

Comparative analysis of molecular interactions in quaternary fluid system performed by classical and *ab initio* molecular dynamics

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1. Input Parameters for Classical Molecular Dynamics

---- Dynamics parameters ----

Ensemble	: NVT
Temperature	: 298.00 K
Control method	: Nose
Q ratio	: 0.0100000
Timestep	: 1.00 fs
Number of steps	: 50000000
Duration	: 50000 ps
Initial velocities	: Random
Random number seed	: 1636139800

---- Energy parameters ----

Forcefield	: Universal
Charges	: Use current
Electrostatic terms:	
Summation method	: Ewald
Accuracy	: 0.001 kcal/mol
Buffer width	: 0.5 Å

van der Waals terms:

Summation method	: Atom based
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Truncation method : Cubic spline
 Cutoff distance : 12.5 A
 Spline width : 1 A
 Long range correction : YES
 Buffer width : 0.5 A

---- Thermostat ----

Nose mass parameter, Q mass: 17.7478 kcal/mol*ps²

2. Input Coordinates of Atoms for Classical Molecular Dynamics

REMARK Materials Studio PDB file

CRYST1 21.527 21.527 21.527 90.00 90.00 90.00 P1

ORIGX1 1.000000 0.000000 0.000000 0.000000

ORIGX2 0.000000 1.000000 0.000000 0.000000

ORIGX3 0.000000 0.000000 1.000000 0.000000

SCALE1 0.046454 0.000000 0.000000 0.000000

SCALE2 0.000000 0.046454 0.000000 0.000000

SCALE3 0.000000 0.000000 0.046454 0.000000

ATOM	1	O_w	MOL	2	8.100	4.197	0.797	1.00	0.00	O
ATOM	2	H_w	MOL	2	8.022	4.006	-0.173	1.00	0.00	H
ATOM	3	H_w	MOL	2	7.232	3.897	1.172	1.00	0.00	H
ATOM	4	O_w	MOL	2	11.511	15.738	4.620	1.00	0.00	O
ATOM	5	H_w	MOL	2	11.241	14.894	5.062	1.00	0.00	H
ATOM	6	H_w	MOL	2	11.190	16.447	5.235	1.00	0.00	H
ATOM	7	O_w	MOL	2	5.451	13.283	17.983	1.00	0.00	O
ATOM	8	H_w	MOL	2	4.502	13.278	18.275	1.00	0.00	H
ATOM	9	H_w	MOL	2	5.382	13.424	17.004	1.00	0.00	H
ATOM	10	O_w	MOL	2	18.257	18.500	12.790	1.00	0.00	O
ATOM	11	H_w	MOL	2	19.088	18.994	12.574	1.00	0.00	H

ATOM	12	H_w	MOL	2	17.592	18.863	12.150	1.00	0.00	H
ATOM	13	O_w	MOL	2	2.251	11.275	3.063	1.00	0.00	O
ATOM	14	H_w	MOL	2	2.723	10.511	2.644	1.00	0.00	H
ATOM	15	H_w	MOL	2	2.314	11.991	2.381	1.00	0.00	H
ATOM	16	O_w	MOL	2	1.175	3.584	15.355	1.00	0.00	O
ATOM	17	H_w	MOL	2	1.895	4.196	15.055	1.00	0.00	H
ATOM	18	H_w	MOL	2	1.141	3.725	16.335	1.00	0.00	H
ATOM	19	O_w	MOL	2	11.435	5.075	21.076	1.00	0.00	O
ATOM	20	H_w	MOL	2	10.488	5.264	20.854	1.00	0.00	H
ATOM	21	H_w	MOL	2	11.454	5.078	22.066	1.00	0.00	H
ATOM	22	O_w	MOL	2	1.281	18.126	16.968	1.00	0.00	O
ATOM	23	H_w	MOL	2	1.650	18.587	17.764	1.00	0.00	H
ATOM	24	H_w	MOL	2	1.668	18.620	16.201	1.00	0.00	H
ATOM	25	O_w	MOL	2	12.900	4.333	2.655	1.00	0.00	O
ATOM	26	H_w	MOL	2	12.541	4.020	3.525	1.00	0.00	H
ATOM	27	H_w	MOL	2	13.298	5.214	2.874	1.00	0.00	H
ATOM	28	O_w	MOL	2	15.274	8.668	15.895	1.00	0.00	O
ATOM	29	H_w	MOL	2	16.256	8.698	15.760	1.00	0.00	H
ATOM	30	H_w	MOL	2	14.904	8.520	14.986	1.00	0.00	H
ATOM	31	O_w	MOL	2	2.167	3.651	19.149	1.00	0.00	O
ATOM	32	H_w	MOL	2	1.287	3.281	18.881	1.00	0.00	H
ATOM	33	H_w	MOL	2	2.173	3.532	20.134	1.00	0.00	H
ATOM	34	O_w	MOL	2	16.420	21.174	3.668	1.00	0.00	O
ATOM	35	H_w	MOL	2	16.709	20.803	4.541	1.00	0.00	H
ATOM	36	H_w	MOL	2	15.492	20.838	3.579	1.00	0.00	H
ATOM	37	O_w	MOL	2	19.942	13.245	7.114	1.00	0.00	O
ATOM	38	H_w	MOL	2	20.292	13.036	8.017	1.00	0.00	H
ATOM	39	H_w	MOL	2	20.275	14.161	6.934	1.00	0.00	H
ATOM	40	O_w	MOL	2	0.243	14.247	16.987	1.00	0.00	O
ATOM	41	H_w	MOL	2	0.990	13.861	16.459	1.00	0.00	H
ATOM	42	H_w	MOL	2	0.285	15.213	16.769	1.00	0.00	H
ATOM	43	O_w	MOL	2	1.406	15.751	19.739	1.00	0.00	O
ATOM	44	H_w	MOL	2	1.908	15.114	20.310	1.00	0.00	H

ATOM	45	H_w	MOL	2	0.533	15.300	19.612	1.00	0.00	H
ATOM	46	O_w	MOL	2	19.360	4.759	6.175	1.00	0.00	O
ATOM	47	H_w	MOL	2	19.961	5.428	5.760	1.00	0.00	H
ATOM	48	H_w	MOL	2	18.471	5.197	6.183	1.00	0.00	H
ATOM	49	O_w	MOL	2	9.797	6.315	2.644	1.00	0.00	O
ATOM	50	H_w	MOL	2	8.821	6.479	2.583	1.00	0.00	H
ATOM	51	H_w	MOL	2	9.878	5.343	2.469	1.00	0.00	H
ATOM	52	O_w	MOL	2	11.037	9.824	4.416	1.00	0.00	O
ATOM	53	H_w	MOL	2	11.415	10.731	4.562	1.00	0.00	H
ATOM	54	H_w	MOL	2	11.379	9.286	5.175	1.00	0.00	H
ATOM	55	O_w	MOL	2	17.372	13.439	2.304	1.00	0.00	O
ATOM	56	H_w	MOL	2	17.256	13.412	3.288	1.00	0.00	H
ATOM	57	H_w	MOL	2	16.468	13.234	1.950	1.00	0.00	H
ATOM	58	O_w	MOL	2	7.673	17.215	19.466	1.00	0.00	O
ATOM	59	H_w	MOL	2	8.647	17.119	19.300	1.00	0.00	H
ATOM	60	H_w	MOL	2	7.371	17.860	18.778	1.00	0.00	H
ATOM	61	O_w	MOL	2	5.994	15.607	2.574	1.00	0.00	O
ATOM	62	H_w	MOL	2	5.026	15.435	2.700	1.00	0.00	H
ATOM	63	H_w	MOL	2	6.425	14.787	2.926	1.00	0.00	H
ATOM	64	O_w	MOL	2	14.206	12.437	21.944	1.00	0.00	O
ATOM	65	H_w	MOL	2	14.832	12.443	21.173	1.00	0.00	H
ATOM	66	H_w	MOL	2	13.416	11.943	21.606	1.00	0.00	H
ATOM	67	O_w	MOL	2	2.820	3.106	11.981	1.00	0.00	O
ATOM	68	H_w	MOL	2	3.222	3.210	11.081	1.00	0.00	H
ATOM	69	H_w	MOL	2	3.374	2.414	12.424	1.00	0.00	H
ATOM	70	O_w	MOL	2	13.045	4.369	5.989	1.00	0.00	O
ATOM	71	H_w	MOL	2	12.336	4.511	6.667	1.00	0.00	H
ATOM	72	H_w	MOL	2	13.643	5.154	6.098	1.00	0.00	H
ATOM	73	O_w	MOL	2	18.678	5.613	13.826	1.00	0.00	O
ATOM	74	H_w	MOL	2	19.473	5.358	14.357	1.00	0.00	H
ATOM	75	H_w	MOL	2	18.089	4.820	13.893	1.00	0.00	H
ATOM	76	C_m	MOL	2	2.638	17.122	1.432	1.00	0.00	C
ATOM	77	C_m	MOL	2	2.135	18.564	1.453	1.00	0.00	C

ATOM	78	C78	MOL	2	0.724	18.648	2.011	1.00	0.00	C
ATOM	79	O_p	MOL	2	0.381	19.994	2.197	1.00	0.00	O
ATOM	80	H80	MOL	2	2.582	16.667	2.440	1.00	0.00	H
ATOM	81	H81	MOL	2	3.695	17.080	1.102	1.00	0.00	H
ATOM	82	H82	MOL	2	2.027	16.518	0.731	1.00	0.00	H
ATOM	83	H83	MOL	2	2.142	18.975	0.422	1.00	0.00	H
ATOM	84	H84	MOL	2	2.797	19.190	2.077	1.00	0.00	H
ATOM	85	H85	MOL	2	0.666	18.124	2.989	1.00	0.00	H
ATOM	86	H86	MOL	2	0.037	18.130	1.310	1.00	0.00	H
ATOM	87	H87	MOL	2	-0.304	20.222	1.511	1.00	0.00	H
ATOM	88	C_m	MOL	2	7.683	5.057	6.024	1.00	0.00	C
ATOM	89	C_m	MOL	2	9.206	5.188	5.947	1.00	0.00	C
ATOM	90	C90	MOL	2	9.662	6.605	6.294	1.00	0.00	C
ATOM	91	O_p	MOL	2	11.051	6.713	6.153	1.00	0.00	O
ATOM	92	H92	MOL	2	7.189	5.800	5.360	1.00	0.00	H
ATOM	93	H93	MOL	2	7.334	5.195	7.065	1.00	0.00	H
ATOM	94	H94	MOL	2	7.369	4.041	5.711	1.00	0.00	H
ATOM	95	H95	MOL	2	9.546	4.938	4.922	1.00	0.00	H
ATOM	96	H96	MOL	2	9.677	4.464	6.647	1.00	0.00	H
ATOM	97	H97	MOL	2	9.397	6.824	7.351	1.00	0.00	H
ATOM	98	H98	MOL	2	9.150	7.350	5.641	1.00	0.00	H
ATOM	99	H99	MOL	2	11.236	6.700	5.174	1.00	0.00	H
ATOM	100	C_m	MOL	2	4.526	6.113	11.081	1.00	0.00	C
ATOM	101	C_m	MOL	2	5.106	6.592	12.412	1.00	0.00	C
ATOM	102	C10	MOL	2	5.072	5.484	13.464	1.00	0.00	C
ATOM	103	O_p	MOL	2	5.565	5.974	14.680	1.00	0.00	O
ATOM	104	4H10	MOL	2	5.031	5.181	10.749	1.00	0.00	H
ATOM	105	5H10	MOL	2	4.684	6.890	10.305	1.00	0.00	H
ATOM	106	6H10	MOL	2	3.436	5.919	11.182	1.00	0.00	H
ATOM	107	7H10	MOL	2	4.528	7.472	12.771	1.00	0.00	H
ATOM	108	8H10	MOL	2	6.162	6.907	12.270	1.00	0.00	H
ATOM	109	9H10	MOL	2	5.717	4.639	13.133	1.00	0.00	H
ATOM	110	0H11	MOL	2	4.035	5.097	13.595	1.00	0.00	H

ATOM	111	1H11	MOL	2	4.885	6.610	15.023	1.00	0.00	H
ATOM	112	C_m	MOL	2	14.666	4.257	19.045	1.00	0.00	C
ATOM	113	C_m	MOL	2	15.553	3.698	20.155	1.00	0.00	C
ATOM	114	C11	MOL	2	14.718	3.064	21.261	1.00	0.00	C
ATOM	115	O_p	MOL	2	15.564	2.425	22.175	1.00	0.00	O
ATOM	116	6H11	MOL	2	14.091	3.442	18.554	1.00	0.00	H
ATOM	117	7H11	MOL	2	15.301	4.745	18.275	1.00	0.00	H
ATOM	118	8H11	MOL	2	13.956	5.007	19.454	1.00	0.00	H
ATOM	119	9H11	MOL	2	16.164	4.518	20.589	1.00	0.00	H
ATOM	120	0H12	MOL	2	16.240	2.936	19.726	1.00	0.00	H
ATOM	121	1H12	MOL	2	14.035	2.308	20.820	1.00	0.00	H
ATOM	122	2H12	MOL	2	14.095	3.835	21.770	1.00	0.00	H
ATOM	123	3H12	MOL	2	15.988	3.138	22.718	1.00	0.00	H
ATOM	124	C_m	MOL	2	14.751	0.710	16.019	1.00	0.00	C
ATOM	125	C_m	MOL	2	15.080	0.255	14.596	1.00	0.00	C
ATOM	126	C12	MOL	2	16.519	-0.240	14.473	1.00	0.00	C
ATOM	127	O_p	MOL	2	16.872	-0.323	13.122	1.00	0.00	O
ATOM	128	8H12	MOL	2	14.784	-0.149	16.721	1.00	0.00	H
ATOM	129	9H12	MOL	2	13.733	1.153	16.043	1.00	0.00	H
ATOM	130	0H13	MOL	2	15.466	1.492	16.354	1.00	0.00	H
ATOM	131	1H13	MOL	2	14.924	1.105	13.901	1.00	0.00	H
ATOM	132	2H13	MOL	2	14.392	-0.561	14.291	1.00	0.00	H
ATOM	133	3H13	MOL	2	16.604	-1.251	14.926	1.00	0.00	H
ATOM	134	4H13	MOL	2	17.217	0.443	15.010	1.00	0.00	H
ATOM	135	5H13	MOL	2	17.117	0.599	12.849	1.00	0.00	H
ATOM	136	C_m	MOL	2	2.172	19.755	9.018	1.00	0.00	C
ATOM	137	C_m	MOL	2	1.800	19.445	10.466	1.00	0.00	C
ATOM	138	C13	MOL	2	1.470	20.721	11.239	1.00	0.00	C
ATOM	139	O_p	MOL	2	1.068	20.399	12.542	1.00	0.00	O
ATOM	140	0H14	MOL	2	1.326	20.273	8.521	1.00	0.00	H
ATOM	141	1H14	MOL	2	2.386	18.813	8.470	1.00	0.00	H
ATOM	142	2H14	MOL	2	3.072	20.405	8.969	1.00	0.00	H
ATOM	143	3H14	MOL	2	2.636	18.905	10.958	1.00	0.00	H

ATOM	144	4H14	MOL	2	0.908	18.785	10.485	1.00	0.00	H
ATOM	145	5H14	MOL	2	0.635	21.249	10.731	1.00	0.00	H
ATOM	146	6H14	MOL	2	2.346	21.409	11.263	1.00	0.00	H
ATOM	147	7H14	MOL	2	1.870	20.037	12.999	1.00	0.00	H
ATOM	148	C_m	MOL	2	8.089	1.105	15.019	1.00	0.00	C
ATOM	149	C_m	MOL	2	7.996	2.459	14.318	1.00	0.00	C
ATOM	150	C15	MOL	2	9.354	2.886	13.772	1.00	0.00	C
ATOM	151	O_p	MOL	2	9.260	4.196	13.282	1.00	0.00	O
ATOM	152	2H15	MOL	2	8.395	0.317	14.298	1.00	0.00	H
ATOM	153	3H15	MOL	2	7.104	0.838	15.457	1.00	0.00	H
ATOM	154	4H15	MOL	2	8.835	1.147	15.841	1.00	0.00	H
ATOM	155	5H15	MOL	2	7.638	3.222	15.041	1.00	0.00	H
ATOM	156	6H15	MOL	2	7.263	2.406	13.484	1.00	0.00	H
ATOM	157	7H15	MOL	2	9.656	2.204	12.946	1.00	0.00	H
ATOM	158	8H15	MOL	2	10.118	2.816	14.585	1.00	0.00	H
ATOM	159	9H15	MOL	2	10.150	4.610	13.434	1.00	0.00	H
ATOM	160	C_m	MOL	2	17.612	-0.376	17.994	1.00	0.00	C
ATOM	161	C_m	MOL	2	19.055	0.107	18.084	1.00	0.00	C
ATOM	162	C16	MOL	2	19.532	0.731	16.782	1.00	0.00	C
ATOM	163	O_p	MOL	2	20.853	1.167	16.945	1.00	0.00	O
ATOM	164	4H16	MOL	2	16.924	0.492	17.958	1.00	0.00	H
ATOM	165	5H16	MOL	2	17.374	-0.996	18.881	1.00	0.00	H
ATOM	166	6H16	MOL	2	17.463	-1.012	17.100	1.00	0.00	H
ATOM	167	7H16	MOL	2	19.715	-0.753	18.318	1.00	0.00	H
ATOM	168	8H16	MOL	2	19.136	0.856	18.900	1.00	0.00	H
ATOM	169	9H16	MOL	2	18.873	1.587	16.510	1.00	0.00	H
ATOM	170	0H17	MOL	2	19.490	-0.035	15.976	1.00	0.00	H
ATOM	171	1H17	MOL	2	21.085	1.651	16.109	1.00	0.00	H
ATOM	172	C_m	MOL	2	9.493	14.186	19.590	1.00	0.00	C
ATOM	173	C_m	MOL	2	9.349	12.667	19.630	1.00	0.00	C
ATOM	174	C17	MOL	2	9.075	12.095	18.242	1.00	0.00	C
ATOM	175	O_p	MOL	2	8.808	10.721	18.321	1.00	0.00	O
ATOM	176	6H17	MOL	2	10.324	14.485	18.913	1.00	0.00	H

