
S	-0.39627920	1.31740596	-1.03543100
N	0.24734180	0.05119396	1.13633600
C	0.88878980	-0.14500504	2.40247400
C	1.46961880	-1.38699404	2.69197800
C	0.87812580	0.89770396	3.33679200
C	2.09629980	-1.54836904	3.92486500
C	1.52095480	0.69248096	4.56058400
C	2.14410980	-0.51645904	4.86583100
H	2.57046380	-2.50033904	4.15387900
H	1.52081280	1.49140996	5.29900100
C	0.21471080	2.21876496	3.03597500
H	0.92827580	2.93851096	2.61841500
H	-0.59985420	2.11623396	2.31373200
H	-0.19105020	2.66003996	3.95080000
C	1.45700280	-2.49188504	1.67203900
H	0.44724980	-2.66714504	1.28906600
H	2.08688480	-2.22610904	0.81504200

H	1. 83520380	-3. 42027904	2. 10416200
C	2. 82728080	-0. 72449104	6. 19313300
H	3. 80415780	-1. 19720104	6. 06086500
H	2. 97222380	0. 22324496	6. 71588100
H	2. 23242980	-1. 37855604	6. 83839400
C	2. 15236580	0. 93225096	-0. 39247000
O	2. 28176880	1. 49428896	-1. 57523000
C	3. 28828680	0. 06882596	0. 09077000
C	3. 79359280	0. 02288796	1. 39395300
C	3. 89278980	-0. 74212404	-0. 88238600
C	4. 80228580	-0. 87143704	1. 74467600
H	3. 39322880	0. 67402996	2. 16409800
C	4. 89186580	-1. 64803404	-0. 55059800
H	3. 54160180	-0. 65347704	-1. 90475700
C	5. 31920980	-1. 71716404	0. 77312400
H	5. 16994180	-0. 91571404	2. 76489800
H	5. 32840680	-2. 30073804	-1. 29939000
Cl	6. 56622080	-2. 86922904	1. 21500100
C	8. 19943580	0. 16256996	1. 31894100
C	7. 72732180	0. 23000996	0. 01994700
C	6. 94918080	1. 32406496	-0. 34303800
C	6. 70364680	2. 34612796	0. 57247800
C	7. 18627580	2. 23120096	1. 87799800
C	7. 91359680	1. 12263796	2. 27591400
H	7. 96021980	-0. 55532904	-0. 68904500
H	6. 54581780	1. 38988996	-1. 34730100
H	8. 28686680	1. 03485596	3. 28895000
N	9. 06861380	-0. 96142104	1. 70622400
S	5. 72728280	3. 69580996	-0. 09839500
O	5. 51922280	4. 80834196	0. 79476400
O	6. 16979180	3. 88716796	-1. 45648900
O	4. 27820080	2. 86438796	-0. 24705600
N	7. 06611480	3. 29261996	2. 89076400
N	3. 13702980	3. 33445096	0. 43110700
C	2. 35059680	4. 29581096	-0. 45650000
H	2. 29841280	3. 68346396	-1. 36084500
C	3. 06181080	5. 61415196	-0. 70045100
H	3. 25721980	6. 14969596	0. 23147400
H	3. 99452980	5. 49254396	-1. 25443500
H	2. 39718480	6. 22482196	-1. 31658100
C	0. 94022880	4. 47451096	0. 09425500
H	0. 31610480	4. 82001396	-0. 73309200
H	0. 51561480	3. 52866296	0. 43904500
H	0. 90187180	5. 21266196	0. 89628600

C	3.48456780	3.64267596	1.85947900
O	4.28706180	2.95276996	2.41955900
O	2.76735780	4.63535796	2.28071800
C	3.01210380	5.23996096	3.63019500
C	1.95441880	6.32969696	3.67573000
H	2.02396580	6.85961796	4.62831500
H	2.10402380	7.04634796	2.86390300
H	0.95470280	5.89498596	3.58943400
C	4.42093880	5.81098696	3.63936600
H	5.17815980	5.02479296	3.64348300
H	4.57930980	6.45825396	2.77322800
H	4.54167580	6.40728396	4.54768900
C	2.79339280	4.19809696	4.71510400
H	1.77626080	3.80349496	4.66766800
H	3.51078780	3.37993396	4.63882300
H	2.92414980	4.68697196	5.68395200
O	9.56154880	-1.61632904	0.81051900
O	9.24133180	-1.14791804	2.89491800
O	6.67722080	2.95892196	3.99197400
O	7.42735380	4.40472596	2.56827000
H	2.49230580	2.32192796	0.42459700
HCO3 ⁻			
C	-1.09500806	0.90982285	0.00000000
O	-2.17372006	1.52241085	0.00011900
O	0.04197094	1.74492085	0.00008500
H	0.78336394	1.12763785	0.00009900
O	-0.84603606	-0.31404115	0.00010500
TS2R-B			
C	-1.80354268	1.69887276	0.00000000
C	-0.93072868	0.87746376	0.62418600
C	0.41767432	2.75455076	0.37149600
C	-3.56153968	0.10854576	1.77995800
H	-3.45375268	1.11999776	2.18937300
H	-4.40248468	-0.34808724	2.31026200
C	-2.29501768	-0.70840724	2.08616700
H	-2.54529468	-1.77429624	2.12220100
H	-1.92470568	-0.44228424	3.08183800
C	-1.16523568	-0.54386824	1.05393100
H	-1.39813768	-1.13253424	0.16101900
H	-0.23815168	-0.95798424	1.45886700
C	-3.24138768	1.45757576	-0.36934300
H	-3.81320768	2.34020376	-0.05612400

