(Supporting Information)

Michael Addition of Stannyl Ketone Enolate to α,β -Unsaturated Esters Catalyzed by Tetrabutylammonium Bromide and an ab Initio Theoretical Study on the Reaction Course

Makoto Yasuda, Kouji Chiba, Noriyuki Ohigashi, Yasuhiro Katoh, and Akio Baba*

Department of Molecular Chemistry and Handai Frontier Research Center, Graduate School of Engineering, Osaka University, 2-1 Yamadaoka, Suita, Osaka 565-0871, Japan and Science and Technology System Division, Ryoka Systems Inc., 1-5-2 Irifune, Urayasu, Chiba 279-0012, Japan

Total energies for all of the calculated species (in hartree). All energies includes zero point vibration energy correction.

ester enolate (Scheme 1)	-267.607889
ketone enolate (Scheme 1)	-192.418136
enone (Scheme 1)	-231.063825
enoate (Scheme 1) = 2a	-306.263640
product in Type A (Scheme 1)	-498.725096
product in Type B (Scheme 1)	-423.529637
product in Type C (Scheme 1)	-573.918737
product in Type D (Scheme 1)	-498.721569
7	-507.009657
8	-507.009812
9	-390.575233
10	-390.583641
7-Br	-3078.526315
A	-813.244464
B	-813.283561
C	-3384.791878
D	-3384.772850
E	-3384.778257
F	-3384.773400
G	-3384.801164

Geometries (PDB)

ester enolate (Scheme 1)

HETATM	1	O1	UNK	0	-1.800	-0.380	1.180	1.00	0.00
HETATM	2	C2	UNK	0	-0.664	-0.316	0.668	1.00	0.00
HETATM	3	O3	UNK	0	-0.272	1.036	0.388	1.00	0.00
HETATM	4	C4	UNK	0	0.976	1.272	-0.196	1.00	0.00
HETATM	5	C5	UNK	0	0.224	-1.336	0.352	1.00	0.00
HETATM	6	7H	UNK	0	1.068	2.360	-0.324	1.00	0.00
HETATM	7	8H	UNK	0	1.076	0.788	-1.180	1.00	0.00
HETATM	8	9H	UNK	0	1.804	0.920	0.440	1.00	0.00
HETATM	9	OH1	UNK	0	-0.076	-2.356	0.564	1.00	0.00
HETATM	10	1H1	UNK	0	1.200	-1.180	-0.096	1.00	0.00
TER	11		UNK	0					
END									

ketone enolate (Scheme 1)

HETATM	1	C1	UNK	0	-0.324	1.460	-0.072	1.00	0.00
HETATM	2	C2	UNK	0	-0.468	-0.068	-0.000	1.00	0.00
HETATM	3	C3	UNK	0	0.684	-0.820	-0.164	1.00	0.00
HETATM	4	O4	UNK	0	-1.652	-0.496	0.212	1.00	0.00
HETATM	5	5H	UNK	0	-0.680	1.908	0.868	1.00	0.00
HETATM	6	6H	UNK	0	0.704	1.796	-0.252	1.00	0.00
HETATM	7	7H	UNK	0	-0.968	1.852	-0.868	1.00	0.00
HETATM	8	8H	UNK	0	1.652	-0.348	-0.340	1.00	0.00
HETATM	9	9H	UNK	0	0.644	-1.908	-0.124	1.00	0.00
TER	10		UNK	0					
END									

enone (Scheme 1)

HETATM	1	C1	UNK	0	-0.348	1.876	-0.052	1.00	0.00
HETATM	2	C2	UNK	0	-0.536	0.380	-0.004	1.00	0.00
HETATM	3	C3	UNK	0	0.696	-0.436	0.180	1.00	0.00
HETATM	4	O4	UNK	0	-1.640	-0.132	-0.112	1.00	0.00
HETATM	5	5H	UNK	0	0.120	2.232	0.872	1.00	0.00
HETATM	6	6H	UNK	0	0.328	2.148	-0.872	1.00	0.00
HETATM	7	7H	UNK	0	-1.308	2.372	-0.192	1.00	0.00
HETATM	8	8H	UNK	0	1.640	0.096	0.268	1.00	0.00
HETATM	9	C12	UNK	0	0.656	-1.772	0.236	1.00	0.00
HETATM	10	3H1	UNK	0	-0.292	-2.296	0.148	1.00	0.00
HETATM	11	4H1	UNK	0	1.552	-2.368	0.372	1.00	0.00
TER	12		UNK	0					
END									

enoate (Scheme 1) = 2a

HETATM	1	C1	UNK	0	-0.836	1.036	-1.008	1.00	0.00
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HETATM	2	C2	UNK	0	-0.800	2.372	-0.992	1.00	0.00
HETATM	3	C3	UNK	0	-0.164	0.240	0.044	1.00	0.00
HETATM	4	O4	UNK	0	0.456	0.688	0.984	1.00	0.00
HETATM	5	O5	UNK	0	-0.336	-1.080	-0.176	1.00	0.00
HETATM	6	C6	UNK	0	0.272	-1.948	0.780	1.00	0.00
HETATM	7	7H	UNK	0	-1.352	0.484	-1.784	1.00	0.00
HETATM	8	8H	UNK	0	-0.272	2.900	-0.200	1.00	0.00
HETATM	9	9H	UNK	0	-1.288	2.964	-1.756	1.00	0.00
HETATM	10	OH1	UNK	0	-0.132	-1.764	1.780	1.00	0.00
HETATM	11	1H1	UNK	0	0.032	-2.960	0.452	1.00	0.00
HETATM	12	2H1	UNK	0	1.356	-1.796	0.800	1.00	0.00
TER	13		UNK	0					
END									

Product in type A (Scheme 1)

HETATM	1	O1	UNK	0	-1.384	3.548	1.676	1.00	0.00
HETATM	2	C2	UNK	0	-1.024	2.744	0.836	1.00	0.00
HETATM	3	O3	UNK	0	-1.460	2.932	-0.432	1.00	0.00
HETATM	4	C4	UNK	0	-0.976	2.116	-1.512	1.00	0.00
HETATM	5	C5	UNK	0	-0.212	1.516	1.144	1.00	0.00
HETATM	6	7H	UNK	0	-1.696	2.256	-2.320	1.00	0.00
HETATM	7	8H	UNK	0	-0.892	1.048	-1.264	1.00	0.00
HETATM	8	9H	UNK	0	0.000	2.492	-1.840	1.00	0.00
HETATM	9	OH1	UNK	0	0.484	1.276	0.336	1.00	0.00
HETATM	10	1H1	UNK	0	0.360	1.720	2.052	1.00	0.00
HETATM	11	C12	UNK	0	-1.112	0.256	1.364	1.00	0.00
HETATM	12	C13	UNK	0	-0.344	-1.024	1.324	1.00	0.00
HETATM	13	C14	UNK	0	0.104	-1.508	0.108	1.00	0.00
HETATM	14	C15	UNK	0	0.892	-2.820	0.080	1.00	0.00
HETATM	15	O16	UNK	0	-0.092	-0.940	-1.024	1.00	0.00
HETATM	16	7H1	UNK	0	-1.640	0.388	2.320	1.00	0.00
HETATM	17	8H1	UNK	0	-1.880	0.252	0.576	1.00	0.00
HETATM	18	9H1	UNK	0	-0.112	-1.544	2.252	1.00	0.00
HETATM	19	OH2	UNK	0	0.376	-3.548	-0.556	1.00	0.00
HETATM	20	1H2	UNK	0	1.884	-2.648	-0.364	1.00	0.00
HETATM	21	2H2	UNK	0	1.028	-3.260	1.080	1.00	0.00
TER	22		UNK	0					
END									