ATOM	177	7H17	MOL	2	9.716	14.571	20.608	1.00	0.00	H
ATOM	178	8H17	MOL	2	8.547	14.650	19.243	1.00	0.00	H
ATOM	179	9H17	MOL	2	8.524	12.399	20.319	1.00	0.00	H
ATOM	180	0H18	MOL	2	10.287	12.221	20.022	1.00	0.00	H
ATOM	181	1H18	MOL	2	9.979	12.248	17.616	1.00	0.00	H
ATOM	182	2H18	MOL	2	8.219	12.620	17.763	1.00	0.00	H
ATOM	183	3H18	MOL	2	7.890	10.631	18.692	1.00	0.00	H
ATOM	184	C_m	MOL	2	16.367	4.186	4.125	1.00	0.00	C
ATOM	185	C_m	MOL	2	17.318	4.922	3.181	1.00	0.00	C
ATOM	186	C18	MOL	2	16.580	5.968	2.351	1.00	0.00	C
ATOM	187	O_p	MOL	2	17.476	6.600	1.478	1.00	0.00	O
ATOM	188	8H18	MOL	2	15.879	4.901	4.821	1.00	0.00	H
ATOM	189	9H18	MOL	2	16.937	3.449	4.727	1.00	0.00	H
ATOM	190	0H19	MOL	2	15.584	3.642	3.557	1.00	0.00	H
ATOM	191	1H19	MOL	2	17.807	4.188	2.511	1.00	0.00	H
ATOM	192	2H19	MOL	2	18.112	5.429	3.769	1.00	0.00	H
ATOM	193	3H19	MOL	2	16.141	6.732	3.029	1.00	0.00	H
ATOM	194	4H19	MOL	2	15.747	5.497	1.781	1.00	0.00	H
ATOM	195	5H19	MOL	2	17.664	5.958	0.744	1.00	0.00	H
ATOM	196	C_m	MOL	2	5.069	11.986	7.472	1.00	0.00	C
ATOM	197	C_m	MOL	2	5.116	12.982	6.318	1.00	0.00	C
ATOM	198	C19	MOL	2	4.146	12.608	5.204	1.00	0.00	C
ATOM	199	O_p	MOL	2	4.463	13.356	4.059	1.00	0.00	O
ATOM	200	0H20	MOL	2	4.037	11.887	7.865	1.00	0.00	H
ATOM	201	1H20	MOL	2	5.732	12.334	8.293	1.00	0.00	H
ATOM	202	2H20	MOL	2	5.428	10.993	7.137	1.00	0.00	H
ATOM	203	3H20	MOL	2	6.145	13.008	5.916	1.00	0.00	H
ATOM	204	4H20	MOL	2	4.876	13.998	6.693	1.00	0.00	H
ATOM	205	5H20	MOL	2	3.109	12.849	5.523	1.00	0.00	H
ATOM	206	6H20	MOL	2	4.189	11.512	5.004	1.00	0.00	H
ATOM	207	7H20	MOL	2	4.548	12.715	3.303	1.00	0.00	H
ATOM	208	C_m	MOL	2	16.435	11.702	9.636	1.00	0.00	C
ATOM	209	C_m	MOL	2	17.597	12.678	9.764	1.00	0.00	C

ATOM	210	C21	MOL	2	18.835	12.002	10.346	1.00	0.00	C
ATOM	211	O_p	MOL	2	19.836	12.961	10.533	1.00	0.00	O
ATOM	212	2H21	MOL	2	16.674	10.893	8.913	1.00	0.00	H
ATOM	213	3H21	MOL	2	15.536	12.250	9.289	1.00	0.00	H
ATOM	214	4H21	MOL	2	16.211	11.264	10.627	1.00	0.00	H
ATOM	215	5H21	MOL	2	17.294	13.524	10.420	1.00	0.00	H
ATOM	216	6H21	MOL	2	17.841	13.080	8.761	1.00	0.00	H
ATOM	217	7H21	MOL	2	19.206	11.222	9.646	1.00	0.00	H
ATOM	218	8H21	MOL	2	18.595	11.502	11.309	1.00	0.00	H
ATOM	219	9H21	MOL	2	19.640	13.403	11.403	1.00	0.00	H
ATOM	220	C_m	MOL	2	5.440	-2.858	3.599	1.00	0.00	C
ATOM	221	C_m	MOL	2	5.682	-1.390	3.935	1.00	0.00	C
ATOM	222	C22	MOL	2	5.063	-0.456	2.906	1.00	0.00	C
ATOM	223	O_p	MOL	2	5.424	0.862	3.203	1.00	0.00	O
ATOM	224	4H22	MOL	2	4.358	-3.065	3.527	1.00	0.00	H
ATOM	225	5H22	MOL	2	5.851	-3.497	4.408	1.00	0.00	H
ATOM	226	6H22	MOL	2	5.932	-3.126	2.641	1.00	0.00	H
ATOM	227	7H22	MOL	2	6.774	-1.199	3.990	1.00	0.00	H
ATOM	228	8H22	MOL	2	5.235	-1.179	4.925	1.00	0.00	H
ATOM	229	9H22	MOL	2	3.957	-0.554	2.926	1.00	0.00	H
ATOM	230	0H23	MOL	2	5.437	-0.729	1.900	1.00	0.00	H
ATOM	231	1H23	MOL	2	5.058	1.421	2.467	1.00	0.00	H
ATOM	232	C_m	MOL	2	22.383	7.206	1.116	1.00	0.00	C
ATOM	233	C_m	MOL	2	22.295	5.842	1.798	1.00	0.00	C
ATOM	234	C23	MOL	2	21.150	5.795	2.808	1.00	0.00	C
ATOM	235	O_p	MOL	2	21.104	4.533	3.417	1.00	0.00	O
ATOM	236	6H23	MOL	2	21.454	7.415	0.544	1.00	0.00	H
ATOM	237	7H23	MOL	2	23.247	7.223	0.417	1.00	0.00	H
ATOM	238	8H23	MOL	2	22.538	8.008	1.869	1.00	0.00	H
ATOM	239	9H23	MOL	2	23.251	5.640	2.322	1.00	0.00	H
ATOM	240	0H24	MOL	2	22.144	5.048	1.033	1.00	0.00	H
ATOM	241	1H24	MOL	2	20.186	5.977	2.285	1.00	0.00	H
ATOM	242	2H24	MOL	2	21.280	6.591	3.576	1.00	0.00	H

ATOM	243	3H24	MOL	2	21.851	4.509	4.073	1.00	0.00	H
ATOM	244	C_m	MOL	2	10.921	20.295	6.637	1.00	0.00	C
ATOM	245	C_m	MOL	2	12.350	20.813	6.728	1.00	0.00	C
ATOM	246	C24	MOL	2	13.333	19.807	6.137	1.00	0.00	C
ATOM	247	O_p	MOL	2	14.616	20.362	6.116	1.00	0.00	O
ATOM	248	8H24	MOL	2	10.624	20.184	5.572	1.00	0.00	H
ATOM	249	9H24	MOL	2	10.235	21.018	7.125	1.00	0.00	H
ATOM	250	0H25	MOL	2	10.827	19.308	7.137	1.00	0.00	H
ATOM	251	1H25	MOL	2	12.611	21.006	7.791	1.00	0.00	H
ATOM	252	2H25	MOL	2	12.428	21.772	6.172	1.00	0.00	H
ATOM	253	3H25	MOL	2	13.036	19.554	5.097	1.00	0.00	H
ATOM	254	4H25	MOL	2	13.329	18.866	6.733	1.00	0.00	H
ATOM	255	5H25	MOL	2	14.890	20.427	7.066	1.00	0.00	H
ATOM	256	C_m	MOL	2	7.321	15.531	11.700	1.00	0.00	C
ATOM	257	C_m	MOL	2	8.506	16.179	10.985	1.00	0.00	C
ATOM	258	C25	MOL	2	9.647	16.456	11.952	1.00	0.00	C
ATOM	259	O_p	MOL	2	10.678	17.094	11.259	1.00	0.00	O
ATOM	260	0H26	MOL	2	7.634	14.619	12.246	1.00	0.00	H
ATOM	261	1H26	MOL	2	6.551	15.251	10.951	1.00	0.00	H
ATOM	262	2H26	MOL	2	6.882	16.236	12.433	1.00	0.00	H
ATOM	263	3H26	MOL	2	8.177	17.134	10.524	1.00	0.00	H
ATOM	264	4H26	MOL	2	8.875	15.516	10.173	1.00	0.00	H
ATOM	265	5H26	MOL	2	10.014	15.492	12.364	1.00	0.00	H
ATOM	266	6H26	MOL	2	9.289	17.107	12.781	1.00	0.00	H
ATOM	267	7H26	MOL	2	11.442	17.154	11.891	1.00	0.00	H
ATOM	268	C_m	MOL	2	18.035	8.677	11.892	1.00	0.00	C
ATOM	269	C_m	MOL	2	16.744	7.995	12.333	1.00	0.00	C
ATOM	270	C27	MOL	2	15.514	8.824	11.976	1.00	0.00	C
ATOM	271	O_p	MOL	2	14.356	8.112	12.302	1.00	0.00	O
ATOM	272	2H27	MOL	2	17.961	9.055	10.852	1.00	0.00	H
ATOM	273	3H27	MOL	2	18.872	7.950	11.940	1.00	0.00	H
ATOM	274	4H27	MOL	2	18.268	9.523	12.566	1.00	0.00	H
ATOM	275	5H27	MOL	2	16.778	7.824	13.429	1.00	0.00	H

ATOM	276	6H27	MOL	2	16.671	7.007	11.839	1.00	0.00	H
ATOM	277	7H27	MOL	2	15.517	9.067	10.889	1.00	0.00	H
ATOM	278	8H27	MOL	2	15.519	9.773	12.553	1.00	0.00	H
ATOM	279	9H27	MOL	2	14.262	7.409	11.605	1.00	0.00	H
ATOM	280	C_m	MOL	2	4.427	5.394	21.569	1.00	0.00	C
ATOM	281	C_m	MOL	2	5.328	6.608	21.351	1.00	0.00	C
ATOM	282	C28	MOL	2	6.060	6.519	20.016	1.00	0.00	C
ATOM	283	O_p	MOL	2	6.754	7.714	19.794	1.00	0.00	O
ATOM	284	4H28	MOL	2	3.655	5.339	20.774	1.00	0.00	H
ATOM	285	5H28	MOL	2	3.907	5.479	22.546	1.00	0.00	H
ATOM	286	6H28	MOL	2	5.018	4.454	21.566	1.00	0.00	H
ATOM	287	7H28	MOL	2	6.074	6.673	22.173	1.00	0.00	H
ATOM	288	8H28	MOL	2	4.707	7.529	21.377	1.00	0.00	H
ATOM	289	9H28	MOL	2	5.331	6.352	19.190	1.00	0.00	H
ATOM	290	0H29	MOL	2	6.770	5.662	20.049	1.00	0.00	H
ATOM	291	1H29	MOL	2	7.364	7.544	19.028	1.00	0.00	H
ATOM	292	C_m	MOL	2	17.470	9.987	4.095	1.00	0.00	C
ATOM	293	C_m	MOL	2	18.929	10.407	3.933	1.00	0.00	C
ATOM	294	C29	MOL	2	19.830	9.196	3.691	1.00	0.00	C
ATOM	295	O_p	MOL	2	21.131	9.613	3.380	1.00	0.00	O
ATOM	296	6H29	MOL	2	17.119	9.445	3.190	1.00	0.00	H
ATOM	297	7H29	MOL	2	16.835	10.887	4.230	1.00	0.00	H
ATOM	298	8H29	MOL	2	17.346	9.328	4.982	1.00	0.00	H
ATOM	299	9H29	MOL	2	19.261	10.939	4.851	1.00	0.00	H
ATOM	300	0H30	MOL	2	19.017	11.105	3.072	1.00	0.00	H
ATOM	301	1H30	MOL	2	19.437	8.603	2.834	1.00	0.00	H
ATOM	302	2H30	MOL	2	19.842	8.538	4.589	1.00	0.00	H
ATOM	303	3H30	MOL	2	21.476	10.112	4.168	1.00	0.00	H
ATOM	304	C_m	MOL	2	8.779	17.699	1.070	1.00	0.00	C
ATOM	305	C_m	MOL	2	9.087	18.378	2.403	1.00	0.00	C
ATOM	306	C30	MOL	2	8.866	17.413	3.565	1.00	0.00	C
ATOM	307	O_p	MOL	2	9.204	18.030	4.777	1.00	0.00	O
ATOM	308	8H30	MOL	2	9.465	16.841	0.902	1.00	0.00	H

ATOM	309	9H30	MOL	2	8.909	18.423	0.241	1.00	0.00	H
ATOM	310	0H31	MOL	2	7.736	17.322	1.058	1.00	0.00	H
ATOM	311	1H31	MOL	2	8.432	19.266	2.527	1.00	0.00	H
ATOM	312	2H31	MOL	2	10.144	18.722	2.414	1.00	0.00	H
ATOM	313	3H31	MOL	2	9.499	16.515	3.420	1.00	0.00	H
ATOM	314	4H31	MOL	2	7.815	17.061	3.591	1.00	0.00	H
ATOM	315	5H31	MOL	2	8.484	18.688	4.973	1.00	0.00	H
ATOM	316	C_m	MOL	2	21.530	13.540	4.232	1.00	0.00	C
ATOM	317	C_m	MOL	2	21.076	13.532	2.775	1.00	0.00	C
ATOM	318	C31	MOL	2	21.859	14.551	1.949	1.00	0.00	C
ATOM	319	O_p	MOL	2	21.338	14.630	0.651	1.00	0.00	O
ATOM	320	0H32	MOL	2	22.613	13.316	4.304	1.00	0.00	H
ATOM	321	1H32	MOL	2	20.976	12.759	4.792	1.00	0.00	H
ATOM	322	2H32	MOL	2	21.329	14.530	4.695	1.00	0.00	H
ATOM	323	3H32	MOL	2	19.992	13.768	2.733	1.00	0.00	H
ATOM	324	4H32	MOL	2	21.229	12.517	2.348	1.00	0.00	H
ATOM	325	5H32	MOL	2	22.925	14.242	1.888	1.00	0.00	H
ATOM	326	6H32	MOL	2	21.823	15.550	2.437	1.00	0.00	H
ATOM	327	7H32	MOL	2	20.423	15.010	0.732	1.00	0.00	H
ATOM	328	C_m	MOL	2	7.728	11.166	14.813	1.00	0.00	C
ATOM	329	C_m	MOL	2	6.387	10.573	15.238	1.00	0.00	C
ATOM	330	C33	MOL	2	6.549	9.172	15.833	1.00	0.00	C
ATOM	331	O_p	MOL	2	5.343	8.753	16.414	1.00	0.00	O
ATOM	332	2H33	MOL	2	8.434	11.185	15.666	1.00	0.00	H
ATOM	333	3H33	MOL	2	7.580	12.209	14.464	1.00	0.00	H
ATOM	334	4H33	MOL	2	8.172	10.567	13.991	1.00	0.00	H
ATOM	335	5H33	MOL	2	5.713	10.521	14.356	1.00	0.00	H
ATOM	336	6H33	MOL	2	5.921	11.242	15.991	1.00	0.00	H
ATOM	337	7H33	MOL	2	7.361	9.161	16.595	1.00	0.00	H
ATOM	338	8H33	MOL	2	6.828	8.458	15.027	1.00	0.00	H
ATOM	339	9H33	MOL	2	5.203	9.328	17.211	1.00	0.00	H
ATOM	340	C_m	MOL	2	11.226	7.895	10.695	1.00	0.00	C
ATOM	341	C_m	MOL	2	11.413	6.492	11.273	1.00	0.00	C