H	-3.33977968	1.40405576	-1.46034700
C	-3.87870268	0.21875076	0.28162600
H	-3.56435168	-0.69218924	-0.23996000
H	-4.95937168	0.29531076	0.13106000
S	-1.06132268	3.24955776	-0.35524600
N	0.32177632	1.48946376	0.83152100
C	1.43541332	0.83743476	1.46939200
C	2.34091632	0.13181376	0.66736500
C	1.58655632	0.96674476	2.84987400
C	3.46740232	-0.40025424	1.28400000
C	2.72736432	0.40067876	3.42565100
C	3.68477032	-0.25804224	2.65768500
H	4.20253432	-0.92640224	0.67872200
H	2.87740032	0.50072276	4.49808800
C	0.58484832	1.73095176	3.67360400
H	0.70410332	2.81305976	3.53212500
H	-0.44208668	1.47689076	3.39084000
H	0.71576532	1.50697276	4.73422700
C	2.08775432	-0.04301124	-0.80566400
H	2.95018732	-0.50377324	-1.29086000
H	1.21441032	-0.68262824	-0.97880200
H	1.89282932	0.91685776	-1.29146900
C	4.95250432	-0.78698724	3.27593000
H	4.90848132	-0.75580024	4.36647500
H	5.14550432	-1.81767324	2.96574500
H	5.80871832	-0.18402124	2.95351700
C	1.43539232	3.77567176	0.50499000
H	1.23882532	4.16387676	1.70550900
O	1.13975432	4.86999076	-0.27299200
C	2.87531632	3.31380976	0.44161400
C	3.64152032	3.15766176	1.59705800
C	3.47139332	3.07211976	-0.79915600
C	4.95038832	2.68669676	1.53076900
H	3.19721532	3.39293376	2.56043800
C	4.77544332	2.59708576	-0.88873400
H	2.89137732	3.25146776	-1.70055200
C	5.49220532	2.39351976	0.28652800
H	5.53739132	2.54078476	2.43179400
H	5.23190332	2.38397876	-1.84941000
Cl	7.12525032	1.75225276	0.19250700
C	0.37066932	5.97677776	2.65213600
O	-0.06335168	6.67243676	3.57962300
O	0.08063332	6.30216076	1.39342700
H	0.58882232	5.69207676	0.63302800

O	1. 10654132	4. 91442876	2. 84476600
TS2S-B			
C	-0. 66022545	0. 39452495	0. 00000000
C	0. 27542655	-0. 54099205	0. 26990600
C	-1. 58222045	-1. 93676205	0. 11408800
C	1. 70313655	1. 40394995	-1. 46064900
H	0. 98847455	0. 99548895	-2. 18586700
H	2. 42718855	1. 98231895	-2. 04204600
C	2. 45108855	0. 25351995	-0. 76160300
H	3. 44356955	0. 59541695	-0. 44918500
H	2. 60977755	-0. 56411805	-1. 47344100
C	1. 74064755	-0. 29162305	0. 48829100
H	1. 84001455	0. 42301695	1. 31047200
H	2. 22575655	-1. 21362605	0. 81657300
C	-0. 49784745	1. 87256495	-0. 22675400
H	-1. 10606745	2. 13309795	-1. 10181600
H	-0. 92148845	2. 43195295	0. 61559600
C	0. 94759355	2. 33064895	-0. 49689000
H	1. 50007755	2. 42907695	0. 44362500
H	0. 88849755	3. 33837695	-0. 91789500
S	-2. 23368145	-0. 35436105	-0. 15974600
N	-0. 25300445	-1. 84241905	0. 31243200
C	0. 61755455	-2. 99378005	0. 22066000
C	1. 05291555	-3. 62771205	1. 38516000
C	1. 02844355	-3. 37708305	-1. 05840500
C	1. 90255755	-4. 72016805	1. 23835200
C	1. 87386455	-4. 48154305	-1. 15172900
C	2. 29717755	-5. 17507805	-0. 02080400
H	2. 23897155	-5. 24804305	2. 12787000
H	2. 17831255	-4. 82699705	-2. 13652500
C	0. 54584155	-2. 67280305	-2. 30023600
H	-0. 41268145	-3. 10904205	-2. 60200300
H	0. 41156155	-1. 59711305	-2. 14537200
H	1. 26013555	-2. 81416105	-3. 11471500
C	0. 57243055	-3. 15584305	2. 72759000
H	0. 83176055	-2. 10503705	2. 90232400
H	-0. 51800545	-3. 25080605	2. 74273600
H	1. 00814855	-3. 75511905	3. 52959000
C	3. 11152255	-6. 43222705	-0. 17114100
H	3. 62291855	-6. 69644305	0. 75730000
H	2. 44701255	-7. 25917305	-0. 44356300
H	3. 85646155	-6. 33506805	-0. 96533800
C	-2. 32771345	-3. 19164205	0. 13744500