Product in type B (Scheme 1)

HETATM	1	C1	UNK	0	-2.836	0.828	-0.428	1.00	0.00
HETATM	2	C2	UNK	0	-1.736	1.856	-0.216	1.00	0.00
HETATM	3	C3	UNK	0	-0.416	1.320	0.244	1.00	0.00
HETATM	4	C4	UNK	0	0.420	0.728	-0.944	1.00	0.00
HETATM	5	C5	UNK	0	1.608	-0.052	-0.480	1.00	0.00
HETATM	6	C6	UNK	0	1.432	-1.308	0.068	1.00	0.00

HETATM	7	C7	UNK	0	2.668	-2.080	0.536	1.00	0.00
HETATM	8	O8	UNK	0	-1.940	3.044	-0.460	1.00	0.00
HETATM	9	O9	UNK	0	0.304	-1.896	0.212	1.00	0.00
HETATM	10	OH1	UNK	0	-2.432	-0.116	-0.800	1.00	0.00
HETATM	11	1H1	UNK	0	-3.296	0.608	0.544	1.00	0.00
HETATM	12	2H1	UNK	0	-3.608	1.220	-1.096	1.00	0.00
HETATM	13	3H1	UNK	0	0.152	2.116	0.728	1.00	0.00
HETATM	14	4H1	UNK	0	-0.568	0.480	0.936	1.00	0.00
HETATM	15	5H1	UNK	0	-0.244	0.068	-1.520	1.00	0.00
HETATM	16	6H1	UNK	0	0.708	1.560	-1.604	1.00	0.00
HETATM	17	7H1	UNK	0	2.596	0.408	-0.524	1.00	0.00
HETATM	18	8H1	UNK	0	2.732	-3.040	0.004	1.00	0.00
HETATM	19	9H1	UNK	0	3.608	-1.528	0.376	1.00	0.00
HETATM	20	OH2	UNK	0	2.576	-2.316	1.604	1.00	0.00
TER	21		UNK	0					
END									

Product in type C (Scheme 1)

HETATM	1	C1	UNK	0	0.576	-1.308	-1.112	1.00	0.00
HETATM	2	C2	UNK	0	1.384	0.040	-0.956	1.00	0.00
HETATM	3	C3	UNK	0	1.208	-2.432	-0.364	1.00	0.00
HETATM	4	O4	UNK	0	2.020	-3.232	-0.800	1.00	0.00
HETATM	5	O5	UNK	0	0.844	-2.444	0.952	1.00	0.00
HETATM	6	C6	UNK	0	1.504	-3.412	1.760	1.00	0.00
HETATM	7	7H	UNK	0	0.548	-1.572	-2.168	1.00	0.00
HETATM	8	8H	UNK	0	1.360	0.296	0.116	1.00	0.00
HETATM	9	9H	UNK	0	2.428	-0.172	-1.220	1.00	0.00
HETATM	10	OH1	UNK	0	2.588	-3.260	1.748	1.00	0.00
HETATM	11	1H1	UNK	0	1.112	-3.268	2.768	1.00	0.00
HETATM	12	2H1	UNK	0	1.288	-4.428	1.408	1.00	0.00
HETATM	13	C13	UNK	0	0.836	1.160	-1.768	1.00	0.00
HETATM	14	C14	UNK	0	-0.216	1.924	-1.300	1.00	0.00
HETATM	15	O15	UNK	0	-0.832	1.860	-0.212	1.00	0.00
HETATM	16	O16	UNK	0	-0.628	2.924	-2.232	1.00	0.00
HETATM	17	C17	UNK	0	-1.680	3.740	-1.788	1.00	0.00
HETATM	18	8H1	UNK	0	-0.436	-1.116	-0.752	1.00	0.00
HETATM	19	9H1	UNK	0	1.212	1.324	-2.772	1.00	0.00
HETATM	20	1H2	UNK	0	-2.584	3.160	-1.544	1.00	0.00
HETATM	21	2H2	UNK	0	-1.408	4.316	-0.892	1.00	0.00
HETATM	22	3H2	UNK	0	-1.896	4.432	-2.608	1.00	0.00
TER	23		UNK	0					
END									

Product in type D (Scheme 1)

HETATM	1	C1	UNK	0	0.720	-1.876	-0.696	1.00	0.00
HETATM	2	C2	UNK	0	1.528	-0.528	-0.512	1.00	0.00

HETATM	3	C3	UNK	0	1.236	-2.964	0.192	1.00	0.00
HETATM	4	O4	UNK	0	2.048	-3.808	-0.176	1.00	0.00
HETATM	5	C5	UNK	0	0.748	-2.944	1.632	1.00	0.00
HETATM	6	7H	UNK	0	0.796	-2.188	-1.740	1.00	0.00
HETATM	7	8H	UNK	0	1.532	-0.300	0.564	1.00	0.00
HETATM	8	9H	UNK	0	2.568	-0.728	-0.804	1.00	0.00
HETATM	9	C13	UNK	0	0.964	0.616	-1.268	1.00	0.00
HETATM	10	C14	UNK	0	-0.136	1.292	-0.768	1.00	0.00
HETATM	11	O15	UNK	0	-0.760	1.100	0.304	1.00	0.00
HETATM	12	O16	UNK	0	-0.592	2.340	-1.620	1.00	0.00
HETATM	13	C17	UNK	0	-1.688	3.060	-1.124	1.00	0.00
HETATM	14	8H1	UNK	0	-0.316	-1.636	-0.456	1.00	0.00
HETATM	15	9H1	UNK	0	1.344	0.864	-2.256	1.00	0.00
HETATM	16	1H2	UNK	0	-2.564	2.420	-0.956	1.00	0.00
HETATM	17	2H2	UNK	0	-1.460	3.564	-0.176	1.00	0.00
HETATM	18	3H2	UNK	0	-1.928	3.812	-1.888	1.00	0.00
HETATM	19	4H2	UNK	0	0.760	-1.920	2.032	1.00	0.00
HETATM	20	5H2	UNK	0	-0.292	-3.276	1.664	1.00	0.00
HETATM	21	6H2	UNK	0	1.360	-3.608	2.252	1.00	0.00
TER	22		UNK	0					
END									