ATOM	342	C34	MOL	2	11.972	5.523	10.231	1.00	0.00	C
ATOM	343	O_p	MOL	2	12.190	4.265	10.806	1.00	0.00	O
ATOM	344	4H34	MOL	2	12.199	8.319	10.372	1.00	0.00	H
ATOM	345	5H34	MOL	2	10.796	8.564	11.469	1.00	0.00	H
ATOM	346	6H34	MOL	2	10.525	7.863	9.834	1.00	0.00	H
ATOM	347	7H34	MOL	2	10.434	6.124	11.636	1.00	0.00	H
ATOM	348	8H34	MOL	2	12.099	6.530	12.145	1.00	0.00	H
ATOM	349	9H34	MOL	2	12.943	5.907	9.852	1.00	0.00	H
ATOM	350	0H35	MOL	2	11.276	5.436	9.366	1.00	0.00	H
ATOM	351	1H35	MOL	2	11.296	3.879	11.009	1.00	0.00	H
ATOM	352	C_m	MOL	2	19.887	5.406	19.451	1.00	0.00	C
ATOM	353	C_m	MOL	2	18.820	4.605	18.703	1.00	0.00	C
ATOM	354	C35	MOL	2	19.044	4.649	17.194	1.00	0.00	C
ATOM	355	O_p	MOL	2	17.987	3.995	16.543	1.00	0.00	O
ATOM	356	6H35	MOL	2	20.889	4.967	19.266	1.00	0.00	H
ATOM	357	7H35	MOL	2	19.687	5.380	20.543	1.00	0.00	H
ATOM	358	8H35	MOL	2	19.895	6.465	19.114	1.00	0.00	H
ATOM	359	9H35	MOL	2	17.821	5.025	18.930	1.00	0.00	H
ATOM	360	0H36	MOL	2	18.839	3.546	19.039	1.00	0.00	H
ATOM	361	1H36	MOL	2	19.997	4.130	16.947	1.00	0.00	H
ATOM	362	2H36	MOL	2	19.131	5.704	16.842	1.00	0.00	H
ATOM	363	3H36	MOL	2	17.237	4.647	16.492	1.00	0.00	H
ATOM	364	C_m	MOL	2	14.129	18.170	16.882	1.00	0.00	C
ATOM	365	C_m	MOL	2	14.688	17.112	17.830	1.00	0.00	C
ATOM	366	C36	MOL	2	15.093	17.735	19.163	1.00	0.00	C
ATOM	367	O_p	MOL	2	15.536	16.734	20.037	1.00	0.00	O
ATOM	368	8H36	MOL	2	13.231	18.639	17.333	1.00	0.00	H
ATOM	369	9H36	MOL	2	13.837	17.700	15.922	1.00	0.00	H
ATOM	370	0H37	MOL	2	14.897	18.944	16.675	1.00	0.00	H
ATOM	371	1H37	MOL	2	15.573	16.625	17.367	1.00	0.00	H
ATOM	372	2H37	MOL	2	13.921	16.326	18.008	1.00	0.00	H
ATOM	373	3H37	MOL	2	14.216	18.244	19.617	1.00	0.00	H
ATOM	374	4H37	MOL	2	15.883	18.505	19.009	1.00	0.00	H

ATOM	375	5H37	MOL	2	16.483	16.554	19.797	1.00	0.00	H
ATOM	376	C_m	MOL	2	15.001	2.102	7.116	1.00	0.00	C
ATOM	377	C37	MOL	2	15.535	3.345	7.740	1.00	0.00	C
ATOM	378	O_O	MOL	2	14.792	4.083	8.657	1.00	0.00	O
ATOM	379	O_O	MOL	2	16.651	3.721	7.443	1.00	0.00	O
ATOM	380	0H38	MOL	2	14.979	2.230	6.016	1.00	0.00	H
ATOM	381	1H38	MOL	2	13.977	1.879	7.468	1.00	0.00	H
ATOM	382	2H38	MOL	2	15.671	1.257	7.369	1.00	0.00	H
ATOM	383	3H38	MOL	2	13.903	3.653	8.871	1.00	0.00	H
ATOM	384	C_m	MOL	2	18.585	14.564	18.840	1.00	0.00	C
ATOM	385	C38	MOL	2	17.414	13.762	19.286	1.00	0.00	C
ATOM	386	O_O	MOL	2	17.133	13.566	20.633	1.00	0.00	O
ATOM	387	O_O	MOL	2	16.695	13.251	18.448	1.00	0.00	O
ATOM	388	8H38	MOL	2	19.214	13.959	18.163	1.00	0.00	H
ATOM	389	9H38	MOL	2	19.205	14.874	19.698	1.00	0.00	H
ATOM	390	0H39	MOL	2	18.219	15.454	18.295	1.00	0.00	H
ATOM	391	1H39	MOL	2	17.741	14.102	21.237	1.00	0.00	H
ATOM	392	C_m	MOL	2	1.749	7.038	18.919	1.00	0.00	C
ATOM	393	C39	MOL	2	1.668	6.524	17.525	1.00	0.00	C
ATOM	394	O_O	MOL	2	2.783	6.481	16.694	1.00	0.00	O
ATOM	395	O_O	MOL	2	0.594	6.148	17.094	1.00	0.00	O
ATOM	396	6H39	MOL	2	1.030	7.873	19.031	1.00	0.00	H
ATOM	397	7H39	MOL	2	2.766	7.399	19.163	1.00	0.00	H
ATOM	398	8H39	MOL	2	1.472	6.226	19.619	1.00	0.00	H
ATOM	399	9H39	MOL	2	3.620	6.810	17.155	1.00	0.00	H
ATOM	400	C_m	MOL	2	2.499	10.137	11.095	1.00	0.00	C
ATOM	401	C40	MOL	2	3.716	10.228	10.261	1.00	0.00	C
ATOM	402	O_O	MOL	2	3.949	9.333	9.224	1.00	0.00	O
ATOM	403	O_O	MOL	2	4.522	11.110	10.486	1.00	0.00	O
ATOM	404	4H40	MOL	2	2.783	9.831	12.120	1.00	0.00	H
ATOM	405	5H40	MOL	2	1.775	9.425	10.662	1.00	0.00	H
ATOM	406	6H40	MOL	2	2.020	11.130	11.132	1.00	0.00	H
ATOM	407	7H40	MOL	2	3.259	8.597	9.197	1.00	0.00	H

ATOM	408	C_m	MOL	2	19.751	18.139	15.996	1.00	0.00	C
ATOM	409	C40	MOL	2	18.407	17.694	16.435	1.00	0.00	C
ATOM	410	O_O	MOL	2	17.599	16.938	15.597	1.00	0.00	O
ATOM	411	O_O	MOL	2	18.009	17.991	17.545	1.00	0.00	O
ATOM	412	2H41	MOL	2	20.232	18.740	16.792	1.00	0.00	H
ATOM	413	3H41	MOL	2	19.646	18.756	15.083	1.00	0.00	H
ATOM	414	4H41	MOL	2	20.370	17.246	15.783	1.00	0.00	H
ATOM	415	5H41	MOL	2	18.085	16.675	14.748	1.00	0.00	H
ATOM	416	C_m	MOL	2	13.836	10.104	2.732	1.00	0.00	C
ATOM	417	C41	MOL	2	13.852	8.799	3.445	1.00	0.00	C
ATOM	418	O_O	MOL	2	12.929	7.795	3.169	1.00	0.00	O
ATOM	419	O_O	MOL	2	14.698	8.605	4.294	1.00	0.00	O
ATOM	420	0H42	MOL	2	14.762	10.200	2.132	1.00	0.00	H
ATOM	421	1H42	MOL	2	13.801	10.923	3.472	1.00	0.00	H
ATOM	422	2H42	MOL	2	12.954	10.196	2.076	1.00	0.00	H
ATOM	423	3H42	MOL	2	12.246	8.077	2.479	1.00	0.00	H
ATOM	424	C_m	MOL	2	1.725	10.152	16.904	1.00	0.00	C
ATOM	425	C42	MOL	2	2.702	10.856	16.032	1.00	0.00	C
ATOM	426	O_O	MOL	2	3.201	10.273	14.872	1.00	0.00	O
ATOM	427	O_O	MOL	2	3.083	11.967	16.348	1.00	0.00	O
ATOM	428	8H42	MOL	2	2.179	10.005	17.901	1.00	0.00	H
ATOM	429	9H42	MOL	2	1.440	9.172	16.479	1.00	0.00	H
ATOM	430	0H43	MOL	2	0.812	10.773	16.994	1.00	0.00	H
ATOM	431	1H43	MOL	2	2.893	9.316	14.765	1.00	0.00	H
ATOM	432	C_m	MOL	2	5.501	18.803	21.224	1.00	0.00	C
ATOM	433	C43	MOL	2	4.840	19.097	19.931	1.00	0.00	C
ATOM	434	O_O	MOL	2	3.639	18.484	19.592	1.00	0.00	O
ATOM	435	O_O	MOL	2	5.354	19.882	19.155	1.00	0.00	O
ATOM	436	6H43	MOL	2	6.445	19.376	21.310	1.00	0.00	H
ATOM	437	7H43	MOL	2	5.721	17.721	21.287	1.00	0.00	H
ATOM	438	8H43	MOL	2	4.817	19.098	22.037	1.00	0.00	H
ATOM	439	9H43	MOL	2	3.383	17.758	20.248	1.00	0.00	H
ATOM	440	C_m	MOL	2	1.021	19.835	5.478	1.00	0.00	C

ATOM	441	C44	MOL	2	1.705	21.116	5.790	1.00	0.00	C
ATOM	442	O_O	MOL	2	1.050	22.135	6.472	1.00	0.00	O
ATOM	443	O_O	MOL	2	2.854	21.286	5.433	1.00	0.00	O
ATOM	444	4H44	MOL	2	0.182	20.041	4.790	1.00	0.00	H
ATOM	445	5H44	MOL	2	0.641	19.364	6.405	1.00	0.00	H
ATOM	446	6H44	MOL	2	1.729	19.145	4.983	1.00	0.00	H
ATOM	447	7H44	MOL	2	0.123	21.854	6.763	1.00	0.00	H
ATOM	448	C_m	MOL	2	10.025	-1.719	18.779	1.00	0.00	C
ATOM	449	C44	MOL	2	9.110	-1.834	17.614	1.00	0.00	C
ATOM	450	O_O	MOL	2	7.963	-1.057	17.523	1.00	0.00	O
ATOM	451	O_O	MOL	2	9.358	-2.639	16.736	1.00	0.00	O
ATOM	452	2H45	MOL	2	10.857	-2.445	18.678	1.00	0.00	H
ATOM	453	3H45	MOL	2	9.469	-1.943	19.707	1.00	0.00	H
ATOM	454	4H45	MOL	2	10.439	-0.697	18.814	1.00	0.00	H
ATOM	455	5H45	MOL	2	7.851	-0.438	18.315	1.00	0.00	H
ATOM	456	C_m	MOL	2	21.011	2.630	12.213	1.00	0.00	C
ATOM	457	C45	MOL	2	19.884	1.999	12.945	1.00	0.00	C
ATOM	458	O_O	MOL	2	20.061	0.812	13.641	1.00	0.00	O
ATOM	459	O_O	MOL	2	18.784	2.518	12.922	1.00	0.00	O
ATOM	460	0H46	MOL	2	20.654	3.526	11.670	1.00	0.00	H
ATOM	461	1H46	MOL	2	21.432	1.912	11.485	1.00	0.00	H
ATOM	462	2H46	MOL	2	21.796	2.921	12.938	1.00	0.00	H
ATOM	463	3H46	MOL	2	21.011	0.475	13.564	1.00	0.00	H
ATOM	464	C_m	MOL	2	12.792	17.110	0.605	1.00	0.00	C
ATOM	465	C46	MOL	2	12.174	16.587	-0.644	1.00	0.00	C
ATOM	466	O_O	MOL	2	12.675	15.450	-1.266	1.00	0.00	O
ATOM	467	O_O	MOL	2	11.206	17.151	-1.119	1.00	0.00	O
ATOM	468	8H46	MOL	2	12.263	18.025	0.940	1.00	0.00	H
ATOM	469	9H46	MOL	2	13.855	17.355	0.419	1.00	0.00	H
ATOM	470	0H47	MOL	2	12.726	16.340	1.396	1.00	0.00	H
ATOM	471	1H47	MOL	2	13.551	15.152	-0.856	1.00	0.00	H
ATOM	472	C_m	MOL	2	10.448	8.387	14.684	1.00	0.00	C
ATOM	473	C47	MOL	2	11.094	9.728	14.696	1.00	0.00	C

ATOM	474	O_O	MOL	2	11.076	10.519	15.838	1.00	0.00	O
ATOM	475	O_O	MOL	2	11.614	10.155	13.682	1.00	0.00	O
ATOM	476	6H47	MOL	2	10.838	7.792	13.836	1.00	0.00	H
ATOM	477	7H47	MOL	2	9.355	8.505	14.575	1.00	0.00	H
ATOM	478	8H47	MOL	2	10.672	7.848	15.621	1.00	0.00	H
ATOM	479	9H47	MOL	2	10.671	10.036	16.629	1.00	0.00	H
ATOM	480	C_m	MOL	2	6.041	13.511	21.586	1.00	0.00	C
ATOM	481	C48	MOL	2	4.903	14.430	21.323	1.00	0.00	C
ATOM	482	O_O	MOL	2	4.972	15.368	20.300	1.00	0.00	O
ATOM	483	O_O	MOL	2	3.899	14.368	22.009	1.00	0.00	O
ATOM	484	4H48	MOL	2	5.794	12.825	22.421	1.00	0.00	H
ATOM	485	5H48	MOL	2	6.940	14.104	21.849	1.00	0.00	H
ATOM	486	6H48	MOL	2	6.238	12.919	20.674	1.00	0.00	H
ATOM	487	7H48	MOL	2	5.858	15.313	19.816	1.00	0.00	H
ATOM	488	C_m	MOL	2	12.874	0.468	1.308	1.00	0.00	C
ATOM	489	C48	MOL	2	12.676	0.074	2.723	1.00	0.00	C
ATOM	490	O_O	MOL	2	13.227	0.832	3.749	1.00	0.00	O
ATOM	491	O_O	MOL	2	11.997	-0.900	2.988	1.00	0.00	O
ATOM	492	2H49	MOL	2	12.390	-0.266	0.632	1.00	0.00	H
ATOM	493	3H49	MOL	2	13.959	0.489	1.110	1.00	0.00	H
ATOM	494	4H49	MOL	2	12.445	1.476	1.151	1.00	0.00	H
ATOM	495	5H49	MOL	2	13.785	1.596	3.393	1.00	0.00	H
ATOM	496	C_m	MOL	2	15.758	16.312	11.991	1.00	0.00	C
ATOM	497	C49	MOL	2	14.872	17.473	12.293	1.00	0.00	C
ATOM	498	O_O	MOL	2	15.028	18.232	13.449	1.00	0.00	O
ATOM	499	O_O	MOL	2	13.969	17.748	11.526	1.00	0.00	O
ATOM	500	0H50	MOL	2	15.142	15.394	11.927	1.00	0.00	H
ATOM	501	1H50	MOL	2	16.525	16.170	12.778	1.00	0.00	H
ATOM	502	2H50	MOL	2	16.264	16.483	11.021	1.00	0.00	H
ATOM	503	3H50	MOL	2	15.811	17.921	14.007	1.00	0.00	H
ATOM	504	C_m	MOL	2	10.702	20.076	10.221	1.00	0.00	C
ATOM	505	C50	MOL	2	9.273	19.859	10.554	1.00	0.00	C
ATOM	506	O_O	MOL	2	8.350	19.573	9.553	1.00	0.00	O