C	-3.81610145	-2.97554205	-0.00172000
C	-4.66070545	-3.33695705	1.05044900
C	-4.38781645	-2.47070505	-1.17532200
C	-6.03810145	-3.16432705	0.95833500
H	-4.20367945	-3.76510505	1.93595800
C	-5.76265845	-2.28554205	-1.28530100
H	-3.74941345	-2.23436305	-2.02374700
C	-6.57276345	-2.63118905	-0.20936000
H	-6.69251445	-3.43944505	1.77875700
H	-6.20234745	-1.89522505	-2.19657900
Cl	-8.30939645	-2.40501205	-0.33602400
O	-1.96098845	-4.04734005	1.14543500
H	-1.98807745	-3.80972405	-0.92441500
C	-1.02735845	-5.81164005	-1.37068700
O	-0.49362145	-6.66620605	-2.09576300
O	-0.91479245	-5.91284405	-0.04907600
H	-1.39250545	-5.09875205	0.49174200
O	-1.71734545	-4.81079905	-1.84517000
M2B			
C	-1.38438856	1.40901769	-0.03625149
C	-0.59931656	0.33446069	0.13740451
C	1.08418044	1.95774469	-0.13308649
C	-2.98488956	-0.19081231	1.86459051
H	-2.56607456	0.67269469	2.39570351
H	-3.75187956	-0.61131331	2.52248851
C	-1.88909856	-1.25193131	1.65439251
H	-2.34482956	-2.24822031	1.62274551
H	-1.20844556	-1.24634731	2.51373751
C	-1.07299856	-1.07697131	0.36350151
H	-1.67370556	-1.38480131	-0.49806149
H	-0.21055156	-1.74804431	0.39096451
C	-2.88210556	1.51838769	-0.03359949
H	-3.14158956	2.40066369	0.56801251
H	-3.25332656	1.72823969	-1.04545249
C	-3.62316456	0.30798269	0.56077751
H	-3.67513756	-0.50739331	-0.16923149
H	-4.65740756	0.61531469	0.74367951
S	-0.42605856	2.89179769	-0.27004949
N	0.78805344	0.58804969	0.07365151
C	1.69738444	-0.20647031	0.85372051
C	2.48590644	-1.16161731	0.19881351
C	1.81061444	0.01604469	2.23192151
C	3.42772244	-1.86698931	0.94458751

C	2.75658244	-0.72492531	2.94376151
C	3.58502044	-1.65265231	2.31506951
H	4.06478644	-2.59173031	0.44107851
H	2.86231744	-0.55286031	4.01301751
C	0.99561944	1.08184969	2.91632051
H	1.42846944	2.07269469	2.72887351
H	-0.03496356	1.10412469	2.54768751
H	0.97815744	0.91733469	3.99611051
C	2.31316044	-1.41948531	-1.27403949
H	3.17968544	-1.94914331	-1.67658949
H	1.42238744	-2.03016831	-1.46307349
H	2.18368644	-0.48364131	-1.82096149
C	4.65930044	-2.38080631	3.08124251
H	4.47371344	-2.34790831	4.15717651
H	4.72832844	-3.42751631	2.77325251
H	5.63676444	-1.92125331	2.89647551
C	2.27412144	2.57321969	-0.25438849
H	1.87399944	4.30868969	1.50131251
O	2.26195444	3.92459169	-0.49459749
C	3.59225344	1.87768269	-0.20241049
C	4.26435244	1.70070969	1.01186051
C	4.17378444	1.38336769	-1.37184049
C	5.45345244	0.98478469	1.07130051
H	3.83059744	2.09821169	1.92520151
C	5.36808644	0.66679269	-1.33389449
H	3.67069144	1.53665369	-2.32209949
C	5.98197644	0.46413969	-0.10491149
H	5.95790744	0.82155769	2.01748351
H	5.80695244	0.26188769	-2.23909049
Cl	7.45614144	-0.48339831	-0.02947849
C	3.62952944	4.69242969	2.19755551
O	4.30439244	4.75826769	3.22083351
O	3.98569444	4.92221169	0.99756151
H	3.04578844	4.36688769	0.02851051
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TS3-B			
C	-0.91787440	1.89210947	0.00000000
C	-1.51790040	2.86089147	-0.74441100
C	0.48373060	3.90796847	-0.26774400
C	-2.61494540	0.34249447	-1.87169300
H	-1.56763540	0.29970747	-2.19596000
H	-3.13662740	-0.44433853	-2.42321700
C	-3.22745140	1.69425047	-2.26343200