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HETATM	1	C1	UNK	0	3.324	-2.068	-2.260	1.00	0.00
HETATM	2	2H	UNK	0	4.372	-2.020	-2.552	1.00	0.00
HETATM	3	C3	UNK	0	2.812	-1.112	-1.384	1.00	0.00
HETATM	4	4H	UNK	0	3.464	-0.324	-1.020	1.00	0.00
HETATM	5	C5	UNK	0	1.464	-1.140	-0.996	1.00	0.00
HETATM	6	C7	UNK	0	0.640	-2.140	-1.532	1.00	0.00
HETATM	7	8H	UNK	0	-0.408	-2.156	-1.252	1.00	0.00
HETATM	8	C9	UNK	0	1.152	-3.096	-2.408	1.00	0.00
HETATM	9	0H1	UNK	0	0.492	-3.868	-2.804	1.00	0.00
HETATM	10	C11	UNK	0	2.496	-3.068	-2.772	1.00	0.00
HETATM	11	2H1	UNK	0	2.896	-3.812	-3.460	1.00	0.00
HETATM	12	C13	UNK	0	0.896	-0.148	-0.044	1.00	0.00
HETATM	13	C14	UNK	0	1.656	0.564	0.812	1.00	0.00
HETATM	14	O15	UNK	0	-0.444	-0.068	-0.120	1.00	0.00
HETATM	15	6H1	UNK	0	2.728	0.424	0.872	1.00	0.00
HETATM	16	7H1	UNK	0	1.224	1.284	1.500	1.00	0.00
HETATM	17	SN18	UNK	0	-1.672	1.164	0.836	1.00	0.00
HETATM	18	C19	UNK	0	-1.188	3.160	0.228	1.00	0.00
HETATM	19	C20	UNK	0	-1.476	0.836	2.944	1.00	0.00
HETATM	20	C21	UNK	0	-3.548	0.492	0.072	1.00	0.00
HETATM	21	2H2	UNK	0	-1.912	3.872	0.644	1.00	0.00
HETATM	22	3H2	UNK	0	-0.188	3.448	0.564	1.00	0.00
HETATM	23	4H2	UNK	0	-1.220	3.236	-0.864	1.00	0.00

HETATM	24	5H2	UNK	0	-2.404	1.108	3.456	1.00	0.00
HETATM	25	6H2	UNK	0	-1.276	-0.220	3.136	1.00	0.00
HETATM	26	7H2	UNK	0	-0.660	1.424	3.368	1.00	0.00
HETATM	27	8H2	UNK	0	-4.368	1.120	0.432	1.00	0.00
HETATM	28	9H2	UNK	0	-3.540	0.524	-1.024	1.00	0.00
HETATM	29	0H3	UNK	0	-3.740	-0.536	0.384	1.00	0.00
TER	30		UNK	0					
END									

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HETATM	1	C1	UNK	0	2.288	-2.624	-1.048	1.00	0.00
HETATM	2	2H	UNK	0	2.684	-3.376	-0.368	1.00	0.00
HETATM	3	C3	UNK	0	2.012	-1.340	-0.580	1.00	0.00
HETATM	4	4H	UNK	0	2.204	-1.116	0.464	1.00	0.00
HETATM	5	C5	UNK	0	1.496	-0.360	-1.440	1.00	0.00
HETATM	6	C7	UNK	0	1.264	-0.696	-2.784	1.00	0.00
HETATM	7	8H	UNK	0	0.864	0.072	-3.440	1.00	0.00
HETATM	8	C9	UNK	0	1.544	-1.976	-3.252	1.00	0.00
HETATM	9	0H1	UNK	0	1.360	-2.220	-4.296	1.00	0.00
HETATM	10	C11	UNK	0	2.052	-2.944	-2.388	1.00	0.00
HETATM	11	2H1	UNK	0	2.272	-3.948	-2.752	1.00	0.00
HETATM	12	C13	UNK	0	1.172	1.040	-1.004	1.00	0.00
HETATM	13	C14	UNK	0	1.392	1.452	0.412	1.00	0.00
HETATM	14	O15	UNK	0	0.696	1.828	-1.820	1.00	0.00
HETATM	15	6H1	UNK	0	2.172	0.892	0.932	1.00	0.00
HETATM	16	7H1	UNK	0	1.644	2.516	0.424	1.00	0.00
HETATM	17	SN18	UNK	0	-0.472	1.324	1.572	1.00	0.00
HETATM	18	C19	UNK	0	-1.660	3.036	1.056	1.00	0.00
HETATM	19	C20	UNK	0	0.104	1.368	3.644	1.00	0.00
HETATM	20	C21	UNK	0	-1.512	-0.496	1.120	1.00	0.00
HETATM	21	2H2	UNK	0	-2.680	2.932	1.432	1.00	0.00
HETATM	22	3H2	UNK	0	-1.224	3.952	1.468	1.00	0.00
HETATM	23	4H2	UNK	0	-1.700	3.140	-0.036	1.00	0.00
HETATM	24	5H2	UNK	0	-0.780	1.376	4.292	1.00	0.00
HETATM	25	6H2	UNK	0	0.704	0.488	3.904	1.00	0.00
HETATM	26	7H2	UNK	0	0.696	2.264	3.868	1.00	0.00
HETATM	27	8H2	UNK	0	-1.728	-0.564	0.048	1.00	0.00
HETATM	28	9H2	UNK	0	-0.920	-1.376	1.404	1.00	0.00
HETATM	29	0H3	UNK	0	-2.460	-0.532	1.664	1.00	0.00
TER	30		UNK	0					
END									

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HETATM	1	SN18	UNK	0	-1.104	0.596	0.068	1.00	0.00
HETATM	2	C19	UNK	0	-1.356	2.548	-0.748	1.00	0.00
HETATM	3	C20	UNK	0	-0.544	0.620	2.136	1.00	0.00