ATOM	507	O_O	MOL	2	8.900	19.952	11.705	1.00	0.00	O
ATOM	508	8H50	MOL	2	11.291	20.154	11.155	1.00	0.00	H
ATOM	509	9H50	MOL	2	10.790	21.007	9.632	1.00	0.00	H
ATOM	510	0H51	MOL	2	11.075	19.215	9.640	1.00	0.00	H
ATOM	511	1H51	MOL	2	8.783	19.527	8.642	1.00	0.00	H
ATOM	512	C_m	MOL	2	17.025	21.248	0.046	1.00	0.00	C
ATOM	513	C51	MOL	2	15.743	20.551	-0.249	1.00	0.00	C
ATOM	514	O_O	MOL	2	14.886	20.994	-1.254	1.00	0.00	O
ATOM	515	O_O	MOL	2	15.426	19.585	0.418	1.00	0.00	O
ATOM	516	6H51	MOL	2	17.866	20.556	-0.141	1.00	0.00	H
ATOM	517	7H51	MOL	2	17.028	21.548	1.112	1.00	0.00	H
ATOM	518	8H51	MOL	2	17.154	22.148	-0.583	1.00	0.00	H
ATOM	519	9H51	MOL	2	15.230	21.826	-1.708	1.00	0.00	H
ATOM	520	C_m	MOL	2	11.529	19.492	14.226	1.00	0.00	C
ATOM	521	C52	MOL	2	11.450	20.890	14.738	1.00	0.00	C
ATOM	522	O_O	MOL	2	11.597	21.182	16.090	1.00	0.00	O
ATOM	523	O_O	MOL	2	11.271	21.800	13.953	1.00	0.00	O
ATOM	524	4H52	MOL	2	12.392	19.406	13.537	1.00	0.00	H
ATOM	525	5H52	MOL	2	10.596	19.264	13.674	1.00	0.00	H
ATOM	526	6H52	MOL	2	11.641	18.762	15.050	1.00	0.00	H
ATOM	527	7H52	MOL	2	11.815	20.360	16.627	1.00	0.00	H
ATOM	528	C_m	MOL	2	18.349	1.769	9.742	1.00	0.00	C
ATOM	529	C52	MOL	2	19.425	0.741	9.746	1.00	0.00	C
ATOM	530	O_O	MOL	2	19.382	-0.356	10.600	1.00	0.00	O
ATOM	531	O_O	MOL	2	20.368	0.861	8.987	1.00	0.00	O
ATOM	532	2H53	MOL	2	17.804	1.705	8.783	1.00	0.00	H
ATOM	533	3H53	MOL	2	18.798	2.776	9.845	1.00	0.00	H
ATOM	534	4H53	MOL	2	17.633	1.606	10.567	1.00	0.00	H
ATOM	535	5H53	MOL	2	18.521	-0.394	11.127	1.00	0.00	H
ATOM	536	C_m	MOL	2	15.634	12.128	15.229	1.00	0.00	C
ATOM	537	C53	MOL	2	16.559	12.999	14.449	1.00	0.00	C
ATOM	538	O_O	MOL	2	17.254	12.501	13.355	1.00	0.00	O
ATOM	539	O_O	MOL	2	16.733	14.153	14.787	1.00	0.00	O

ATOM	540	0H54	MOL	2	14.809	11.781	14.577	1.00	0.00	H
ATOM	541	1H54	MOL	2	15.212	12.695	16.082	1.00	0.00	H
ATOM	542	2H54	MOL	2	16.188	11.257	15.621	1.00	0.00	H
ATOM	543	3H54	MOL	2	17.045	11.526	13.202	1.00	0.00	H
ATOM	544	C_m	MOL	2	19.455	22.848	4.059	1.00	0.00	C
ATOM	545	C54	MOL	2	19.166	22.160	5.341	1.00	0.00	C
ATOM	546	O_O	MOL	2	18.619	22.853	6.411	1.00	0.00	O
ATOM	547	O_O	MOL	2	19.408	20.974	5.460	1.00	0.00	O
ATOM	548	8H54	MOL	2	19.936	22.142	3.350	1.00	0.00	H
ATOM	549	9H54	MOL	2	20.130	23.705	4.248	1.00	0.00	H
ATOM	550	0H55	MOL	2	18.501	23.210	3.632	1.00	0.00	H
ATOM	551	1H55	MOL	2	18.525	23.840	6.213	1.00	0.00	H
ATOM	552	C_m	MOL	2	12.850	11.496	10.741	1.00	0.00	C
ATOM	553	C55	MOL	2	13.356	12.630	11.558	1.00	0.00	C
ATOM	554	O_O	MOL	2	12.600	13.782	11.729	1.00	0.00	O
ATOM	555	O_O	MOL	2	14.460	12.561	12.063	1.00	0.00	O
ATOM	556	6H55	MOL	2	13.604	10.686	10.714	1.00	0.00	H
ATOM	557	7H55	MOL	2	12.653	11.850	9.712	1.00	0.00	H
ATOM	558	8H55	MOL	2	11.928	11.099	11.206	1.00	0.00	H
ATOM	559	9H55	MOL	2	11.685	13.702	11.310	1.00	0.00	H
ATOM	560	C_m	MOL	2	4.424	13.510	13.045	1.00	0.00	C
ATOM	561	C56	MOL	2	3.370	14.559	13.111	1.00	0.00	C
ATOM	562	O_O	MOL	2	3.547	15.792	12.493	1.00	0.00	O
ATOM	563	O_O	MOL	2	2.327	14.330	13.696	1.00	0.00	O
ATOM	564	4H56	MOL	2	4.086	12.602	13.584	1.00	0.00	H
ATOM	565	5H56	MOL	2	5.348	13.888	13.522	1.00	0.00	H
ATOM	566	6H56	MOL	2	4.623	13.257	11.986	1.00	0.00	H
ATOM	567	7H56	MOL	2	4.456	15.862	12.061	1.00	0.00	H
ATOM	568	C_m	MOL	2	4.818	17.237	17.098	1.00	0.00	C
ATOM	569	C56	MOL	2	4.302	16.064	16.358	1.00	0.00	C
ATOM	570	O_O	MOL	2	3.159	15.402	16.784	1.00	0.00	O
ATOM	571	O_O	MOL	2	4.898	15.662	15.378	1.00	0.00	O
ATOM	572	2H57	MOL	2	5.715	17.648	16.605	1.00	0.00	H

ATOM	573	3H57	MOL	2	5.079	16.919	18.121	1.00	0.00	H
ATOM	574	4H57	MOL	2	4.043	18.025	17.115	1.00	0.00	H
ATOM	575	5H57	MOL	2	2.749	15.853	17.591	1.00	0.00	H
ATOM	576	C_e	MOL	2	8.001	11.603	4.067	1.00	0.00	C
ATOM	577	C_m	MOL	2	7.327	10.309	4.522	1.00	0.00	C
ATOM	578	C57	MOL	2	7.475	9.202	3.479	1.00	0.00	C
ATOM	579	O_b	MOL	2	6.639	8.093	3.818	1.00	0.00	O
ATOM	580	0H58	MOL	2	7.445	12.047	3.213	1.00	0.00	H
ATOM	581	1H58	MOL	2	9.053	11.420	3.769	1.00	0.00	H
ATOM	582	2H58	MOL	2	8.021	12.341	4.893	1.00	0.00	H
ATOM	583	3H58	MOL	2	6.252	10.504	4.702	1.00	0.00	H
ATOM	584	4H58	MOL	2	7.777	9.968	5.477	1.00	0.00	H
ATOM	585	5H58	MOL	2	8.533	8.859	3.468	1.00	0.00	H
ATOM	586	6H58	MOL	2	7.243	9.580	2.457	1.00	0.00	H
ATOM	587	C_M	MOL	2	4.405	7.035	3.646	1.00	0.00	C
ATOM	588	C58	MOL	2	5.313	8.159	3.353	1.00	0.00	C
ATOM	589	O_O	MOL	2	4.897	9.119	2.725	1.00	0.00	O
ATOM	590	0H59	MOL	2	3.413	7.220	3.188	1.00	0.00	H
ATOM	591	1H59	MOL	2	4.309	6.954	4.742	1.00	0.00	H
ATOM	592	2H59	MOL	2	4.837	6.104	3.231	1.00	0.00	H
ATOM	593	C_e	MOL	2	9.631	8.142	-0.130	1.00	0.00	C
ATOM	594	C_m	MOL	2	9.843	9.652	-0.227	1.00	0.00	C
ATOM	595	C59	MOL	2	9.997	10.314	1.140	1.00	0.00	C
ATOM	596	O_b	MOL	2	10.885	11.434	1.042	1.00	0.00	O
ATOM	597	7H59	MOL	2	8.701	7.911	0.432	1.00	0.00	H
ATOM	598	8H59	MOL	2	10.500	7.658	0.362	1.00	0.00	H
ATOM	599	9H59	MOL	2	9.534	7.720	-1.154	1.00	0.00	H
ATOM	600	0H60	MOL	2	8.970	10.098	-0.742	1.00	0.00	H
ATOM	601	1H60	MOL	2	10.738	9.854	-0.847	1.00	0.00	H
ATOM	602	2H60	MOL	2	10.435	9.598	1.866	1.00	0.00	H
ATOM	603	3H60	MOL	2	8.992	10.585	1.515	1.00	0.00	H
ATOM	604	C_M	MOL	2	11.349	13.763	1.740	1.00	0.00	C
ATOM	605	C60	MOL	2	10.385	12.694	1.410	1.00	0.00	C

ATOM	606	O_O	MOL	2	9.187	12.929	1.448	1.00	0.00	O
ATOM	607	7H60	MOL	2	10.817	14.695	2.019	1.00	0.00	H
ATOM	608	8H60	MOL	2	11.989	13.942	0.858	1.00	0.00	H
ATOM	609	9H60	MOL	2	11.971	13.420	2.588	1.00	0.00	H
ATOM	610	C_e	MOL	2	0.298	5.981	12.520	1.00	0.00	C
ATOM	611	C_m	MOL	2	0.703	7.440	12.690	1.00	0.00	C
ATOM	612	C61	MOL	2	-0.040	8.099	13.856	1.00	0.00	C
ATOM	613	O_b	MOL	2	0.446	9.427	14.074	1.00	0.00	O
ATOM	614	4H61	MOL	2	-0.764	5.918	12.200	1.00	0.00	H
ATOM	615	5H61	MOL	2	0.431	5.424	13.470	1.00	0.00	H
ATOM	616	6H61	MOL	2	0.929	5.502	11.741	1.00	0.00	H
ATOM	617	7H61	MOL	2	0.459	7.973	11.751	1.00	0.00	H
ATOM	618	8H61	MOL	2	1.798	7.503	12.871	1.00	0.00	H
ATOM	619	9H61	MOL	2	0.152	7.511	14.779	1.00	0.00	H
ATOM	620	0H62	MOL	2	-1.142	8.091	13.699	1.00	0.00	H
ATOM	621	C_M	MOL	2	0.409	11.827	13.455	1.00	0.00	C
ATOM	622	C62	MOL	2	-0.006	10.429	13.200	1.00	0.00	C
ATOM	623	O_O	MOL	2	-0.681	10.169	12.216	1.00	0.00	O
ATOM	624	4H62	MOL	2	-0.043	12.510	12.710	1.00	0.00	H
ATOM	625	5H62	MOL	2	1.509	11.890	13.393	1.00	0.00	H
ATOM	626	6H62	MOL	2	0.094	12.124	14.470	1.00	0.00	H
ATOM	627	C_e	MOL	2	10.655	10.240	7.920	1.00	0.00	C
ATOM	628	C_m	MOL	2	9.819	11.382	7.340	1.00	0.00	C
ATOM	629	C62	MOL	2	10.480	12.742	7.570	1.00	0.00	C
ATOM	630	O_b	MOL	2	9.811	13.762	6.821	1.00	0.00	O
ATOM	631	1H63	MOL	2	10.187	9.267	7.662	1.00	0.00	H
ATOM	632	2H63	MOL	2	11.687	10.255	7.510	1.00	0.00	H
ATOM	633	3H63	MOL	2	10.703	10.312	9.023	1.00	0.00	H
ATOM	634	4H63	MOL	2	8.803	11.372	7.793	1.00	0.00	H
ATOM	635	5H63	MOL	2	9.708	11.226	6.251	1.00	0.00	H
ATOM	636	6H63	MOL	2	11.528	12.688	7.207	1.00	0.00	H
ATOM	637	7H63	MOL	2	10.521	12.997	8.652	1.00	0.00	H
ATOM	638	C_M	MOL	2	7.907	15.345	6.630	1.00	0.00	C

ATOM	639	C63 MOL	2	8.601	14.247	7.342	1.00	0.00	C
ATOM	640	O_O MOL	2	8.123	13.800	8.374	1.00	0.00	O
ATOM	641	1H64 MOL	2	8.564	16.235	6.618	1.00	0.00	H
ATOM	642	2H64 MOL	2	6.957	15.597	7.142	1.00	0.00	H
ATOM	643	3H64 MOL	2	7.699	15.025	5.590	1.00	0.00	H
ATOM	644	C_e MOL	2	14.959	17.521	3.647	1.00	0.00	C
ATOM	645	C_m MOL	2	15.521	16.096	3.645	1.00	0.00	C
ATOM	646	C64 MOL	2	14.512	15.102	4.213	1.00	0.00	C
ATOM	647	O_b MOL	2	15.193	13.949	4.713	1.00	0.00	O
ATOM	648	8H64 MOL	2	14.882	17.895	4.690	1.00	0.00	H
ATOM	649	9H64 MOL	2	13.952	17.557	3.180	1.00	0.00	H
ATOM	650	0H65 MOL	2	15.629	18.204	3.090	1.00	0.00	H
ATOM	651	1H65 MOL	2	16.441	16.075	4.266	1.00	0.00	H
ATOM	652	2H65 MOL	2	15.787	15.796	2.608	1.00	0.00	H
ATOM	653	3H65 MOL	2	13.788	14.822	3.416	1.00	0.00	H
ATOM	654	4H65 MOL	2	13.963	15.585	5.045	1.00	0.00	H
ATOM	655	C_M MOL	2	14.941	12.007	6.253	1.00	0.00	C
ATOM	656	C65 MOL	2	14.358	12.994	5.318	1.00	0.00	C
ATOM	657	O_O MOL	2	13.162	12.951	5.087	1.00	0.00	O
ATOM	658	8H65 MOL	2	14.405	12.086	7.217	1.00	0.00	H
ATOM	659	9H65 MOL	2	16.016	12.227	6.408	1.00	0.00	H
ATOM	660	0H66 MOL	2	14.818	10.991	5.834	1.00	0.00	H
ATOM	661	C_e MOL	2	19.883	7.626	8.460	1.00	0.00	C
ATOM	662	C_m MOL	2	18.456	8.020	8.080	1.00	0.00	C
ATOM	663	C66 MOL	2	17.427	7.070	8.698	1.00	0.00	C
ATOM	664	O_b MOL	2	16.128	7.672	8.671	1.00	0.00	O
ATOM	665	5H66 MOL	2	20.113	6.597	8.110	1.00	0.00	H
ATOM	666	6H66 MOL	2	20.023	7.672	9.562	1.00	0.00	H
ATOM	667	7H66 MOL	2	20.596	8.336	7.991	1.00	0.00	H
ATOM	668	8H66 MOL	2	18.343	8.012	6.975	1.00	0.00	H
ATOM	669	9H66 MOL	2	18.263	9.054	8.436	1.00	0.00	H
ATOM	670	0H67 MOL	2	17.693	6.873	9.754	1.00	0.00	H
ATOM	671	1H67 MOL	2	17.443	6.076	8.198	1.00	0.00	H

ATOM	672	C_M	MOL	2	14.016	8.081	7.438	1.00	0.00	C
ATOM	673	C67	MOL	2	15.377	7.497	7.499	1.00	0.00	C
ATOM	674	O_O	MOL	2	15.813	6.876	6.543	1.00	0.00	O
ATOM	675	5H67	MOL	2	13.525	7.809	6.483	1.00	0.00	H
ATOM	676	6H67	MOL	2	14.097	9.180	7.520	1.00	0.00	H
ATOM	677	7H67	MOL	2	13.418	7.686	8.279	1.00	0.00	H
ATOM	678	C_e	MOL	2	19.178	17.692	4.191	1.00	0.00	C
ATOM	679	C_m	MOL	2	18.939	17.214	2.758	1.00	0.00	C
ATOM	680	C68	MOL	2	18.322	18.314	1.872	1.00	0.00	C
ATOM	681	O_b	MOL	2	19.177	18.623	0.767	1.00	0.00	O
ATOM	682	2H68	MOL	2	18.218	17.989	4.668	1.00	0.00	H
ATOM	683	3H68	MOL	2	19.861	18.567	4.189	1.00	0.00	H
ATOM	684	4H68	MOL	2	19.651	16.882	4.787	1.00	0.00	H
ATOM	685	5H68	MOL	2	18.277	16.323	2.760	1.00	0.00	H
ATOM	686	6H68	MOL	2	19.903	16.878	2.335	1.00	0.00	H
ATOM	687	7H68	MOL	2	18.173	19.249	2.456	1.00	0.00	H
ATOM	688	8H68	MOL	2	17.315	18.009	1.508	1.00	0.00	H
ATOM	689	C_M	MOL	2	20.110	17.949	-1.426	1.00	0.00	C
ATOM	690	C69	MOL	2	19.245	17.670	-0.259	1.00	0.00	C
ATOM	691	O_O	MOL	2	18.618	16.624	-0.203	1.00	0.00	O
ATOM	692	2H69	MOL	2	20.054	17.128	-2.165	1.00	0.00	H
ATOM	693	3H69	MOL	2	21.156	18.066	-1.083	1.00	0.00	H
ATOM	694	4H69	MOL	2	19.757	18.883	-1.894	1.00	0.00	H
ATOM	695	C_e	MOL	2	11.122	1.815	19.865	1.00	0.00	C
ATOM	696	C_m	MOL	2	10.140	2.434	18.867	1.00	0.00	C
ATOM	697	C69	MOL	2	10.850	3.415	17.931	1.00	0.00	C
ATOM	698	O_b	MOL	2	9.923	4.006	17.015	1.00	0.00	O
ATOM	699	9H69	MOL	2	11.570	2.602	20.505	1.00	0.00	H
ATOM	700	0H70	MOL	2	11.936	1.276	19.334	1.00	0.00	H
ATOM	701	1H70	MOL	2	10.592	1.098	20.526	1.00	0.00	H
ATOM	702	2H70	MOL	2	9.338	2.963	19.423	1.00	0.00	H
ATOM	703	3H70	MOL	2	9.662	1.636	18.259	1.00	0.00	H
ATOM	704	4H70	MOL	2	11.605	2.853	17.336	1.00	0.00	H

