

Juliusz A. Wolny, Konstatin Gröpl, Jonathan Kiehl, Eva Rentschler, Volker Schünemann

Quantification of the thermodynamic effects of the low-spin – high-spin interaction in molecular crystals of a mononuclear iron(II) spin crossover complex

Supplementary Materials.

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Table 1. PDB file of the optimised structure of the 15-nuclear model of the LS centre in LS matrix

TITLE	CSD ENTRY	jmk-126-9-90kslow				
REMARK	1	File created by GaussView 6.0.16				
HETATM	1	Fe	0	18.380	6.240	0.757
Fe						
HETATM	2	S	0	22.643	7.032	1.570
S						
HETATM	3	S	0	17.251	8.932	4.482
S						
HETATM	4	N	0	19.242	5.025	2.125
N						
HETATM	5	N	0	20.219	7.028	0.793
N						
HETATM	6	N	0	20.790	8.090	0.144
N						
HETATM	7	N	0	17.855	7.422	2.205
N						
HETATM	8	C	0	18.673	4.046	2.816
C						
HETATM	9	H	0	17.744	3.888	2.703
H						
HETATM	10	C	0	19.386	3.246	3.698
C						
HETATM	11	H	0	18.946	2.540	4.158
H						
HETATM	12	C	0	20.720	3.472	3.909
C						
HETATM	13	H	0	21.216	2.928	4.509
H						
HETATM	14	C	0	21.329	4.509	3.227
C						
HETATM	15	H	0	22.250	4.701	3.360
H						
HETATM	16	C	0	20.568	5.267	2.345
C						

HETATM	17	C	0	21.051	6.389	1.575
C						
HETATM	18	C	0	22.054	8.216	0.434
C						
HETATM	19	C	0	22.947	9.241	-0.123
C						
HETATM	20	C	0	22.423	10.314	-0.881
C						
HETATM	21	H	0	21.484	10.385	-1.004
H						
HETATM	22	C	0	23.240	11.240	-1.433
C						
HETATM	23	H	0	22.866	11.958	-1.930
H						
HETATM	24	C	0	24.651	11.155	-1.281
C						
HETATM	25	C	0	25.538	12.085	-1.862
C						
HETATM	26	H	0	25.191	12.809	-2.371
H						
HETATM	27	C	0	26.895	11.959	-1.704
C						
HETATM	28	H	0	27.476	12.596	-2.103
H						
HETATM	29	C	0	27.434	10.893	-0.955
C						
HETATM	30	H	0	28.374	10.814	-0.850
H						
HETATM	31	C	0	26.604	9.974	-0.381
C						
HETATM	32	H	0	26.973	9.259	0.121
H						
HETATM	33	C	0	25.192	10.075	-0.528
C						
HETATM	34	C	0	24.314	9.138	0.042
C						
HETATM	35	H	0	24.668	8.418	0.552
H						
HETATM	36	C	0	17.614	8.050	3.134
C						
HETATM	37	S	0	14.117	5.447	-0.057
S						
HETATM	38	S	0	19.509	3.547	-2.970
S						
HETATM	39	N	0	17.518	7.455	-0.613
N						
HETATM	40	N	0	16.541	5.451	0.719
N						
HETATM	41	N	0	15.970	4.389	1.368
N						
HETATM	42	N	0	18.905	5.058	-0.693
N						
HETATM	43	C	0	18.087	8.433	-1.303
C						
HETATM	44	H	0	19.017	8.592	-1.190
H						

HETATM	45	C	0	17.374	9.233	-2.185
C						
HETATM	46	H	0	17.814	9.939	-2.646
H						
HETATM	47	C	0	16.040	9.007	-2.397
C						
HETATM	48	H	0	15.545	9.551	-2.997
H						
HETATM	49	C	0	15.431	7.970	-1.715
C						
HETATM	50	H	0	14.511	7.778	-1.848
H						
HETATM	51	C	0	16.192	7.212	-0.832
C						
HETATM	52	C	0	15.709	6.090	-0.063
C						
HETATM	53	C	0	14.707	4.263	1.079
C						
HETATM	54	C	0	13.813	3.238	1.636
C						
HETATM	55	C	0	14.337	2.166	2.393
C						
HETATM	56	H	0	15.277	2.094	2.516
H						
HETATM	57	C	0	13.520	1.239	2.945
C						
HETATM	58	H	0	13.895	0.521	3.442
H						
HETATM	59	C	0	12.109	1.324	2.793
C						
HETATM	60	C	0	11.222	0.394	3.375
C						
HETATM	61	H	0	11.569	-0.329	3.883
H						
HETATM	62	C	0	9.866	0.521	3.217
C						
HETATM	63	H	0	9.284	-0.116	3.615
H						
HETATM	64	C	0	9.327	1.587	2.467
C						
HETATM	65	H	0	8.386	1.665	2.362
H						
HETATM	66	C	0	10.157	2.504	1.893
C						
HETATM	67	H	0	9.788	3.220	1.391
H						
HETATM	68	C	0	11.568	2.404	2.040
C						
HETATM	69	C	0	12.446	3.341	1.470
C						
HETATM	70	H	0	12.093	4.061	0.960
H						
HETATM	71	C	0	19.148	4.430	-1.622
C						
HETATM	72	Fe	0	14.551	-5.509	0.284
Fe						