HETATM	4	C21	UNK	0	-2.744	-0.712	-0.360	1.00	0.00
HETATM	5	2H2	UNK	0	-2.200	3.072	-0.284	1.00	0.00
HETATM	6	3H2	UNK	0	-0.448	3.144	-0.592	1.00	0.00
HETATM	7	4H2	UNK	0	-1.540	2.484	-1.828	1.00	0.00
HETATM	8	5H2	UNK	0	-1.308	1.136	2.732	1.00	0.00
HETATM	9	6H2	UNK	0	-0.428	-0.392	2.528	1.00	0.00
HETATM	10	7H2	UNK	0	0.404	1.148	2.260	1.00	0.00
HETATM	11	8H2	UNK	0	-2.852	-0.828	-1.444	1.00	0.00
HETATM	12	9H2	UNK	0	-2.584	-1.700	0.076	1.00	0.00
HETATM	13	0H3	UNK	0	-3.676	-0.304	0.040	1.00	0.00
HETATM	14	O31	UNK	0	0.460	-0.016	-0.976	1.00	0.00
HETATM	15	C32	UNK	0	1.108	-1.172	-0.936	1.00	0.00
HETATM	16	C33	UNK	0	0.832	-2.228	-0.140	1.00	0.00
HETATM	17	O34	UNK	0	2.116	-1.124	-1.840	1.00	0.00
HETATM	18	C35	UNK	0	2.944	-2.264	-1.964	1.00	0.00
HETATM	19	6H3	UNK	0	0.012	-2.192	0.560	1.00	0.00
HETATM	20	7H3	UNK	0	1.412	-3.144	-0.164	1.00	0.00
HETATM	21	8H3	UNK	0	3.460	-2.484	-1.024	1.00	0.00
HETATM	22	9H3	UNK	0	2.364	-3.140	-2.276	1.00	0.00
HETATM	23	0H4	UNK	0	3.676	-2.016	-2.736	1.00	0.00
TER	24		UNK	0					
END									

1 0

HETATM	1	SN18	UNK	0	-1.092	0.404	0.068	1.00	0.00
HETATM	2	C19	UNK	0	-1.252	2.212	-1.072	1.00	0.00
HETATM	3	C20	UNK	0	-0.624	0.768	2.132	1.00	0.00
HETATM	4	C21	UNK	0	-2.944	-0.696	-0.064	1.00	0.00
HETATM	5	2H2	UNK	0	-2.028	2.864	-0.660	1.00	0.00
HETATM	6	3H2	UNK	0	-0.296	2.744	-1.052	1.00	0.00
HETATM	7	4H2	UNK	0	-1.508	1.992	-2.116	1.00	0.00
HETATM	8	5H2	UNK	0	-1.388	1.400	2.596	1.00	0.00
HETATM	9	6H2	UNK	0	-0.568	-0.168	2.692	1.00	0.00
HETATM	10	7H2	UNK	0	0.340	1.280	2.204	1.00	0.00
HETATM	11	8H2	UNK	0	-3.196	-0.928	-1.100	1.00	0.00
HETATM	12	9H2	UNK	0	-2.884	-1.644	0.488	1.00	0.00
HETATM	13	0H3	UNK	0	-3.772	-0.116	0.360	1.00	0.00
HETATM	14	O31	UNK	0	1.924	0.916	-0.288	1.00	0.00
HETATM	15	C32	UNK	0	1.768	-0.192	-0.756	1.00	0.00
HETATM	16	C33	UNK	0	0.428	-0.884	-0.804	1.00	0.00
HETATM	17	O34	UNK	0	2.860	-0.824	-1.256	1.00	0.00
HETATM	18	C35	UNK	0	2.760	-2.124	-1.820	1.00	0.00
HETATM	19	6H3	UNK	0	0.472	-1.840	-0.268	1.00	0.00
HETATM	20	7H3	UNK	0	0.168	-1.136	-1.840	1.00	0.00
HETATM	21	8H3	UNK	0	2.416	-2.860	-1.084	1.00	0.00
HETATM	22	9H3	UNK	0	2.100	-2.136	-2.696	1.00	0.00

HETATM	23	OH4	UNK	0	3.776	-2.384	-2.136	1.00	0.00
TER	24		UNK	0					
END									

7 - Br

HETATM	1	SN1	UNK	0	2.620	0.092	-0.112	1.00	0.00
HETATM	2	BR2	UNK	0	5.464	0.156	-0.040	1.00	0.00
HETATM	3	O3	UNK	0	0.476	0.184	-0.180	1.00	0.00
HETATM	4	C4	UNK	0	-0.436	-0.744	0.008	1.00	0.00
HETATM	5	C5	UNK	0	-1.844	-0.220	-0.044	1.00	0.00
HETATM	6	C6	UNK	0	-2.964	-1.040	-0.252	1.00	0.00
HETATM	7	C7	UNK	0	-4.252	-0.504	-0.276	1.00	0.00
HETATM	8	C8	UNK	0	-4.456	0.864	-0.100	1.00	0.00
HETATM	9	C9	UNK	0	-3.348	1.692	0.092	1.00	0.00
HETATM	10	C10	UNK	0	-2.060	1.156	0.112	1.00	0.00
HETATM	11	1H1	UNK	0	-1.188	1.792	0.248	1.00	0.00
HETATM	12	2H1	UNK	0	-3.484	2.764	0.220	1.00	0.00
HETATM	13	3H1	UNK	0	-5.460	1.280	-0.120	1.00	0.00
HETATM	14	4H1	UNK	0	-5.104	-1.164	-0.448	1.00	0.00
HETATM	15	5H1	UNK	0	-2.828	-2.104	-0.416	1.00	0.00
HETATM	16	C16	UNK	0	-0.200	-2.060	0.256	1.00	0.00
HETATM	17	7H1	UNK	0	-1.004	-2.760	0.456	1.00	0.00
HETATM	18	8H1	UNK	0	0.812	-2.452	0.300	1.00	0.00
HETATM	19	C19	UNK	0	2.636	2.188	-0.572	1.00	0.00
HETATM	20	OH2	UNK	0	3.076	2.748	0.256	1.00	0.00
HETATM	21	1H2	UNK	0	3.256	2.368	-1.456	1.00	0.00
HETATM	22	2H2	UNK	0	1.612	2.532	-0.756	1.00	0.00
HETATM	23	C23	UNK	0	2.764	-1.320	-1.720	1.00	0.00
HETATM	24	4H2	UNK	0	1.768	-1.616	-2.064	1.00	0.00
HETATM	25	5H2	UNK	0	3.324	-0.868	-2.544	1.00	0.00
HETATM	26	6H2	UNK	0	3.320	-2.204	-1.388	1.00	0.00
HETATM	27	C27	UNK	0	2.656	-0.540	1.936	1.00	0.00
HETATM	28	8H2	UNK	0	1.640	-0.716	2.304	1.00	0.00
HETATM	29	9H2	UNK	0	3.248	-1.456	2.036	1.00	0.00
HETATM	30	OH3	UNK	0	3.144	0.232	2.540	1.00	0.00
TER	31		UNK	0					
END									