ATOM	705	5H70	MOL	2	11.403	4.192	18.506	1.00	0.00	H
ATOM	706	C_M	MOL	2	8.301	5.834	16.536	1.00	0.00	C
ATOM	707	C70	MOL	2	9.151	5.081	17.486	1.00	0.00	C
ATOM	708	O_O	MOL	2	9.170	5.421	18.658	1.00	0.00	O
ATOM	709	9H70	MOL	2	8.569	6.904	16.578	1.00	0.00	H
ATOM	710	0H71	MOL	2	7.236	5.707	16.808	1.00	0.00	H
ATOM	711	1H71	MOL	2	8.462	5.456	15.507	1.00	0.00	H
ATOM	712	C_e	MOL	2	5.100	3.144	16.914	1.00	0.00	C
ATOM	713	C_m	MOL	2	6.227	2.963	17.930	1.00	0.00	C
ATOM	714	C71	MOL	2	5.824	2.037	19.068	1.00	0.00	C
ATOM	715	O_b	MOL	2	6.979	1.789	19.873	1.00	0.00	O
ATOM	716	6H71	MOL	2	4.182	3.541	17.400	1.00	0.00	H
ATOM	717	7H71	MOL	2	4.872	2.179	16.416	1.00	0.00	H
ATOM	718	8H71	MOL	2	5.421	3.861	16.131	1.00	0.00	H
ATOM	719	9H71	MOL	2	6.505	3.948	18.356	1.00	0.00	H
ATOM	720	0H72	MOL	2	7.122	2.546	17.419	1.00	0.00	H
ATOM	721	1H72	MOL	2	5.441	1.075	18.655	1.00	0.00	H
ATOM	722	2H72	MOL	2	5.019	2.523	19.669	1.00	0.00	H
ATOM	723	C_M	MOL	2	7.932	0.478	21.746	1.00	0.00	C
ATOM	724	C72	MOL	2	6.762	1.005	21.013	1.00	0.00	C
ATOM	725	O_O	MOL	2	5.638	0.767	21.419	1.00	0.00	O
ATOM	726	6H72	MOL	2	7.608	-0.036	22.673	1.00	0.00	H
ATOM	727	7H72	MOL	2	8.591	1.326	22.000	1.00	0.00	H
ATOM	728	8H72	MOL	2	8.469	-0.234	21.095	1.00	0.00	H
ATOM	729	C_e	MOL	2	7.108	18.676	14.037	1.00	0.00	C
ATOM	730	C_m	MOL	2	6.047	19.664	14.515	1.00	0.00	C
ATOM	731	C73	MOL	2	4.625	19.186	14.199	1.00	0.00	C
ATOM	732	O_b	MOL	2	3.679	19.823	15.065	1.00	0.00	O
ATOM	733	3H73	MOL	2	7.047	18.537	12.939	1.00	0.00	H
ATOM	734	4H73	MOL	2	6.981	17.694	14.533	1.00	0.00	H
ATOM	735	5H73	MOL	2	8.117	19.066	14.286	1.00	0.00	H
ATOM	736	6H73	MOL	2	6.218	20.642	14.018	1.00	0.00	H
ATOM	737	7H73	MOL	2	6.157	19.813	15.611	1.00	0.00	H

ATOM	738	8H73	MOL	2	4.551	18.091	14.360	1.00	0.00	H
ATOM	739	9H73	MOL	2	4.373	19.360	13.132	1.00	0.00	H
ATOM	740	C_M	MOL	2	2.662	21.937	15.860	1.00	0.00	C
ATOM	741	C74	MOL	2	3.467	21.196	14.868	1.00	0.00	C
ATOM	742	O_O	MOL	2	3.898	21.777	13.883	1.00	0.00	O
ATOM	743	3H74	MOL	2	2.590	23.002	15.571	1.00	0.00	H
ATOM	744	4H74	MOL	2	3.159	21.850	16.844	1.00	0.00	H
ATOM	745	5H74	MOL	2	1.649	21.494	15.907	1.00	0.00	H
ATOM	746	C_e	MOL	2	8.010	15.599	16.181	1.00	0.00	C
ATOM	747	C_m	MOL	2	9.470	15.718	15.763	1.00	0.00	C
ATOM	748	C74	MOL	2	9.937	14.444	15.052	1.00	0.00	C
ATOM	749	O_b	MOL	2	11.221	14.638	14.454	1.00	0.00	O
ATOM	750	0H75	MOL	2	7.869	14.768	16.900	1.00	0.00	H
ATOM	751	1H75	MOL	2	7.374	15.419	15.290	1.00	0.00	H
ATOM	752	2H75	MOL	2	7.698	16.541	16.671	1.00	0.00	H
ATOM	753	3H75	MOL	2	10.089	15.906	16.666	1.00	0.00	H
ATOM	754	4H75	MOL	2	9.592	16.590	15.085	1.00	0.00	H
ATOM	755	5H75	MOL	2	9.217	14.200	14.242	1.00	0.00	H
ATOM	756	6H75	MOL	2	9.946	13.578	15.746	1.00	0.00	H
ATOM	757	C_M	MOL	2	13.648	15.036	14.767	1.00	0.00	C
ATOM	758	C75	MOL	2	12.316	14.732	15.328	1.00	0.00	C
ATOM	759	O_O	MOL	2	12.188	14.588	16.533	1.00	0.00	O
ATOM	760	0H76	MOL	2	14.398	15.123	15.580	1.00	0.00	H
ATOM	761	1H76	MOL	2	13.585	15.986	14.213	1.00	0.00	H
ATOM	762	2H76	MOL	2	13.943	14.227	14.075	1.00	0.00	H
ATOM	763	C_e	MOL	2	-1.158	17.508	8.342	1.00	0.00	C
ATOM	764	C_m	MOL	2	-2.086	17.443	9.558	1.00	0.00	C
ATOM	765	C76	MOL	2	-1.682	16.336	10.530	1.00	0.00	C
ATOM	766	O_b	MOL	2	-0.485	16.721	11.222	1.00	0.00	O
ATOM	767	7H76	MOL	2	-1.186	16.555	7.776	1.00	0.00	H
ATOM	768	8H76	MOL	2	-0.117	17.705	8.662	1.00	0.00	H
ATOM	769	9H76	MOL	2	-1.466	18.327	7.660	1.00	0.00	H
ATOM	770	0H77	MOL	2	-3.123	17.249	9.212	1.00	0.00	H

ATOM	771	1H77	MOL	2	-2.078	18.420	10.087	1.00	0.00	H
ATOM	772	2H77	MOL	2	-1.488	15.406	9.957	1.00	0.00	H
ATOM	773	3H77	MOL	2	-2.543	16.134	11.209	1.00	0.00	H
ATOM	774	C_M	MOL	2	0.643	17.229	13.382	1.00	0.00	C
ATOM	775	C77	MOL	2	-0.480	16.629	12.625	1.00	0.00	C
ATOM	776	O_O	MOL	2	-1.374	16.066	13.239	1.00	0.00	O
ATOM	777	7H77	MOL	2	1.022	16.502	14.126	1.00	0.00	H
ATOM	778	8H77	MOL	2	0.286	18.140	13.895	1.00	0.00	H
ATOM	779	9H77	MOL	2	1.457	17.493	12.682	1.00	0.00	H
ATOM	780	C_e	MOL	2	13.223	22.358	11.465	1.00	0.00	C
ATOM	781	C_m	MOL	2	14.575	22.346	10.757	1.00	0.00	C
ATOM	782	C78	MOL	2	14.992	20.938	10.349	1.00	0.00	C
ATOM	783	O_b	MOL	2	16.122	21.037	9.481	1.00	0.00	O
ATOM	784	4H78	MOL	2	13.144	21.513	12.180	1.00	0.00	H
ATOM	785	5H78	MOL	2	12.406	22.295	10.721	1.00	0.00	H
ATOM	786	6H78	MOL	2	13.087	23.305	12.028	1.00	0.00	H
ATOM	787	7H78	MOL	2	15.350	22.768	11.426	1.00	0.00	H
ATOM	788	8H78	MOL	2	14.519	22.990	9.859	1.00	0.00	H
ATOM	789	9H78	MOL	2	14.152	20.430	9.821	1.00	0.00	H
ATOM	790	0H79	MOL	2	15.246	20.350	11.262	1.00	0.00	H
ATOM	791	C_M	MOL	2	17.574	19.820	7.883	1.00	0.00	C
ATOM	792	C79	MOL	2	16.641	19.815	9.031	1.00	0.00	C
ATOM	793	O_O	MOL	2	16.341	18.761	9.567	1.00	0.00	O
ATOM	794	4H79	MOL	2	17.651	18.805	7.449	1.00	0.00	H
ATOM	795	5H79	MOL	2	18.565	20.166	8.222	1.00	0.00	H
ATOM	796	6H79	MOL	2	17.201	20.515	7.109	1.00	0.00	H
ATOM	797	C_e	MOL	2	1.403	13.759	10.228	1.00	0.00	C
ATOM	798	C_m	MOL	2	1.765	14.264	8.837	1.00	0.00	C
ATOM	799	C79	MOL	2	2.537	15.585	8.901	1.00	0.00	C
ATOM	800	O_b	MOL	2	3.221	15.824	7.668	1.00	0.00	O
ATOM	801	1H80	MOL	2	0.819	14.519	10.788	1.00	0.00	H
ATOM	802	2H80	MOL	2	2.322	13.513	10.796	1.00	0.00	H
ATOM	803	3H80	MOL	2	0.788	12.841	10.135	1.00	0.00	H

ATOM	804	4H80	MOL	2	0.834	14.410	8.252	1.00	0.00	H
ATOM	805	5H80	MOL	2	2.382	13.499	8.322	1.00	0.00	H
ATOM	806	6H80	MOL	2	3.305	15.521	9.701	1.00	0.00	H
ATOM	807	7H80	MOL	2	1.860	16.430	9.160	1.00	0.00	H
ATOM	808	C_M	MOL	2	3.075	16.128	5.213	1.00	0.00	C
ATOM	809	C80	MOL	2	2.431	16.092	6.540	1.00	0.00	C
ATOM	810	O_O	MOL	2	1.232	16.309	6.626	1.00	0.00	O
ATOM	811	1H81	MOL	2	2.915	17.126	4.774	1.00	0.00	H
ATOM	812	2H81	MOL	2	2.625	15.346	4.571	1.00	0.00	H
ATOM	813	3H81	MOL	2	4.160	15.937	5.323	1.00	0.00	H
ATOM	814	C_e	MOL	2	9.124	12.156	11.316	1.00	0.00	C
ATOM	815	C_m	MOL	2	7.661	11.724	11.231	1.00	0.00	C
ATOM	816	C81	MOL	2	7.523	10.210	11.062	1.00	0.00	C
ATOM	817	O_b	MOL	2	7.513	9.899	9.668	1.00	0.00	O
ATOM	818	8H81	MOL	2	9.687	11.737	10.464	1.00	0.00	H
ATOM	819	9H81	MOL	2	9.581	11.810	12.268	1.00	0.00	H
ATOM	820	0H82	MOL	2	9.199	13.259	11.261	1.00	0.00	H
ATOM	821	1H82	MOL	2	7.167	12.235	10.374	1.00	0.00	H
ATOM	822	2H82	MOL	2	7.127	12.046	12.147	1.00	0.00	H
ATOM	823	3H82	MOL	2	6.564	9.885	11.526	1.00	0.00	H
ATOM	824	4H82	MOL	2	8.352	9.673	11.579	1.00	0.00	H
ATOM	825	C_M	MOL	2	6.826	8.201	8.002	1.00	0.00	C
ATOM	826	C82	MOL	2	7.283	8.555	9.361	1.00	0.00	C
ATOM	827	O_O	MOL	2	7.472	7.672	10.184	1.00	0.00	O
ATOM	828	8H82	MOL	2	7.622	8.462	7.285	1.00	0.00	H
ATOM	829	9H82	MOL	2	5.920	8.784	7.766	1.00	0.00	H
ATOM	830	0H83	MOL	2	6.583	7.125	7.952	1.00	0.00	H
ATOM	831	C_e	MOL	2	14.198	7.416	21.438	1.00	0.00	C
ATOM	832	C_m	MOL	2	13.658	8.757	20.948	1.00	0.00	C
ATOM	833	C83	MOL	2	13.182	8.679	19.494	1.00	0.00	C
ATOM	834	O_b	MOL	2	12.667	9.941	19.055	1.00	0.00	O
ATOM	835	5H83	MOL	2	15.008	7.051	20.775	1.00	0.00	H
ATOM	836	6H83	MOL	2	13.389	6.660	21.473	1.00	0.00	H

ATOM	837	7H83	MOL	2	14.614	7.537	22.458	1.00	0.00	H
ATOM	838	8H83	MOL	2	14.460	9.519	21.048	1.00	0.00	H
ATOM	839	9H83	MOL	2	12.806	9.067	21.584	1.00	0.00	H
ATOM	840	0H84	MOL	2	12.364	7.929	19.429	1.00	0.00	H
ATOM	841	1H84	MOL	2	13.998	8.340	18.823	1.00	0.00	H
ATOM	842	C_M	MOL	2	13.138	12.265	18.319	1.00	0.00	C
ATOM	843	C84	MOL	2	13.612	10.946	18.785	1.00	0.00	C
ATOM	844	O_O	MOL	2	14.807	10.758	18.942	1.00	0.00	O
ATOM	845	5H84	MOL	2	13.991	12.962	18.196	1.00	0.00	H
ATOM	846	6H84	MOL	2	12.435	12.686	19.059	1.00	0.00	H
ATOM	847	7H84	MOL	2	12.628	12.133	17.346	1.00	0.00	H
ATOM	848	C_e	MOL	2	17.257	7.910	18.943	1.00	0.00	C
ATOM	849	C_m	MOL	2	17.943	9.202	19.384	1.00	0.00	C
ATOM	850	C85	MOL	2	18.047	10.202	18.237	1.00	0.00	C
ATOM	851	O_b	MOL	2	18.852	9.643	17.198	1.00	0.00	O
ATOM	852	2H85	MOL	2	17.829	7.432	18.120	1.00	0.00	H
ATOM	853	3H85	MOL	2	16.235	8.123	18.574	1.00	0.00	H
ATOM	854	4H85	MOL	2	17.201	7.209	19.800	1.00	0.00	H
ATOM	855	5H85	MOL	2	18.964	8.969	19.757	1.00	0.00	H
ATOM	856	6H85	MOL	2	17.361	9.662	20.213	1.00	0.00	H
ATOM	857	7H85	MOL	2	18.497	11.139	18.624	1.00	0.00	H
ATOM	858	8H85	MOL	2	17.029	10.434	17.852	1.00	0.00	H
ATOM	859	C_M	MOL	2	19.225	11.905	16.131	1.00	0.00	C
ATOM	860	C86	MOL	2	18.985	10.438	16.053	1.00	0.00	C
ATOM	861	O_O	MOL	2	18.930	9.906	14.962	1.00	0.00	O
ATOM	862	2H86	MOL	2	19.365	12.323	15.114	1.00	0.00	H
ATOM	863	3H86	MOL	2	20.133	12.091	16.734	1.00	0.00	H
ATOM	864	4H86	MOL	2	18.351	12.402	16.587	1.00	0.00	H
ATOM	865	C_e	MOL	2	15.424	4.180	12.122	1.00	0.00	C
ATOM	866	C_m	MOL	2	14.955	4.939	13.362	1.00	0.00	C
ATOM	867	C86	MOL	2	14.532	3.987	14.481	1.00	0.00	C
ATOM	868	O_b	MOL	2	14.258	4.715	15.681	1.00	0.00	O
ATOM	869	9H86	MOL	2	14.589	3.581	11.707	1.00	0.00	H