H	-4.31729840	1.60040847	-2.30951200
H	-2.90047940	1.96793447	-3.27118800
C	-2.92304940	2.84047547	-1.27985800
H	-3.58891140	2.76100447	-0.41476300
H	-3.14799140	3.80062547	-1.74934300
C	-1.42327740	0.52869247	0.38795800
H	-0.61683340	-0.18577653	0.18500300
H	-1.59305640	0.50080647	1.47017100
C	-2.68147040	0.06411647	-0.36324700
H	-3.57571740	0.52819647	0.06682900
H	-2.78060240	-1.00905853	-0.18092200
S	0.65189760	2.40323947	0.52753300
N	-0.69857640	3.98520047	-0.90041500
C	-1.06779940	5.09709447	-1.74662700
C	-1.55709440	6.26209447	-1.15383400
C	-0.89040340	4.94557947	-3.12369400
C	-1.82961140	7.33581647	-1.99842300
C	-1.19848340	6.04234847	-3.92665300
C	-1.64388840	7.24718947	-3.37982700
H	-2.19254440	8.26517947	-1.56664100
H	-1.05569340	5.96255347	-5.00134700
C	-0.30101840	3.68272347	-3.69488700
H	0.70943160	3.51084547	-3.30274400
H	-0.89403940	2.80095347	-3.43381900
H	-0.24384940	3.74531647	-4.78234600
C	-1.76212640	6.34701747	0.33446300
H	-2.23285140	7.29373147	0.60260100
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C	-1.87662340	8.44854147	-4.25685500
H	-2.10597340	8.15474647	-5.28321400
H	-2.69499640	9.06489047	-3.87791700
H	-0.97673640	9.07316047	-4.28076600
C	1.57254060	4.86024747	-0.12873300
O	2.48069460	4.48204947	0.67019200
C	1.65063660	6.19170347	-0.78328700
C	1.66251260	6.35177347	-2.17063200
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C	1.74576460	8.59654947	-0.50658200
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C	1.70659460	8.72893547	-1.88991000
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Cl	1. 69585760	10. 33139147	-2. 59056600
H	3. 33521260	3. 65092647	0. 03290600
N	5. 96010060	1. 90051347	-2. 63705800
O	4. 77725760	2. 60875247	-2. 79761900
C	5. 89518060	0. 55354147	-3. 26366600
C	5. 69342560	0. 69030247	-4. 77285000
C	4. 82650560	-0. 32331653	-2. 63477100
C	7. 11893760	2. 60594447	-2. 97077800
O	8. 18713860	2. 03432447	-3. 09583000
O	6. 92563260	3. 91928747	-3. 09871900
C	8. 04988760	4. 76800347	-3. 49843500
C	8. 55743560	4. 34338547	-4. 87438600
C	9. 13811960	4. 73699347	-2. 43051000
C	7. 43878560	6. 16273547	-3. 58635800
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H	5. 67501160	-0. 29580653	-5. 24461900
H	6. 50496960	1. 26853147	-5. 22520300
H	4. 74427860	1. 19251347	-4. 97884900
H	3. 83442160	0. 10999747	-2. 77831900
H	4. 98971860	-0. 44478753	-1. 56432000
H	4. 85601560	-1. 30375253	-3. 11934600
H	9. 30805760	5. 06192247	-5. 21481700
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H	7. 18716460	6. 54709547	-2. 59418800
C	5. 34175760	3. 98525047	-0. 64908500
C	6. 14719660	3. 31827947	0. 28372100
C	7. 05774860	4. 01145847	1. 06407800
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N	4. 79526860	6. 13224347	-1. 81793000
O	4. 68310160	7. 33763847	-1. 65720600
O	4. 42346860	5. 52328447	-2. 79844800
N	8. 06126960	6. 14433947	1. 78327900
O	8. 74426260	5. 51101247	2. 56818200
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S	3. 95327460	2. 96489747	-1. 26180500

O	4.02235760	1.61755347	-0.66306700
O	2.79020760	3.51431547	-2.00308600
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H	7.70214260	3.49808647	1.76673300
H	6.42491760	7.16972647	-0.06414200