A

ATOM	1	SN	UNK	1	0.880	1.620	0.008	1.00	0.00
ATOM	2	O	UNK	1	-0.708	0.364	-0.128	1.00	0.00
ATOM	3	C	UNK	1	-0.960	-0.852	0.300	1.00	0.00
ATOM	4	C	UNK	1	-2.364	-1.276	0.168	1.00	0.00
ATOM	5	C	UNK	1	-3.328	-0.352	-0.264	1.00	0.00
ATOM	6	C	UNK	1	-4.664	-0.716	-0.388	1.00	0.00
ATOM	7	C	UNK	1	-5.068	-2.020	-0.088	1.00	0.00

ATOM	8	C	UNK	1	-4.120	-2.956	0.332	1.00	0.00
ATOM	9	C	UNK	1	-2.784	-2.588	0.464	1.00	0.00
ATOM	10	H	UNK	1	-2.064	-3.336	0.792	1.00	0.00
ATOM	11	H	UNK	1	-4.420	-3.972	0.560	1.00	0.00
ATOM	12	H	UNK	1	-6.112	-2.308	-0.188	1.00	0.00
ATOM	13	H	UNK	1	-5.396	0.012	-0.720	1.00	0.00
ATOM	14	H	UNK	1	-3.016	0.660	-0.500	1.00	0.00
ATOM	15	C	UNK	1	0.080	-1.732	0.668	1.00	0.00
ATOM	16	C	UNK	1	0.780	-2.464	-0.892	1.00	0.00
ATOM	17	C	UNK	1	1.924	-3.232	-0.588	1.00	0.00
ATOM	18	C	UNK	1	3.136	-2.564	-0.248	1.00	0.00
ATOM	19	O	UNK	1	4.172	-3.416	0.004	1.00	0.00
ATOM	20	C	UNK	1	5.408	-2.796	0.340	1.00	0.00
ATOM	21	H	UNK	1	5.764	-2.156	-0.468	1.00	0.00
ATOM	22	H	UNK	1	5.312	-2.192	1.248	1.00	0.00
ATOM	23	H	UNK	1	6.112	-3.616	0.508	1.00	0.00
ATOM	24	O	UNK	1	3.280	-1.332	-0.156	1.00	0.00
ATOM	25	H	UNK	1	1.864	-4.308	-0.448	1.00	0.00
ATOM	26	H	UNK	1	0.964	-1.524	-1.416	1.00	0.00
ATOM	27	H	UNK	1	-0.072	-3.008	-1.300	1.00	0.00
ATOM	28	H	UNK	1	-0.196	-2.608	1.248	1.00	0.00
ATOM	29	H	UNK	1	0.988	-1.256	1.028	1.00	0.00
ATOM	30	C	UNK	1	1.908	1.232	1.840	1.00	0.00
ATOM	31	H	UNK	1	2.424	2.144	2.172	1.00	0.00
ATOM	32	H	UNK	1	1.208	0.932	2.628	1.00	0.00
ATOM	33	H	UNK	1	2.644	0.440	1.684	1.00	0.00
ATOM	34	C	UNK	1	-0.220	3.452	0.056	1.00	0.00
ATOM	35	H	UNK	1	0.456	4.312	0.080	1.00	0.00
ATOM	36	H	UNK	1	-0.852	3.540	-0.832	1.00	0.00
ATOM	37	H	UNK	1	-0.864	3.496	0.940	1.00	0.00
ATOM	38	C	UNK	1	1.984	1.352	-1.788	1.00	0.00
ATOM	39	H	UNK	1	2.604	2.236	-1.984	1.00	0.00
ATOM	40	H	UNK	1	2.636	0.476	-1.676	1.00	0.00
ATOM	41	H	UNK	1	1.308	1.208	-2.632	1.00	0.00
TER	42		UNK	1					
END									

B

HETATM	1	SN1	UNK	0	3.384	1.992	0.744	1.00	0.00
HETATM	2	O2	UNK	0	-3.036	0.644	-1.488	1.00	0.00
HETATM	3	C3	UNK	0	-3.012	-0.084	-0.504	1.00	0.00
HETATM	4	C4	UNK	0	-3.824	-1.348	-0.500	1.00	0.00
HETATM	5	C5	UNK	0	-4.528	-1.688	-1.664	1.00	0.00
HETATM	6	C6	UNK	0	-5.304	-2.840	-1.716	1.00	0.00
HETATM	7	C7	UNK	0	-5.392	-3.672	-0.596	1.00	0.00
HETATM	8	C8	UNK	0	-4.704	-3.344	0.568	1.00	0.00

HETATM	9	C9	UNK	0	-3.924	-2.188	0.616	1.00	0.00
HETATM	10	OH1	UNK	0	-3.396	-1.948	1.536	1.00	0.00
HETATM	11	1H1	UNK	0	-4.772	-3.988	1.440	1.00	0.00
HETATM	12	2H1	UNK	0	-6.000	-4.572	-0.636	1.00	0.00
HETATM	13	3H1	UNK	0	-5.840	-3.092	-2.628	1.00	0.00
HETATM	14	4H1	UNK	0	-4.448	-1.024	-2.524	1.00	0.00
HETATM	15	C15	UNK	0	-2.136	0.252	0.680	1.00	0.00
HETATM	16	C16	UNK	0	-0.812	-0.560	0.712	1.00	0.00
HETATM	17	C17	UNK	0	0.072	-0.316	-0.468	1.00	0.00
HETATM	18	C18	UNK	0	1.236	0.356	-0.372	1.00	0.00
HETATM	19	O19	UNK	0	2.072	0.636	-1.428	1.00	0.00
HETATM	20	C20	UNK	0	1.652	0.300	-2.736	1.00	0.00
HETATM	21	1H2	UNK	0	1.552	-0.788	-2.844	1.00	0.00
HETATM	22	2H2	UNK	0	0.696	0.780	-2.976	1.00	0.00
HETATM	23	3H2	UNK	0	2.432	0.660	-3.408	1.00	0.00
HETATM	24	O24	UNK	0	1.752	0.832	0.752	1.00	0.00
HETATM	25	5H2	UNK	0	-0.256	-0.664	-1.436	1.00	0.00
HETATM	26	6H2	UNK	0	-1.052	-1.632	0.792	1.00	0.00
HETATM	27	7H2	UNK	0	-0.280	-0.288	1.628	1.00	0.00
HETATM	28	8H2	UNK	0	-2.684	0.088	1.616	1.00	0.00
HETATM	29	9H2	UNK	0	-1.900	1.316	0.608	1.00	0.00
HETATM	30	C30	UNK	0	3.476	2.408	2.840	1.00	0.00
HETATM	31	1H3	UNK	0	4.352	3.016	3.084	1.00	0.00
HETATM	32	2H3	UNK	0	2.580	2.944	3.164	1.00	0.00
HETATM	33	3H3	UNK	0	3.536	1.472	3.408	1.00	0.00
HETATM	34	C34	UNK	0	2.988	3.752	-0.404	1.00	0.00
HETATM	35	5H3	UNK	0	3.640	4.576	-0.088	1.00	0.00
HETATM	36	6H3	UNK	0	3.156	3.568	-1.468	1.00	0.00
HETATM	37	7H3	UNK	0	1.948	4.064	-0.268	1.00	0.00
HETATM	38	C38	UNK	0	5.068	0.848	0.088	1.00	0.00
HETATM	39	9H3	UNK	0	5.028	-0.156	0.524	1.00	0.00
HETATM	40	OH4	UNK	0	5.064	0.748	-1.000	1.00	0.00
HETATM	41	1H4	UNK	0	6.004	1.320	0.400	1.00	0.00
TER	42		UNK	0					
END									