ATOM	870	0H87	MOL	2	16.277	3.512	12.367	1.00	0.00	H
ATOM	871	1H87	MOL	2	15.747	4.892	11.335	1.00	0.00	H
ATOM	872	2H87	MOL	2	14.094	5.580	13.088	1.00	0.00	H
ATOM	873	3H87	MOL	2	15.768	5.594	13.736	1.00	0.00	H
ATOM	874	4H87	MOL	2	15.382	3.303	14.689	1.00	0.00	H
ATOM	875	5H87	MOL	2	13.657	3.367	14.174	1.00	0.00	H
ATOM	876	C_M	MOL	2	12.918	6.498	16.767	1.00	0.00	C
ATOM	877	C87	MOL	2	13.096	5.503	15.690	1.00	0.00	C
ATOM	878	O_O	MOL	2	12.229	5.383	14.839	1.00	0.00	O
ATOM	879	9H87	MOL	2	11.987	6.279	17.322	1.00	0.00	H
ATOM	880	0H88	MOL	2	12.875	7.509	16.321	1.00	0.00	H
ATOM	881	1H88	MOL	2	13.790	6.452	17.442	1.00	0.00	H
ATOM	882	C_e	MOL	2	-0.699	11.941	20.614	1.00	0.00	C
ATOM	883	C_m	MOL	2	0.790	11.659	20.436	1.00	0.00	C
ATOM	884	C88	MOL	2	1.171	10.310	21.057	1.00	0.00	C
ATOM	885	O_b	MOL	2	2.403	9.825	20.513	1.00	0.00	O
ATOM	886	6H88	MOL	2	-0.967	11.979	21.690	1.00	0.00	H
ATOM	887	7H88	MOL	2	-1.298	11.149	20.125	1.00	0.00	H
ATOM	888	8H88	MOL	2	-0.949	12.917	20.153	1.00	0.00	H
ATOM	889	9H88	MOL	2	1.381	12.473	20.912	1.00	0.00	H
ATOM	890	0H89	MOL	2	1.029	11.654	19.351	1.00	0.00	H
ATOM	891	1H89	MOL	2	0.383	9.566	20.813	1.00	0.00	H
ATOM	892	2H89	MOL	2	1.212	10.381	22.168	1.00	0.00	H
ATOM	893	C_M	MOL	2	4.841	10.170	20.199	1.00	0.00	C
ATOM	894	C89	MOL	2	3.573	10.508	20.879	1.00	0.00	C
ATOM	895	O_O	MOL	2	3.570	11.371	21.739	1.00	0.00	O
ATOM	896	6H89	MOL	2	5.603	9.904	20.959	1.00	0.00	H
ATOM	897	7H89	MOL	2	5.181	11.038	19.606	1.00	0.00	H
ATOM	898	8H89	MOL	2	4.674	9.306	19.530	1.00	0.00	H
ATOM	899	C_e	MOL	2	9.958	1.986	2.831	1.00	0.00	C
ATOM	900	C_m	MOL	2	8.675	2.062	3.651	1.00	0.00	C
ATOM	901	C90	MOL	2	8.771	1.207	4.911	1.00	0.00	C
ATOM	902	O_b	MOL	2	7.589	1.410	5.692	1.00	0.00	O

ATOM	903	3H90	MOL	2	10.078	0.960	2.425	1.00	0.00	H
ATOM	904	4H90	MOL	2	10.835	2.241	3.461	1.00	0.00	H
ATOM	905	5H90	MOL	2	9.916	2.704	1.985	1.00	0.00	H
ATOM	906	6H90	MOL	2	7.816	1.711	3.041	1.00	0.00	H
ATOM	907	7H90	MOL	2	8.476	3.115	3.924	1.00	0.00	H
ATOM	908	8H90	MOL	2	9.655	1.514	5.511	1.00	0.00	H
ATOM	909	9H90	MOL	2	8.902	0.145	4.597	1.00	0.00	H
ATOM	910	C_M	MOL	2	5.810	0.415	7.102	1.00	0.00	C
ATOM	911	C91	MOL	2	7.118	0.309	6.424	1.00	0.00	C
ATOM	912	O_O	MOL	2	7.754	-0.730	6.510	1.00	0.00	O
ATOM	913	3H91	MOL	2	5.505	-0.571	7.502	1.00	0.00	H
ATOM	914	4H91	MOL	2	5.059	0.760	6.368	1.00	0.00	H
ATOM	915	5H91	MOL	2	5.896	1.150	7.918	1.00	0.00	H
ATOM	916	C_e	MOL	2	2.386	9.090	6.106	1.00	0.00	C
ATOM	917	C_m	MOL	2	1.550	7.812	6.008	1.00	0.00	C
ATOM	918	C91	MOL	2	1.727	6.940	7.244	1.00	0.00	C
ATOM	919	O_b	MOL	2	1.014	5.717	7.051	1.00	0.00	O
ATOM	920	0H92	MOL	2	3.462	8.852	6.245	1.00	0.00	H
ATOM	921	1H92	MOL	2	2.039	9.720	6.954	1.00	0.00	H
ATOM	922	2H92	MOL	2	2.279	9.676	5.169	1.00	0.00	H
ATOM	923	3H92	MOL	2	1.846	7.234	5.107	1.00	0.00	H
ATOM	924	4H92	MOL	2	0.476	8.076	5.897	1.00	0.00	H
ATOM	925	5H92	MOL	2	1.331	7.478	8.134	1.00	0.00	H
ATOM	926	6H92	MOL	2	2.809	6.730	7.405	1.00	0.00	H
ATOM	927	C_M	MOL	2	0.363	3.524	8.032	1.00	0.00	C
ATOM	928	C92	MOL	2	1.064	4.822	8.134	1.00	0.00	C
ATOM	929	O_O	MOL	2	1.671	5.093	9.156	1.00	0.00	O
ATOM	930	0H93	MOL	2	1.077	2.704	8.241	1.00	0.00	H
ATOM	931	1H93	MOL	2	-0.055	3.398	7.014	1.00	0.00	H
ATOM	932	2H93	MOL	2	-0.458	3.501	8.774	1.00	0.00	H
ATOM	933	C_e	MOL	2	11.710	16.095	8.447	1.00	0.00	C
ATOM	934	C_m	MOL	2	13.016	15.663	7.788	1.00	0.00	C
ATOM	935	C93	MOL	2	14.156	15.580	8.804	1.00	0.00	C

ATOM	936	O_b	MOL	2	15.329	15.013	8.207	1.00	0.00	O
ATOM	937	7H93	MOL	2	11.825	17.104	8.893	1.00	0.00	H
ATOM	938	8H93	MOL	2	11.413	15.379	9.242	1.00	0.00	H
ATOM	939	9H93	MOL	2	10.900	16.139	7.691	1.00	0.00	H
ATOM	940	0H94	MOL	2	13.273	16.408	7.009	1.00	0.00	H
ATOM	941	1H94	MOL	2	12.883	14.674	7.304	1.00	0.00	H
ATOM	942	2H94	MOL	2	13.845	14.918	9.639	1.00	0.00	H
ATOM	943	3H94	MOL	2	14.370	16.582	9.242	1.00	0.00	H
ATOM	944	C_M	MOL	2	17.437	15.422	6.958	1.00	0.00	C
ATOM	945	C94	MOL	2	16.103	15.875	7.411	1.00	0.00	C
ATOM	946	O_O	MOL	2	15.710	16.985	7.094	1.00	0.00	O
ATOM	947	7H94	MOL	2	18.054	15.196	7.846	1.00	0.00	H
ATOM	948	8H94	MOL	2	17.927	16.221	6.373	1.00	0.00	H
ATOM	949	9H94	MOL	2	17.323	14.516	6.333	1.00	0.00	H
ATOM	950	C_e	MOL	2	4.295	3.737	7.118	1.00	0.00	C
ATOM	951	C_m	MOL	2	3.970	4.209	5.698	1.00	0.00	C
ATOM	952	C95	MOL	2	3.252	3.150	4.867	1.00	0.00	C
ATOM	953	O_b	MOL	2	3.057	3.680	3.553	1.00	0.00	O
ATOM	954	4H95	MOL	2	5.252	3.180	7.118	1.00	0.00	H
ATOM	955	5H95	MOL	2	3.491	3.090	7.531	1.00	0.00	H
ATOM	956	6H95	MOL	2	4.419	4.612	7.793	1.00	0.00	H
ATOM	957	7H95	MOL	2	4.911	4.495	5.182	1.00	0.00	H
ATOM	958	8H95	MOL	2	3.316	5.100	5.747	1.00	0.00	H
ATOM	959	9H95	MOL	2	2.280	2.935	5.359	1.00	0.00	H
ATOM	960	0H96	MOL	2	3.870	2.226	4.821	1.00	0.00	H
ATOM	961	C_M	MOL	2	1.475	1.775	2.893	1.00	0.00	C
ATOM	962	C96	MOL	2	2.482	2.837	2.585	1.00	0.00	C
ATOM	963	O_O	MOL	2	2.780	3.014	1.418	1.00	0.00	O
ATOM	964	4H96	MOL	2	1.923	0.780	2.714	1.00	0.00	H
ATOM	965	5H96	MOL	2	0.611	1.904	2.213	1.00	0.00	H
ATOM	966	6H96	MOL	2	1.095	1.837	3.924	1.00	0.00	H
ATOM	967	C_e	MOL	2	5.565	-0.885	10.765	1.00	0.00	C
ATOM	968	C_m	MOL	2	5.625	0.636	10.830	1.00	0.00	C

ATOM	969	C96	MOL	2	7.037	1.136	10.552	1.00	0.00	C
ATOM	970	O_b	MOL	2	6.980	2.543	10.330	1.00	0.00	O
ATOM	971	1H97	MOL	2	6.273	-1.322	11.494	1.00	0.00	H
ATOM	972	2H97	MOL	2	5.830	-1.249	9.751	1.00	0.00	H
ATOM	973	3H97	MOL	2	4.544	-1.231	11.004	1.00	0.00	H
ATOM	974	4H97	MOL	2	5.320	0.982	11.840	1.00	0.00	H
ATOM	975	5H97	MOL	2	4.915	1.068	10.091	1.00	0.00	H
ATOM	976	6H97	MOL	2	7.454	0.628	9.652	1.00	0.00	H
ATOM	977	7H97	MOL	2	7.688	0.903	11.427	1.00	0.00	H
ATOM	978	C_M	MOL	2	8.237	4.619	9.845	1.00	0.00	C
ATOM	979	C97	MOL	2	8.211	3.161	10.069	1.00	0.00	C
ATOM	980	O_O	MOL	2	9.254	2.523	10.013	1.00	0.00	O
ATOM	981	1H98	MOL	2	8.555	5.110	10.782	1.00	0.00	H
ATOM	982	2H98	MOL	2	7.218	4.965	9.587	1.00	0.00	H
ATOM	983	3H98	MOL	2	8.934	4.862	9.023	1.00	0.00	H
ATOM	984	C_e	MOL	2	24.043	0.157	-1.740	1.00	0.00	C
ATOM	985	C_m	MOL	2	23.029	0.423	-0.633	1.00	0.00	C
ATOM	986	C98	MOL	2	21.608	0.209	-1.147	1.00	0.00	C
ATOM	987	O_b	MOL	2	20.641	0.649	-0.188	1.00	0.00	O
ATOM	988	8H98	MOL	2	23.966	0.942	-2.521	1.00	0.00	H
ATOM	989	9H98	MOL	2	23.870	-0.835	-2.208	1.00	0.00	H
ATOM	990	0H99	MOL	2	25.066	0.181	-1.320	1.00	0.00	H
ATOM	991	1H99	MOL	2	23.151	1.464	-0.276	1.00	0.00	H
ATOM	992	2H99	MOL	2	23.218	-0.246	0.231	1.00	0.00	H
ATOM	993	3H99	MOL	2	21.457	-0.877	-1.325	1.00	0.00	H
ATOM	994	4H99	MOL	2	21.470	0.725	-2.124	1.00	0.00	H
ATOM	995	C_M	MOL	2	19.331	2.551	0.732	1.00	0.00	C
ATOM	996	C99	MOL	2	20.405	2.033	-0.138	1.00	0.00	C
ATOM	997	O_O	MOL	2	21.057	2.820	-0.804	1.00	0.00	O
ATOM	998	8H99	MOL	2	18.591	3.091	0.111	1.00	0.00	H
ATOM	999	9H99	MOL	2	19.780	3.236	1.477	1.00	0.00	H
ATOM	1000	H10	MOL	2	18.838	1.706	1.244	1.00	0.00	H
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```

3. Input Parameters for Ab initio Molecular Dynamics

```

# Task parameters
Calculate          molecular_dynamics
Write_HIS_File     on
Write_ARC_File     on
MD_Velocity        random
MD_Time_Step       1.0000
MD_Simann_panel
  5000   NVT_NH   300.0000  2.0000
#
Symmetry           off
Max_memory         16384
File_usage         smart

# Electronic parameters
Spin_polarization  restricted
Charge            0
Basis             dnp

```

```

basis_version      basfile_v4.4
Pseudopotential    none
Functional          pbe
Aux_density        octupole
Integration_grid    fine
Occupation          fermi
Cutoff_Global       3.7000 angstrom
Scf_density_convergence 1.0000e-006
Scf_charge_mixing   2.0000e-001
Scf_iterations      50
Scf_diis            6 pulay
Kpoints             off

# Calculated properties
Plot                density
Mulliken_analysis   charge
Grid                msbox 3 0.2500 0.2500 0.2500 3.0000

```

4. Input Coordinates of Atoms for Ab initio Molecular Dynamics

```

REMARK  Materials Studio PDB file
CRYST1  15.861  15.861  15.861  90.00  90.00  90.00 P1
ORIGX1   1.000000  0.000000  0.000000    0.000000
ORIGX2   0.000000  1.000000  0.000000    0.000000
ORIGX3   0.000000  0.000000  1.000000    0.000000
SCALE1   0.063048  0.000000  0.000000    0.000000
SCALE2   0.000000  0.063048  0.000000    0.000000
SCALE3   0.000000  0.000000  0.063048    0.000000
ATOM      1  O_w MOL      2      1.431  15.588  12.578  1.00  0.00      O
ATOM      2  H_w MOL      2      2.356  15.971  12.709  1.00  0.00      H
ATOM      3  H_w MOL      2      0.883  16.318  12.920  1.00  0.00      H
ATOM      4  O_w MOL      2      3.263   7.815   9.682  1.00  0.00      O
ATOM      5  H_w MOL      2      2.927   6.972  10.040  1.00  0.00      H

```

ATOM	6	H_w	MOL	2	2.406	8.354	9.698	1.00	0.00	H
ATOM	7	O_w	MOL	2	0.049	13.640	14.262	1.00	0.00	O
ATOM	8	H_w	MOL	2	0.888	14.026	13.974	1.00	0.00	H
ATOM	9	H_w	MOL	2	-0.445	14.473	14.541	1.00	0.00	H
ATOM	10	O_w	MOL	2	0.126	11.698	2.916	1.00	0.00	O
ATOM	11	H_w	MOL	2	1.080	11.986	3.094	1.00	0.00	H
ATOM	12	H_w	MOL	2	0.034	11.812	1.930	1.00	0.00	H
ATOM	13	O_w	MOL	2	13.837	3.451	8.047	1.00	0.00	O
ATOM	14	H_w	MOL	2	14.467	3.160	7.353	1.00	0.00	H
ATOM	15	H_w	MOL	2	13.100	2.763	8.077	1.00	0.00	H
ATOM	16	O_w	MOL	2	7.355	14.575	13.218	1.00	0.00	O
ATOM	17	H_w	MOL	2	7.041	14.191	12.332	1.00	0.00	H
ATOM	18	H_w	MOL	2	7.673	13.756	13.652	1.00	0.00	H
ATOM	19	O_w	MOL	2	7.696	0.697	9.022	1.00	0.00	O
ATOM	20	H_w	MOL	2	8.130	0.629	9.879	1.00	0.00	H
ATOM	21	H_w	MOL	2	8.381	1.041	8.427	1.00	0.00	H
ATOM	22	O_w	MOL	2	6.555	14.391	9.999	1.00	0.00	O
ATOM	23	H_w	MOL	2	7.029	15.076	9.450	1.00	0.00	H
ATOM	24	H_w	MOL	2	6.115	13.619	9.534	1.00	0.00	H
ATOM	25	O_w	MOL	2	8.794	0.768	11.749	1.00	0.00	O
ATOM	26	H_w	MOL	2	8.315	0.174	12.388	1.00	0.00	H
ATOM	27	H_w	MOL	2	9.515	0.156	11.514	1.00	0.00	H
ATOM	28	O_w	MOL	2	15.996	11.685	15.865	1.00	0.00	O
ATOM	29	H_w	MOL	2	16.053	12.556	15.432	1.00	0.00	H
ATOM	30	H_w	MOL	2	15.045	11.453	15.750	1.00	0.00	H
ATOM	31	C_m	MOL	2	12.129	1.435	4.281	1.00	0.00	C
ATOM	32	C_m	MOL	2	10.760	1.971	3.950	1.00	0.00	C
ATOM	33	C33	MOL	2	10.886	3.447	3.921	1.00	0.00	C
ATOM	34	O_p	MOL	2	9.682	4.111	3.386	1.00	0.00	O
ATOM	35	H35	MOL	2	12.909	1.866	3.635	1.00	0.00	H
ATOM	36	H36	MOL	2	12.209	0.312	4.244	1.00	0.00	H
ATOM	37	H37	MOL	2	12.389	1.765	5.329	1.00	0.00	H
ATOM	38	H38	MOL	2	10.004	1.577	4.704	1.00	0.00	H