C

HETATM	1	SN1	UNK	0	1.716	-0.604	-0.180	1.00	0.00
HETATM	2	BR2	UNK	0	-1.072	-1.304	-0.360	1.00	0.00
HETATM	3	O3	UNK	0	3.752	0.032	-0.108	1.00	0.00
HETATM	4	C4	UNK	0	4.832	-0.588	0.320	1.00	0.00
HETATM	5	C5	UNK	0	6.088	0.216	0.168	1.00	0.00
HETATM	6	C6	UNK	0	6.088	1.312	-0.704	1.00	0.00
HETATM	7	C7	UNK	0	7.236	2.084	-0.892	1.00	0.00
HETATM	8	C8	UNK	0	8.408	1.784	-0.200	1.00	0.00
HETATM	9	C9	UNK	0	8.416	0.704	0.684	1.00	0.00

HETATM	10	C10	UNK	0	7.272	-0.064	0.868	1.00	0.00
HETATM	11	1H1	UNK	0	7.292	-0.880	1.584	1.00	0.00
HETATM	12	2H1	UNK	0	9.320	0.468	1.248	1.00	0.00
HETATM	13	3H1	UNK	0	9.304	2.388	-0.340	1.00	0.00
HETATM	14	4H1	UNK	0	7.208	2.928	-1.580	1.00	0.00
HETATM	15	5H1	UNK	0	5.164	1.544	-1.224	1.00	0.00
HETATM	16	C16	UNK	0	4.872	-1.848	0.836	1.00	0.00
HETATM	17	7H1	UNK	0	5.804	-2.316	1.124	1.00	0.00
HETATM	18	8H1	UNK	0	3.968	-2.440	0.948	1.00	0.00
HETATM	19	C19	UNK	0	2.104	-2.260	-1.492	1.00	0.00
HETATM	20	0H2	UNK	0	1.552	-2.112	-2.428	1.00	0.00
HETATM	21	1H2	UNK	0	3.176	-2.340	-1.700	1.00	0.00
HETATM	22	2H2	UNK	0	1.744	-3.188	-1.036	1.00	0.00
HETATM	23	C23	UNK	0	1.204	1.304	-1.012	1.00	0.00
HETATM	24	4H2	UNK	0	0.452	1.788	-0.388	1.00	0.00
HETATM	25	5H2	UNK	0	2.100	1.928	-1.068	1.00	0.00
HETATM	26	6H2	UNK	0	0.776	1.172	-2.012	1.00	0.00
HETATM	27	C27	UNK	0	1.548	-0.896	1.940	1.00	0.00
HETATM	28	8H2	UNK	0	0.776	-0.228	2.332	1.00	0.00
HETATM	29	9H2	UNK	0	1.236	-1.924	2.148	1.00	0.00
HETATM	30	0H3	UNK	0	2.504	-0.692	2.428	1.00	0.00
HETATM	31	O31	UNK	0	-7.532	-0.404	-0.144	1.00	0.00
HETATM	32	C32	UNK	0	-6.804	0.540	0.100	1.00	0.00
HETATM	33	O33	UNK	0	-5.468	0.492	0.088	1.00	0.00
HETATM	34	C34	UNK	0	-4.868	-0.772	-0.240	1.00	0.00
HETATM	35	5H3	UNK	0	-5.180	-1.528	0.484	1.00	0.00
HETATM	36	6H3	UNK	0	-5.180	-1.080	-1.240	1.00	0.00
HETATM	37	7H3	UNK	0	-3.788	-0.620	-0.200	1.00	0.00
HETATM	38	C38	UNK	0	-7.268	1.904	0.460	1.00	0.00
HETATM	39	C39	UNK	0	-8.572	2.196	0.540	1.00	0.00
HETATM	40	0H4	UNK	0	-9.316	1.428	0.344	1.00	0.00
HETATM	41	1H4	UNK	0	-8.916	3.192	0.804	1.00	0.00
HETATM	42	2H4	UNK	0	-6.500	2.648	0.652	1.00	0.00
TER	43		UNK	0					
END									

D

HETATM	1	SN1	UNK	0	2.276	0.116	-0.228	1.00	0.00
HETATM	2	BR2	UNK	0	4.772	-0.976	0.128	1.00	0.00
HETATM	3	O3	UNK	0	0.296	1.204	-0.496	1.00	0.00
HETATM	4	C4	UNK	0	-0.868	1.136	0.044	1.00	0.00
HETATM	5	C5	UNK	0	-1.656	2.408	0.032	1.00	0.00
HETATM	6	C6	UNK	0	-1.000	3.604	-0.304	1.00	0.00
HETATM	7	C7	UNK	0	-1.680	4.820	-0.316	1.00	0.00
HETATM	8	C8	UNK	0	-3.040	4.868	-0.004	1.00	0.00
HETATM	9	C9	UNK	0	-3.708	3.688	0.320	1.00	0.00

HETATM	10	C10	UNK	0	-3.024	2.472	0.340	1.00	0.00
HETATM	11	1H1	UNK	0	-3.568	1.564	0.584	1.00	0.00
HETATM	12	2H1	UNK	0	-4.772	3.708	0.556	1.00	0.00
HETATM	13	3H1	UNK	0	-3.572	5.816	-0.016	1.00	0.00
HETATM	14	4H1	UNK	0	-1.148	5.732	-0.576	1.00	0.00
HETATM	15	5H1	UNK	0	0.056	3.552	-0.556	1.00	0.00
HETATM	16	C16	UNK	0	-1.456	-0.048	0.516	1.00	0.00
HETATM	17	C17	UNK	0	-2.412	-0.884	-1.092	1.00	0.00
HETATM	18	C18	UNK	0	-3.352	-1.832	-0.688	1.00	0.00
HETATM	19	C19	UNK	0	-2.960	-3.168	-0.356	1.00	0.00
HETATM	20	O20	UNK	0	-4.040	-3.944	0.028	1.00	0.00
HETATM	21	C21	UNK	0	-3.720	-5.288	0.348	1.00	0.00
HETATM	22	2H2	UNK	0	-3.292	-5.812	-0.508	1.00	0.00
HETATM	23	3H2	UNK	0	-3.004	-5.340	1.176	1.00	0.00
HETATM	24	4H2	UNK	0	-4.668	-5.756	0.640	1.00	0.00
HETATM	25	O25	UNK	0	-1.828	-3.648	-0.384	1.00	0.00
HETATM	26	6H2	UNK	0	-4.388	-1.556	-0.512	1.00	0.00
HETATM	27	7H2	UNK	0	-1.480	-1.236	-1.524	1.00	0.00
HETATM	28	8H2	UNK	0	-2.788	0.036	-1.532	1.00	0.00
HETATM	29	9H2	UNK	0	-2.304	0.024	1.184	1.00	0.00
HETATM	30	OH3	UNK	0	-0.800	-0.892	0.708	1.00	0.00
HETATM	31	C31	UNK	0	1.960	0.080	1.892	1.00	0.00
HETATM	32	2H3	UNK	0	2.772	0.632	2.372	1.00	0.00
HETATM	33	3H3	UNK	0	0.996	0.524	2.164	1.00	0.00
HETATM	34	4H3	UNK	0	2.000	-0.948	2.248	1.00	0.00
HETATM	35	C35	UNK	0	3.124	1.856	-1.152	1.00	0.00
HETATM	36	6H3	UNK	0	3.884	1.552	-1.880	1.00	0.00
HETATM	37	7H3	UNK	0	2.340	2.436	-1.648	1.00	0.00
HETATM	38	8H3	UNK	0	3.616	2.480	-0.396	1.00	0.00
HETATM	39	C39	UNK	0	1.600	-1.452	-1.520	1.00	0.00
HETATM	40	OH4	UNK	0	2.460	-2.028	-1.872	1.00	0.00
HETATM	41	1H4	UNK	0	0.912	-2.124	-1.000	1.00	0.00
HETATM	42	2H4	UNK	0	1.076	-1.008	-2.372	1.00	0.00
TER	43		UNK	0					
END									

E

HETATM	1	SN1	UNK	0	2.284	-0.208	-0.204	1.00	0.00
HETATM	2	BR2	UNK	0	4.664	-1.392	0.112	1.00	0.00
HETATM	3	O3	UNK	0	0.220	1.096	-0.448	1.00	0.00
HETATM	4	C4	UNK	0	-0.952	1.136	-0.000	1.00	0.00
HETATM	5	C5	UNK	0	-1.636	2.456	0.016	1.00	0.00
HETATM	6	C6	UNK	0	-0.884	3.612	-0.256	1.00	0.00
HETATM	7	C7	UNK	0	-1.472	4.872	-0.236	1.00	0.00
HETATM	8	C8	UNK	0	-2.836	5.008	0.044	1.00	0.00
HETATM	9	C9	UNK	0	-3.600	3.868	0.308	1.00	0.00

HETATM	10	C10	UNK	0	-3.008	2.604	0.296	1.00	0.00
HETATM	11	1H1	UNK	0	-3.620	1.732	0.496	1.00	0.00
HETATM	12	2H1	UNK	0	-4.664	3.960	0.520	1.00	0.00
HETATM	13	3H1	UNK	0	-3.300	5.992	0.056	1.00	0.00
HETATM	14	4H1	UNK	0	-0.872	5.752	-0.448	1.00	0.00
HETATM	15	5H1	UNK	0	0.172	3.492	-0.480	1.00	0.00
HETATM	16	C16	UNK	0	-1.692	-0.084	0.360	1.00	0.00
HETATM	17	C17	UNK	0	-2.392	-0.728	-0.952	1.00	0.00
HETATM	18	C18	UNK	0	-3.224	-1.896	-0.624	1.00	0.00
HETATM	19	C19	UNK	0	-2.612	-3.084	-0.216	1.00	0.00
HETATM	20	O20	UNK	0	-3.532	-4.092	0.116	1.00	0.00
HETATM	21	C21	UNK	0	-2.944	-5.316	0.512	1.00	0.00
HETATM	22	2H2	UNK	0	-2.328	-5.748	-0.284	1.00	0.00
HETATM	23	3H2	UNK	0	-2.312	-5.196	1.400	1.00	0.00
HETATM	24	4H2	UNK	0	-3.780	-5.988	0.740	1.00	0.00
HETATM	25	O25	UNK	0	-1.392	-3.324	-0.128	1.00	0.00
HETATM	26	6H2	UNK	0	-4.304	-1.796	-0.540	1.00	0.00
HETATM	27	7H2	UNK	0	-1.548	-0.980	-1.604	1.00	0.00
HETATM	28	8H2	UNK	0	-2.984	0.056	-1.444	1.00	0.00
HETATM	29	9H2	UNK	0	-2.476	0.096	1.100	1.00	0.00
HETATM	30	OH3	UNK	0	-1.020	-0.864	0.728	1.00	0.00
HETATM	31	C31	UNK	0	1.808	-0.300	1.884	1.00	0.00
HETATM	32	2H3	UNK	0	2.700	-0.044	2.460	1.00	0.00
HETATM	33	3H3	UNK	0	0.992	0.380	2.140	1.00	0.00
HETATM	34	4H3	UNK	0	1.516	-1.324	2.140	1.00	0.00
HETATM	35	C35	UNK	0	3.124	1.612	-0.968	1.00	0.00
HETATM	36	6H3	UNK	0	3.992	1.380	-1.592	1.00	0.00
HETATM	37	7H3	UNK	0	2.372	2.152	-1.552	1.00	0.00
HETATM	38	8H3	UNK	0	3.456	2.248	-0.136	1.00	0.00
HETATM	39	C39	UNK	0	1.460	-1.596	-1.600	1.00	0.00
HETATM	40	OH4	UNK	0	2.240	-2.292	-1.924	1.00	0.00
HETATM	41	1H4	UNK	0	0.640	-2.160	-1.140	1.00	0.00
HETATM	42	2H4	UNK	0	1.072	-1.052	-2.464	1.00	0.00
TER	43		UNK	0					
END									

F

ATOM	1	SN	UNK	1	-3.572	-1.532	-0.092	1.00	0.00
ATOM	2	BR	UNK	1	-6.032	-2.304	-0.072	1.00	0.00
ATOM	3	O	UNK	1	0.288	-2.356	0.100	1.00	0.00
ATOM	4	C	UNK	1	1.356	-1.744	0.244	1.00	0.00
ATOM	5	C	UNK	1	2.644	-2.508	0.112	1.00	0.00
ATOM	6	C	UNK	1	2.588	-3.908	0.048	1.00	0.00
ATOM	7	C	UNK	1	3.748	-4.668	-0.064	1.00	0.00
ATOM	8	C	UNK	1	4.996	-4.040	-0.124	1.00	0.00
ATOM	9	C	UNK	1	5.068	-2.648	-0.072	1.00	0.00