ATOM	39	H39 MOL	2	10.370	1.684	2.952	1.00	0.00	H
ATOM	40	H40 MOL	2	11.738	3.644	3.285	1.00	0.00	H
ATOM	41	H41 MOL	2	11.074	3.890	4.925	1.00	0.00	H
ATOM	42	H42 MOL	2	9.659	3.990	2.398	1.00	0.00	H
ATOM	43	C_m MOL	2	3.771	1.722	6.242	1.00	0.00	C
ATOM	44	C_m MOL	2	3.782	3.028	7.157	1.00	0.00	C
ATOM	45	C45 MOL	2	4.536	3.028	8.513	1.00	0.00	C
ATOM	46	O_p MOL	2	4.507	4.286	9.211	1.00	0.00	O
ATOM	47	H47 MOL	2	4.717	1.155	6.066	1.00	0.00	H
ATOM	48	H48 MOL	2	3.456	2.059	5.273	1.00	0.00	H
ATOM	49	H49 MOL	2	2.986	1.026	6.607	1.00	0.00	H
ATOM	50	H50 MOL	2	2.683	3.122	7.324	1.00	0.00	H
ATOM	51	H51 MOL	2	4.275	3.815	6.552	1.00	0.00	H
ATOM	52	H52 MOL	2	5.589	2.649	8.398	1.00	0.00	H
ATOM	53	H53 MOL	2	4.006	2.227	9.054	1.00	0.00	H
ATOM	54	H54 MOL	2	3.526	4.462	9.421	1.00	0.00	H
ATOM	55	C_m MOL	2	1.934	4.675	15.180	1.00	0.00	C
ATOM	56	C_m MOL	2	0.982	3.871	14.315	1.00	0.00	C
ATOM	57	C57 MOL	2	1.112	2.365	14.553	1.00	0.00	C
ATOM	58	O_p MOL	2	0.154	1.771	13.648	1.00	0.00	O
ATOM	59	H59 MOL	2	1.645	4.488	16.215	1.00	0.00	H
ATOM	60	H60 MOL	2	1.759	5.737	15.045	1.00	0.00	H
ATOM	61	H61 MOL	2	2.977	4.315	15.170	1.00	0.00	H
ATOM	62	H62 MOL	2	1.232	3.995	13.305	1.00	0.00	H
ATOM	63	H63 MOL	2	-0.027	4.250	14.551	1.00	0.00	H
ATOM	64	H64 MOL	2	0.842	2.141	15.578	1.00	0.00	H
ATOM	65	H65 MOL	2	2.166	2.119	14.402	1.00	0.00	H
ATOM	66	H66 MOL	2	-0.458	1.157	14.147	1.00	0.00	H
ATOM	67	C_m MOL	2	10.931	7.927	9.654	1.00	0.00	C
ATOM	68	C_m MOL	2	12.087	8.800	9.496	1.00	0.00	C
ATOM	69	C69 MOL	2	13.368	8.306	10.196	1.00	0.00	C
ATOM	70	O_p MOL	2	14.510	9.168	10.062	1.00	0.00	O
ATOM	71	H71 MOL	2	10.092	8.167	8.984	1.00	0.00	H

ATOM	72	H72 MOL	2	10.424	7.882	10.614	1.00	0.00	H
ATOM	73	H73 MOL	2	11.047	6.836	9.330	1.00	0.00	H
ATOM	74	H74 MOL	2	11.784	9.778	9.880	1.00	0.00	H
ATOM	75	H75 MOL	2	12.362	8.914	8.418	1.00	0.00	H
ATOM	76	H76 MOL	2	13.582	7.243	9.867	1.00	0.00	H
ATOM	77	H77 MOL	2	13.164	8.289	11.295	1.00	0.00	H
ATOM	78	H78 MOL	2	14.704	9.363	9.075	1.00	0.00	H
ATOM	79	C_m MOL	2	3.724	9.802	-1.793	1.00	0.00	C
ATOM	80	C_m MOL	2	4.507	10.185	-0.535	1.00	0.00	C
ATOM	81	C81 MOL	2	3.460	10.548	0.552	1.00	0.00	C
ATOM	82	O_p MOL	2	4.122	10.930	1.815	1.00	0.00	O
ATOM	83	H83 MOL	2	2.898	10.559	-1.958	1.00	0.00	H
ATOM	84	H84 MOL	2	3.238	8.826	-1.655	1.00	0.00	H
ATOM	85	H85 MOL	2	4.388	9.743	-2.711	1.00	0.00	H
ATOM	86	H86 MOL	2	5.161	11.076	-0.598	1.00	0.00	H
ATOM	87	H87 MOL	2	5.058	9.356	-0.057	1.00	0.00	H
ATOM	88	H88 MOL	2	2.698	9.774	0.771	1.00	0.00	H
ATOM	89	H89 MOL	2	2.867	11.390	0.172	1.00	0.00	H
ATOM	90	H90 MOL	2	3.667	11.679	2.249	1.00	0.00	H
ATOM	91	C_m MOL	2	12.164	7.555	3.906	1.00	0.00	C
ATOM	92	C_m MOL	2	12.816	7.601	5.290	1.00	0.00	C
ATOM	93	C93 MOL	2	12.787	6.116	5.954	1.00	0.00	C
ATOM	94	O_p MOL	2	13.413	6.043	7.220	1.00	0.00	O
ATOM	95	H95 MOL	2	11.130	7.239	3.898	1.00	0.00	H
ATOM	96	H96 MOL	2	12.704	6.923	3.148	1.00	0.00	H
ATOM	97	H97 MOL	2	12.092	8.572	3.433	1.00	0.00	H
ATOM	98	H98 MOL	2	12.258	8.245	5.942	1.00	0.00	H
ATOM	99	H99 MOL	2	13.850	7.986	5.243	1.00	0.00	H
ATOM	100	OH10 MOL	2	13.341	5.428	5.334	1.00	0.00	H
ATOM	101	1H10 MOL	2	11.701	5.832	5.850	1.00	0.00	H
ATOM	102	2H10 MOL	2	13.576	5.081	7.470	1.00	0.00	H
ATOM	103	C_m MOL	2	15.032	7.745	15.068	1.00	0.00	C
ATOM	104	C_m MOL	2	15.004	7.750	13.560	1.00	0.00	C

ATOM	105	C10	MOL	2	16.277	8.257	12.953	1.00	0.00	C
ATOM	106	O_p	MOL	2	16.242	7.881	11.568	1.00	0.00	O
ATOM	107	7H10	MOL	2	14.056	7.413	15.448	1.00	0.00	H
ATOM	108	8H10	MOL	2	15.131	8.745	15.490	1.00	0.00	H
ATOM	109	9H10	MOL	2	15.622	7.039	15.587	1.00	0.00	H
ATOM	110	0H11	MOL	2	14.204	8.502	13.218	1.00	0.00	H
ATOM	111	1H11	MOL	2	14.808	6.754	13.092	1.00	0.00	H
ATOM	112	2H11	MOL	2	17.105	7.739	13.521	1.00	0.00	H
ATOM	113	3H11	MOL	2	16.516	9.330	13.141	1.00	0.00	H
ATOM	114	4H11	MOL	2	15.533	8.403	11.057	1.00	0.00	H
ATOM	115	C_m	MOL	2	16.499	7.811	2.763	1.00	0.00	C
ATOM	116	C_m	MOL	2	17.617	6.888	2.197	1.00	0.00	C
ATOM	117	C11	MOL	2	18.433	6.133	3.224	1.00	0.00	C
ATOM	118	O_p	MOL	2	19.268	5.058	2.653	1.00	0.00	O
ATOM	119	9H11	MOL	2	15.536	7.184	2.994	1.00	0.00	H
ATOM	120	0H12	MOL	2	16.102	8.461	1.949	1.00	0.00	H
ATOM	121	1H12	MOL	2	16.862	8.434	3.584	1.00	0.00	H
ATOM	122	2H12	MOL	2	18.271	7.466	1.565	1.00	0.00	H
ATOM	123	3H12	MOL	2	17.070	6.184	1.599	1.00	0.00	H
ATOM	124	4H12	MOL	2	17.846	5.589	3.960	1.00	0.00	H
ATOM	125	5H12	MOL	2	19.071	6.748	3.843	1.00	0.00	H
ATOM	126	6H12	MOL	2	20.043	5.506	2.173	1.00	0.00	H
ATOM	127	C_m	MOL	2	5.230	10.622	6.305	1.00	0.00	C
ATOM	128	C_m	MOL	2	5.540	9.142	5.973	1.00	0.00	C
ATOM	129	C12	MOL	2	5.237	8.978	4.496	1.00	0.00	C
ATOM	130	O_p	MOL	2	3.904	9.348	4.038	1.00	0.00	O
ATOM	131	1H13	MOL	2	5.931	11.366	5.889	1.00	0.00	H
ATOM	132	2H13	MOL	2	5.220	10.822	7.394	1.00	0.00	H
ATOM	133	3H13	MOL	2	4.159	10.858	5.905	1.00	0.00	H
ATOM	134	4H13	MOL	2	4.979	8.496	6.724	1.00	0.00	H
ATOM	135	5H13	MOL	2	6.571	8.924	6.008	1.00	0.00	H
ATOM	136	6H13	MOL	2	5.428	7.887	4.268	1.00	0.00	H
ATOM	137	7H13	MOL	2	5.813	9.664	3.851	1.00	0.00	H

ATOM	138	8H13	MOL	2	3.969	9.907	3.187	1.00	0.00	H
ATOM	139	C_m	MOL	2	7.115	2.459	5.168	1.00	0.00	C
ATOM	140	C_m	MOL	2	6.667	3.284	3.947	1.00	0.00	C
ATOM	141	C14	MOL	2	6.624	2.478	2.684	1.00	0.00	C
ATOM	142	O_p	MOL	2	6.306	3.382	1.557	1.00	0.00	O
ATOM	143	3H14	MOL	2	6.514	1.550	5.152	1.00	0.00	H
ATOM	144	4H14	MOL	2	6.679	2.867	6.115	1.00	0.00	H
ATOM	145	5H14	MOL	2	8.189	2.311	5.199	1.00	0.00	H
ATOM	146	6H14	MOL	2	7.383	4.114	3.814	1.00	0.00	H
ATOM	147	7H14	MOL	2	5.676	3.743	4.108	1.00	0.00	H
ATOM	148	8H14	MOL	2	5.774	1.781	2.685	1.00	0.00	H
ATOM	149	9H14	MOL	2	7.516	1.867	2.506	1.00	0.00	H
ATOM	150	0H15	MOL	2	5.708	2.795	1.032	1.00	0.00	H
ATOM	151	C_m	MOL	2	5.734	1.784	11.668	1.00	0.00	C
ATOM	152	C15	MOL	2	4.616	0.828	12.148	1.00	0.00	C
ATOM	153	O_O	MOL	2	4.446	-0.351	11.469	1.00	0.00	O
ATOM	154	O_O	MOL	2	3.847	1.203	13.009	1.00	0.00	O
ATOM	155	5H15	MOL	2	6.621	1.481	12.148	1.00	0.00	H
ATOM	156	6H15	MOL	2	5.451	2.804	11.876	1.00	0.00	H
ATOM	157	7H15	MOL	2	5.853	1.808	10.591	1.00	0.00	H
ATOM	158	8H15	MOL	2	5.149	-0.526	10.753	1.00	0.00	H
ATOM	159	C_m	MOL	2	12.934	15.555	7.818	1.00	0.00	C
ATOM	160	C16	MOL	2	11.694	16.333	7.859	1.00	0.00	C
ATOM	161	O_O	MOL	2	10.509	15.788	8.141	1.00	0.00	O
ATOM	162	O_O	MOL	2	11.642	17.578	7.650	1.00	0.00	O
ATOM	163	3H16	MOL	2	13.629	15.938	7.074	1.00	0.00	H
ATOM	164	4H16	MOL	2	12.715	14.480	7.727	1.00	0.00	H
ATOM	165	5H16	MOL	2	13.458	15.672	8.751	1.00	0.00	H
ATOM	166	6H16	MOL	2	10.513	14.774	8.305	1.00	0.00	H
ATOM	167	C_m	MOL	2	8.075	2.659	14.434	1.00	0.00	C
ATOM	168	C16	MOL	2	9.183	3.309	15.281	1.00	0.00	C
ATOM	169	O_O	MOL	2	8.733	3.763	16.498	1.00	0.00	O
ATOM	170	O_O	MOL	2	10.324	3.487	14.916	1.00	0.00	O

ATOM	171	1H17	MOL	2	8.052	3.175	13.462	1.00	0.00	H
ATOM	172	2H17	MOL	2	7.105	2.813	14.948	1.00	0.00	H
ATOM	173	3H17	MOL	2	8.144	1.582	14.321	1.00	0.00	H
ATOM	174	4H17	MOL	2	7.721	3.609	16.741	1.00	0.00	H
ATOM	175	C_m	MOL	2	-2.960	10.783	4.792	1.00	0.00	C
ATOM	176	C17	MOL	2	-2.659	12.282	5.141	1.00	0.00	C
ATOM	177	O_O	MOL	2	-1.833	12.934	4.321	1.00	0.00	O
ATOM	178	O_O	MOL	2	-3.279	12.821	6.083	1.00	0.00	O
ATOM	179	9H17	MOL	2	-2.071	10.390	4.270	1.00	0.00	H
ATOM	180	0H18	MOL	2	-3.832	10.931	4.162	1.00	0.00	H
ATOM	181	1H18	MOL	2	-3.057	10.299	5.733	1.00	0.00	H
ATOM	182	2H18	MOL	2	-1.144	12.438	3.807	1.00	0.00	H
ATOM	183	C_m	MOL	2	9.123	10.052	-1.494	1.00	0.00	C
ATOM	184	C18	MOL	2	8.369	11.298	-1.830	1.00	0.00	C
ATOM	185	O_O	MOL	2	7.278	11.160	-2.600	1.00	0.00	O
ATOM	186	O_O	MOL	2	8.647	12.448	-1.415	1.00	0.00	O
ATOM	187	7H18	MOL	2	8.855	9.756	-0.487	1.00	0.00	H
ATOM	188	8H18	MOL	2	10.191	10.326	-1.383	1.00	0.00	H
ATOM	189	9H18	MOL	2	8.866	9.199	-2.156	1.00	0.00	H
ATOM	190	0H19	MOL	2	7.191	10.178	-2.893	1.00	0.00	H
ATOM	191	C_m	MOL	2	15.431	4.876	10.401	1.00	0.00	C
ATOM	192	C19	MOL	2	16.864	4.869	10.328	1.00	0.00	C
ATOM	193	O_O	MOL	2	17.656	5.724	11.047	1.00	0.00	O
ATOM	194	O_O	MOL	2	17.420	4.132	9.527	1.00	0.00	O
ATOM	195	5H19	MOL	2	15.105	4.593	11.387	1.00	0.00	H
ATOM	196	6H19	MOL	2	15.046	4.102	9.695	1.00	0.00	H
ATOM	197	7H19	MOL	2	14.990	5.845	10.101	1.00	0.00	H
ATOM	198	8H19	MOL	2	17.134	6.532	11.330	1.00	0.00	H
ATOM	199	C_m	MOL	2	3.745	14.955	4.513	1.00	0.00	C
ATOM	200	C20	MOL	2	3.641	13.798	3.624	1.00	0.00	C
ATOM	201	O_O	MOL	2	4.556	13.751	2.619	1.00	0.00	O
ATOM	202	O_O	MOL	2	2.783	12.929	3.697	1.00	0.00	O
ATOM	203	3H20	MOL	2	4.469	14.835	5.305	1.00	0.00	H

ATOM	204	4H20	MOL	2	2.731	15.108	4.978	1.00	0.00	H
ATOM	205	5H20	MOL	2	4.018	15.885	3.952	1.00	0.00	H
ATOM	206	6H20	MOL	2	5.297	14.456	2.716	1.00	0.00	H
ATOM	207	C_m	MOL	2	2.628	11.678	9.480	1.00	0.00	C
ATOM	208	C20	MOL	2	3.781	12.552	9.118	1.00	0.00	C
ATOM	209	O_O	MOL	2	3.518	13.675	8.431	1.00	0.00	O
ATOM	210	O_O	MOL	2	4.918	12.339	9.433	1.00	0.00	O
ATOM	211	1H21	MOL	2	1.728	12.276	9.591	1.00	0.00	H
ATOM	212	2H21	MOL	2	2.963	11.085	10.376	1.00	0.00	H
ATOM	213	3H21	MOL	2	2.516	11.037	8.530	1.00	0.00	H
ATOM	214	4H21	MOL	2	2.581	13.820	8.314	1.00	0.00	H
ATOM	215	C_m	MOL	2	11.114	10.694	17.445	1.00	0.00	C
ATOM	216	C21	MOL	2	12.354	10.902	16.590	1.00	0.00	C
ATOM	217	O_O	MOL	2	12.679	9.862	15.776	1.00	0.00	O
ATOM	218	O_O	MOL	2	12.942	11.967	16.448	1.00	0.00	O
ATOM	219	9H21	MOL	2	11.087	11.403	18.284	1.00	0.00	H
ATOM	220	0H22	MOL	2	10.914	9.728	17.841	1.00	0.00	H
ATOM	221	1H22	MOL	2	10.242	10.854	16.811	1.00	0.00	H
ATOM	222	2H22	MOL	2	12.219	8.981	15.909	1.00	0.00	H
ATOM	223	C_m	MOL	2	0.347	16.671	9.889	1.00	0.00	C
ATOM	224	C22	MOL	2	0.919	15.397	9.366	1.00	0.00	C
ATOM	225	O_O	MOL	2	1.234	14.447	10.258	1.00	0.00	O
ATOM	226	O_O	MOL	2	1.112	15.135	8.120	1.00	0.00	O
ATOM	227	7H22	MOL	2	-0.650	16.325	10.416	1.00	0.00	H
ATOM	228	8H22	MOL	2	0.111	17.456	9.147	1.00	0.00	H
ATOM	229	9H22	MOL	2	0.983	16.946	10.718	1.00	0.00	H
ATOM	230	0H23	MOL	2	1.267	15.013	11.138	1.00	0.00	H
ATOM	231	C_e	MOL	2	14.110	4.448	17.068	1.00	0.00	C
ATOM	232	C_m	MOL	2	14.850	3.308	17.706	1.00	0.00	C
ATOM	233	C23	MOL	2	15.409	3.664	19.099	1.00	0.00	C
ATOM	234	O_b	MOL	2	16.124	2.405	19.531	1.00	0.00	O
ATOM	235	5H23	MOL	2	14.708	5.322	16.892	1.00	0.00	H
ATOM	236	6H23	MOL	2	13.316	4.799	17.731	1.00	0.00	H