ATOM	10	C	UNK	1	3.904	-1.888	0.048	1.00	0.00
ATOM	11	H	UNK	1	3.976	-0.808	0.080	1.00	0.00
ATOM	12	H	UNK	1	6.032	-2.148	-0.128	1.00	0.00
ATOM	13	H	UNK	1	5.904	-4.632	-0.216	1.00	0.00
ATOM	14	H	UNK	1	3.684	-5.756	-0.104	1.00	0.00
ATOM	15	H	UNK	1	1.608	-4.380	0.084	1.00	0.00
ATOM	16	C	UNK	1	1.380	-0.272	0.432	1.00	0.00
ATOM	17	C	UNK	1	1.236	0.488	-0.960	1.00	0.00
ATOM	18	C	UNK	1	1.256	1.960	-0.820	1.00	0.00
ATOM	19	C	UNK	1	0.180	2.616	-0.236	1.00	0.00
ATOM	20	O	UNK	1	0.360	4.008	-0.116	1.00	0.00
ATOM	21	C	UNK	1	-0.732	4.704	0.432	1.00	0.00
ATOM	22	H	UNK	1	-1.636	4.600	-0.180	1.00	0.00
ATOM	23	H	UNK	1	-0.972	4.356	1.444	1.00	0.00
ATOM	24	H	UNK	1	-0.432	5.756	0.464	1.00	0.00
ATOM	25	O	UNK	1	-0.896	2.120	0.184	1.00	0.00
ATOM	26	H	UNK	1	2.156	2.524	-1.064	1.00	0.00
ATOM	27	H	UNK	1	0.292	0.120	-1.384	1.00	0.00
ATOM	28	H	UNK	1	2.044	0.148	-1.624	1.00	0.00
ATOM	29	H	UNK	1	2.288	0.080	0.928	1.00	0.00
ATOM	30	H	UNK	1	0.508	0.036	1.020	1.00	0.00
ATOM	31	C	UNK	1	-2.904	-2.036	1.872	1.00	0.00
ATOM	32	H	UNK	1	-3.216	-3.052	2.128	1.00	0.00
ATOM	33	H	UNK	1	-1.812	-1.976	1.892	1.00	0.00
ATOM	34	H	UNK	1	-3.324	-1.340	2.608	1.00	0.00
ATOM	35	C	UNK	1	-2.724	-2.760	-1.628	1.00	0.00
ATOM	36	H	UNK	1	-3.072	-2.436	-2.612	1.00	0.00
ATOM	37	H	UNK	1	-1.632	-2.684	-1.572	1.00	0.00
ATOM	38	H	UNK	1	-3.020	-3.804	-1.476	1.00	0.00
ATOM	39	C	UNK	1	-3.700	0.544	-0.528	1.00	0.00
ATOM	40	H	UNK	1	-4.436	1.008	0.136	1.00	0.00
ATOM	41	H	UNK	1	-2.724	1.032	-0.380	1.00	0.00
ATOM	42	H	UNK	1	-4.028	0.688	-1.560	1.00	0.00
TER	43		UNK	1					
END									

G

HETATM	1	O	2	2	-2.988	0.852	-1.612	1.00	0.00
HETATM	2	C	2	2	-2.428	0.256	-0.704	1.00	0.00
HETATM	3	C	2	2	-3.044	-1.008	-0.168	1.00	0.00
HETATM	4	C	2	2	-2.428	-1.792	0.816	1.00	0.00
HETATM	5	C	2	2	-3.036	-2.956	1.280	1.00	0.00
HETATM	6	C	2	2	-4.272	-3.356	0.764	1.00	0.00
HETATM	7	C	2	2	-4.892	-2.580	-0.220	1.00	0.00
HETATM	8	C	2	2	-4.280	-1.420	-0.680	1.00	0.00
HETATM	9	H	2	2	-4.744	-0.804	-1.448	1.00	0.00

HETATM	10	H	2	2	-5.856	-2.888	-0.624	1.00	0.00
HETATM	11	H	2	2	-4.744	-4.264	1.124	1.00	0.00
HETATM	12	H	2	2	-2.544	-3.556	2.040	1.00	0.00
HETATM	13	H	2	2	-1.464	-1.496	1.224	1.00	0.00
HETATM	14	C	2	2	-1.144	0.752	-0.084	1.00	0.00
HETATM	15	C	2	2	-0.544	2.008	-0.724	1.00	0.00
HETATM	16	C	2	2	0.668	2.516	0.004	1.00	0.00
HETATM	17	C	2	2	1.808	1.772	0.080	1.00	0.00
HETATM	18	O	2	2	1.964	0.596	-0.440	1.00	0.00
HETATM	19	SN	2	2	3.696	-0.716	-0.268	1.00	0.00
HETATM	20	BR	2	2	5.856	-2.548	-0.100	1.00	0.00
HETATM	21	C	2	2	2.612	-2.136	-1.460	1.00	0.00
HETATM	22	H	2	2	3.216	-2.420	-2.328	1.00	0.00
HETATM	23	H	2	2	2.424	-3.044	-0.876	1.00	0.00
HETATM	24	H	2	2	1.668	-1.700	-1.788	1.00	0.00
HETATM	25	C	2	2	3.536	-0.840	1.868	1.00	0.00
HETATM	26	H	2	2	3.528	-1.896	2.164	1.00	0.00
HETATM	27	H	2	2	4.408	-0.372	2.328	1.00	0.00
HETATM	28	H	2	2	2.628	-0.344	2.212	1.00	0.00
HETATM	29	C	2	2	5.012	0.640	-1.284	1.00	0.00
HETATM	30	H	2	2	5.784	0.992	-0.588	1.00	0.00
HETATM	31	H	2	2	5.512	0.112	-2.104	1.00	0.00
HETATM	32	H	2	2	4.448	1.496	-1.664	1.00	0.00
HETATM	33	O	2	2	2.948	2.204	0.740	1.00	0.00
HETATM	34	C	2	2	2.932	3.464	1.360	1.00	0.00
HETATM	35	H	2	2	2.164	3.516	2.148	1.00	0.00
HETATM	36	H	2	2	3.920	3.596	1.808	1.00	0.00
HETATM	37	H	2	2	2.748	4.268	0.636	1.00	0.00
HETATM	38	H	2	2	0.616	3.492	0.468	1.00	0.00
HETATM	39	H	2	2	-0.308	1.768	-1.772	1.00	0.00
HETATM	40	H	2	2	-1.312	2.792	-0.764	1.00	0.00
HETATM	41	H	2	2	-0.388	-0.040	-0.108	1.00	0.00
HETATM	42	H	2	2	-1.336	0.936	0.984	1.00	0.00
TER	43		2	2					
END									