ATOM	237	7H23	MOL	2	13.717	4.102	16.055	1.00	0.00	H
ATOM	238	8H23	MOL	2	15.637	3.016	17.042	1.00	0.00	H
ATOM	239	9H23	MOL	2	14.098	2.474	17.769	1.00	0.00	H
ATOM	240	0H24	MOL	2	14.604	3.876	19.794	1.00	0.00	H
ATOM	241	1H24	MOL	2	16.046	4.598	19.057	1.00	0.00	H
ATOM	242	C_M	MOL	2	16.525	0.656	20.998	1.00	0.00	C
ATOM	243	C24	MOL	2	16.065	2.061	20.840	1.00	0.00	C
ATOM	244	O_O	MOL	2	15.739	2.814	21.754	1.00	0.00	O
ATOM	245	5H24	MOL	2	17.398	0.535	20.357	1.00	0.00	H
ATOM	246	6H24	MOL	2	15.701	0.101	20.444	1.00	0.00	H
ATOM	247	7H24	MOL	2	16.821	0.278	21.989	1.00	0.00	H
ATOM	248	C_e	MOL	2	6.324	7.242	17.376	1.00	0.00	C
ATOM	249	C_m	MOL	2	7.523	6.603	18.093	1.00	0.00	C
ATOM	250	C25	MOL	2	8.895	7.072	17.679	1.00	0.00	C
ATOM	251	O_b	MOL	2	9.092	6.663	16.282	1.00	0.00	O
ATOM	252	2H25	MOL	2	6.472	8.306	17.211	1.00	0.00	H
ATOM	253	3H25	MOL	2	5.379	7.214	17.934	1.00	0.00	H
ATOM	254	4H25	MOL	2	6.111	6.794	16.402	1.00	0.00	H
ATOM	255	5H25	MOL	2	7.539	5.516	18.023	1.00	0.00	H
ATOM	256	6H25	MOL	2	7.363	6.877	19.186	1.00	0.00	H
ATOM	257	7H25	MOL	2	9.571	6.510	18.355	1.00	0.00	H
ATOM	258	8H25	MOL	2	9.122	8.091	17.854	1.00	0.00	H
ATOM	259	C_M	MOL	2	10.389	6.502	14.396	1.00	0.00	C
ATOM	260	C26	MOL	2	10.250	7.031	15.742	1.00	0.00	C
ATOM	261	O_O	MOL	2	11.152	7.676	16.283	1.00	0.00	O
ATOM	262	2H26	MOL	2	10.735	5.498	14.433	1.00	0.00	H
ATOM	263	3H26	MOL	2	11.093	7.086	13.804	1.00	0.00	H
ATOM	264	4H26	MOL	2	9.529	6.443	13.767	1.00	0.00	H
ATOM	265	C_e	MOL	2	13.505	11.476	12.332	1.00	0.00	C
ATOM	266	C_m	MOL	2	13.241	12.910	12.873	1.00	0.00	C
ATOM	267	C26	MOL	2	13.470	13.849	11.699	1.00	0.00	C
ATOM	268	O_b	MOL	2	13.415	15.240	12.127	1.00	0.00	O
ATOM	269	9H26	MOL	2	14.518	11.406	11.925	1.00	0.00	H

ATOM	270	0H27	MOL	2	12.755	11.236	11.553	1.00	0.00	H
ATOM	271	1H27	MOL	2	13.408	10.764	13.134	1.00	0.00	H
ATOM	272	2H27	MOL	2	13.984	13.258	13.594	1.00	0.00	H
ATOM	273	3H27	MOL	2	12.201	13.077	13.154	1.00	0.00	H
ATOM	274	4H27	MOL	2	12.711	13.751	10.902	1.00	0.00	H
ATOM	275	5H27	MOL	2	14.408	13.751	11.273	1.00	0.00	H
ATOM	276	C_M	MOL	2	12.265	17.241	12.664	1.00	0.00	C
ATOM	277	C27	MOL	2	12.277	15.951	11.919	1.00	0.00	C
ATOM	278	O_O	MOL	2	11.362	15.544	11.189	1.00	0.00	O
ATOM	279	9H27	MOL	2	12.136	16.963	13.703	1.00	0.00	H
ATOM	280	0H28	MOL	2	11.492	17.891	12.275	1.00	0.00	H
ATOM	281	1H28	MOL	2	13.251	17.676	12.559	1.00	0.00	H
ATOM	282	C_e	MOL	2	17.729	7.361	6.685	1.00	0.00	C
ATOM	283	C_m	MOL	2	16.739	8.266	7.431	1.00	0.00	C
ATOM	284	C28	MOL	2	16.388	9.564	6.680	1.00	0.00	C
ATOM	285	O_b	MOL	2	15.489	10.347	7.540	1.00	0.00	O
ATOM	286	6H28	MOL	2	17.079	6.985	5.770	1.00	0.00	H
ATOM	287	7H28	MOL	2	17.828	6.393	7.144	1.00	0.00	H
ATOM	288	8H28	MOL	2	18.736	7.650	6.244	1.00	0.00	H
ATOM	289	9H28	MOL	2	17.100	8.577	8.454	1.00	0.00	H
ATOM	290	0H29	MOL	2	15.818	7.611	7.638	1.00	0.00	H
ATOM	291	1H29	MOL	2	15.969	9.420	5.658	1.00	0.00	H
ATOM	292	2H29	MOL	2	17.328	10.116	6.712	1.00	0.00	H
ATOM	293	C_M	MOL	2	15.021	12.384	8.698	1.00	0.00	C
ATOM	294	C29	MOL	2	15.784	11.695	7.616	1.00	0.00	C
ATOM	295	O_O	MOL	2	16.645	12.168	6.935	1.00	0.00	O
ATOM	296	6H29	MOL	2	15.174	11.968	9.689	1.00	0.00	H
ATOM	297	7H29	MOL	2	13.973	12.376	8.564	1.00	0.00	H
ATOM	298	8H29	MOL	2	15.382	13.441	8.663	1.00	0.00	H
ATOM	299	C_e	MOL	2	4.152	13.117	-1.907	1.00	0.00	C
ATOM	300	C_m	MOL	2	3.333	13.991	-0.946	1.00	0.00	C
ATOM	301	C30	MOL	2	4.168	15.060	-0.365	1.00	0.00	C
ATOM	302	O_b	MOL	2	3.294	15.919	0.494	1.00	0.00	O

ATOM	303	3H30	MOL	2	4.850	12.579	-1.329	1.00	0.00	H
ATOM	304	4H30	MOL	2	4.581	13.837	-2.632	1.00	0.00	H
ATOM	305	5H30	MOL	2	3.547	12.458	-2.524	1.00	0.00	H
ATOM	306	6H30	MOL	2	2.806	13.520	-0.164	1.00	0.00	H
ATOM	307	7H30	MOL	2	2.527	14.513	-1.554	1.00	0.00	H
ATOM	308	8H30	MOL	2	4.506	15.706	-1.160	1.00	0.00	H
ATOM	309	9H30	MOL	2	5.088	14.813	0.185	1.00	0.00	H
ATOM	310	C_M	MOL	2	3.154	17.875	1.814	1.00	0.00	C
ATOM	311	C31	MOL	2	3.862	17.126	0.726	1.00	0.00	C
ATOM	312	O_O	MOL	2	4.887	17.576	0.174	1.00	0.00	O
ATOM	313	3H31	MOL	2	3.826	18.338	2.548	1.00	0.00	H
ATOM	314	4H31	MOL	2	2.262	17.508	2.278	1.00	0.00	H
ATOM	315	5H31	MOL	2	2.837	18.816	1.396	1.00	0.00	H
ATOM	316	C_e	MOL	2	11.122	4.464	10.747	1.00	0.00	C
ATOM	317	C_m	MOL	2	9.687	4.338	10.298	1.00	0.00	C
ATOM	318	C31	MOL	2	9.551	4.465	8.732	1.00	0.00	C
ATOM	319	O_b	MOL	2	8.164	4.561	8.269	1.00	0.00	O
ATOM	320	0H32	MOL	2	11.777	3.766	10.239	1.00	0.00	H
ATOM	321	1H32	MOL	2	11.218	4.223	11.788	1.00	0.00	H
ATOM	322	2H32	MOL	2	11.678	5.373	10.536	1.00	0.00	H
ATOM	323	3H32	MOL	2	9.052	5.105	10.828	1.00	0.00	H
ATOM	324	4H32	MOL	2	9.368	3.299	10.563	1.00	0.00	H
ATOM	325	5H32	MOL	2	9.940	3.510	8.273	1.00	0.00	H
ATOM	326	6H32	MOL	2	10.000	5.335	8.310	1.00	0.00	H
ATOM	327	C_M	MOL	2	6.455	5.871	7.374	1.00	0.00	C
ATOM	328	C32	MOL	2	7.888	5.786	7.776	1.00	0.00	C
ATOM	329	O_O	MOL	2	8.654	6.713	7.561	1.00	0.00	O
ATOM	330	0H33	MOL	2	6.120	6.894	7.344	1.00	0.00	H
ATOM	331	1H33	MOL	2	5.767	5.286	8.043	1.00	0.00	H
ATOM	332	2H33	MOL	2	6.452	5.553	6.326	1.00	0.00	H
ATOM	333	C_e	MOL	2	9.694	15.503	16.222	1.00	0.00	C
ATOM	334	C_m	MOL	2	10.965	14.953	16.907	1.00	0.00	C
ATOM	335	C33	MOL	2	12.237	15.480	16.225	1.00	0.00	C

ATOM	336	O_b	MOL	2	13.366	15.379	17.164	1.00	0.00	O
ATOM	337	7H33	MOL	2	9.867	16.618	16.009	1.00	0.00	H
ATOM	338	8H33	MOL	2	8.755	15.489	16.824	1.00	0.00	H
ATOM	339	9H33	MOL	2	9.558	15.073	15.212	1.00	0.00	H
ATOM	340	0H34	MOL	2	10.900	13.880	16.929	1.00	0.00	H
ATOM	341	1H34	MOL	2	10.946	15.343	17.911	1.00	0.00	H
ATOM	342	2H34	MOL	2	12.161	16.553	16.115	1.00	0.00	H
ATOM	343	3H34	MOL	2	12.508	14.974	15.286	1.00	0.00	H
ATOM	344	C_M	MOL	2	15.658	15.759	17.494	1.00	0.00	C
ATOM	345	C34	MOL	2	14.521	15.637	16.569	1.00	0.00	C
ATOM	346	O_O	MOL	2	14.571	15.832	15.327	1.00	0.00	O
ATOM	347	7H34	MOL	2	16.669	15.715	17.036	1.00	0.00	H
ATOM	348	8H34	MOL	2	15.616	14.901	18.150	1.00	0.00	H
ATOM	349	9H34	MOL	2	15.634	16.757	18.010	1.00	0.00	H
ATOM	350	C_e	MOL	2	9.063	10.034	5.007	1.00	0.00	C
ATOM	351	C_m	MOL	2	8.815	10.382	6.498	1.00	0.00	C
ATOM	352	C35	MOL	2	9.958	10.923	7.195	1.00	0.00	C
ATOM	353	O_b	MOL	2	9.462	11.088	8.560	1.00	0.00	O
ATOM	354	4H35	MOL	2	9.842	9.297	4.898	1.00	0.00	H
ATOM	355	5H35	MOL	2	9.414	10.915	4.409	1.00	0.00	H
ATOM	356	6H35	MOL	2	8.112	9.737	4.567	1.00	0.00	H
ATOM	357	7H35	MOL	2	8.550	9.431	6.942	1.00	0.00	H
ATOM	358	8H35	MOL	2	7.890	11.001	6.635	1.00	0.00	H
ATOM	359	9H35	MOL	2	10.329	11.891	6.728	1.00	0.00	H
ATOM	360	0H36	MOL	2	10.714	10.123	7.342	1.00	0.00	H
ATOM	361	C_M	MOL	2	9.303	12.555	10.530	1.00	0.00	C
ATOM	362	C36	MOL	2	9.845	12.268	9.095	1.00	0.00	C
ATOM	363	O_O	MOL	2	10.587	13.088	8.516	1.00	0.00	O
ATOM	364	4H36	MOL	2	10.141	12.764	11.247	1.00	0.00	H
ATOM	365	5H36	MOL	2	8.679	11.725	10.894	1.00	0.00	H
ATOM	366	6H36	MOL	2	8.739	13.416	10.377	1.00	0.00	H
ATOM	367	C_e	MOL	2	7.085	14.508	5.815	1.00	0.00	C
ATOM	368	C_m	MOL	2	8.503	14.027	5.548	1.00	0.00	C

ATOM	369	C36	MOL	2	8.982	14.686	4.193	1.00	0.00	C
ATOM	370	O_b	MOL	2	8.680	13.731	3.069	1.00	0.00	O
ATOM	371	1H37	MOL	2	6.676	14.103	6.810	1.00	0.00	H
ATOM	372	2H37	MOL	2	6.384	14.293	5.022	1.00	0.00	H
ATOM	373	3H37	MOL	2	7.030	15.624	5.972	1.00	0.00	H
ATOM	374	4H37	MOL	2	8.515	12.959	5.370	1.00	0.00	H
ATOM	375	5H37	MOL	2	9.160	14.279	6.434	1.00	0.00	H
ATOM	376	6H37	MOL	2	10.049	14.763	4.033	1.00	0.00	H
ATOM	377	7H37	MOL	2	8.473	15.602	3.999	1.00	0.00	H
ATOM	378	C_M	MOL	2	7.265	12.805	1.278	1.00	0.00	C
ATOM	379	C37	MOL	2	7.515	13.898	2.367	1.00	0.00	C
ATOM	380	O_O	MOL	2	6.775	14.897	2.526	1.00	0.00	O
ATOM	381	1H38	MOL	2	6.595	13.172	0.491	1.00	0.00	H
ATOM	382	2H38	MOL	2	6.721	11.883	1.699	1.00	0.00	H
ATOM	383	3H38	MOL	2	8.152	12.370	0.819	1.00	0.00	H
ATOM	384	C_e	MOL	2	4.961	5.137	-2.127	1.00	0.00	C
ATOM	385	C_m	MOL	2	5.114	6.347	-3.020	1.00	0.00	C
ATOM	386	C38	MOL	2	6.112	6.190	-4.116	1.00	0.00	C
ATOM	387	O_b	MOL	2	6.177	7.275	-5.063	1.00	0.00	O
ATOM	388	8H38	MOL	2	5.933	4.784	-1.760	1.00	0.00	H
ATOM	389	9H38	MOL	2	4.547	4.315	-2.670	1.00	0.00	H
ATOM	390	0H39	MOL	2	4.409	5.379	-1.260	1.00	0.00	H
ATOM	391	1H39	MOL	2	5.385	7.260	-2.478	1.00	0.00	H
ATOM	392	2H39	MOL	2	4.224	6.547	-3.639	1.00	0.00	H
ATOM	393	3H39	MOL	2	5.785	5.419	-4.775	1.00	0.00	H
ATOM	394	4H39	MOL	2	7.185	6.058	-3.919	1.00	0.00	H
ATOM	395	C_M	MOL	2	6.545	9.515	-5.773	1.00	0.00	C
ATOM	396	C39	MOL	2	6.560	8.441	-4.674	1.00	0.00	C
ATOM	397	O_O	MOL	2	7.062	8.674	-3.558	1.00	0.00	O
ATOM	398	8H39	MOL	2	6.130	10.451	-5.365	1.00	0.00	H
ATOM	399	9H39	MOL	2	5.834	9.147	-6.611	1.00	0.00	H
ATOM	400	0H40	MOL	2	7.615	9.572	-6.178	1.00	0.00	H
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