HETATM	73	S	0	18.813	-4.717	1.098
S						
HETATM	74	S	0	13.422	-2.816	4.010
S						
HETATM	75	N	0	15.413	-6.724	1.653
N						
HETATM	76	N	0	16.390	-4.720	0.321
N						
HETATM	77	N	0	16.961	-3.658	-0.327
N						
HETATM	78	N	0	14.026	-4.326	1.734
N						
HETATM	79	C	0	14.844	-7.701	2.344
C						
HETATM	80	H	0	13.914	-7.861	2.231
H						
HETATM	81	C	0	15.556	-8.503	3.226
C						
HETATM	82	H	0	15.116	-9.209	3.686
H						
HETATM	83	C	0	16.890	-8.277	3.438
C						
HETATM	84	H	0	17.386	-8.821	4.037
H						
HETATM	85	C	0	17.499	-7.240	2.756
C						
HETATM	86	H	0	18.420	-7.047	2.889
H						
HETATM	87	C	0	16.738	-6.482	1.873
C						
HETATM	88	C	0	17.222	-5.360	1.104
C						
HETATM	89	C	0	18.224	-3.533	-0.038
C						
HETATM	90	C	0	19.118	-2.507	-0.596
C						
HETATM	91	C	0	18.594	-1.435	-1.352
C						
HETATM	92	H	0	17.654	-1.364	-1.475
H						
HETATM	93	C	0	19.410	-0.509	-1.905
C						
HETATM	94	H	0	19.036	0.210	-2.401
H						
HETATM	95	C	0	20.821	-0.594	-1.753
C						
HETATM	96	C	0	21.709	0.336	-2.335
C						
HETATM	97	H	0	21.362	1.060	-2.842
H						
HETATM	98	C	0	23.065	0.210	-2.176
C						
HETATM	99	H	0	23.647	0.847	-2.574
H						
HETATM	100	C	0	23.604	-0.856	-1.427
C						

HETATM	101	H	0	24.545	-0.934	-1.321
H						
HETATM	102	C	0	22.774	-1.774	-0.853
C						
HETATM	103	H	0	23.143	-2.490	-0.350
H						
HETATM	104	C	0	21.363	-1.673	-1.000
C						
HETATM	105	C	0	20.484	-2.611	-0.429
C						
HETATM	106	H	0	20.838	-3.331	0.081
H						
HETATM	107	C	0	13.783	-3.699	2.662
C						
HETATM	108	S	0	10.288	-6.301	-0.530
S						
HETATM	109	S	0	15.680	-8.202	-3.441
S						
HETATM	110	N	0	13.689	-4.294	-1.084
N						
HETATM	111	N	0	12.712	-6.297	0.248
N						
HETATM	112	N	0	12.141	-7.360	0.896
N						
HETATM	113	N	0	15.076	-6.691	-1.165
N						
HETATM	114	C	0	14.258	-3.316	-1.775
C						
HETATM	115	H	0	15.187	-3.157	-1.663
H						
HETATM	116	C	0	13.545	-2.515	-2.658
C						
HETATM	117	H	0	13.985	-1.809	-3.117
H						
HETATM	118	C	0	12.211	-2.741	-2.868
C						
HETATM	119	H	0	11.714	-2.198	-3.468
H						
HETATM	120	C	0	11.602	-3.779	-2.187
C						
HETATM	121	H	0	10.681	-3.971	-2.320
H						
HETATM	122	C	0	12.363	-4.536	-1.304
C						
HETATM	123	C	0	11.879	-5.659	-0.535
C						
HETATM	124	C	0	10.876	-7.486	0.606
C						
HETATM	125	C	0	9.983	-8.511	1.164
C						
HETATM	126	C	0	10.508	-9.583	1.922
C						
HETATM	127	H	0	11.446	-9.655	2.044
H						
HETATM	128	C	0	9.691	-10.510	2.473
C						

HETATM	129	H	0	10.065	-11.227	2.970
H						
HETATM	130	C	0	8.280	-10.425	2.322
C						
HETATM	131	C	0	7.393	-11.354	2.903
C						
HETATM	132	H	0	7.740	-12.078	3.412
H						
HETATM	133	C	0	6.036	-11.227	2.745
C						
HETATM	134	H	0	5.455	-11.865	3.143
H						
HETATM	135	C	0	5.497	-10.162	1.996
C						
HETATM	136	H	0	4.557	-10.084	1.890
H						
HETATM	137	C	0	6.327	-9.243	1.422
C						
HETATM	138	H	0	5.957	-8.528	0.920
H						
HETATM	139	C	0	7.739	-9.345	1.569
C						
HETATM	140	C	0	8.617	-8.407	0.998
C						
HETATM	141	H	0	8.262	-7.688	0.489
H						
HETATM	142	C	0	15.317	-7.319	-2.093
C						
HETATM	143	Fe	0	10.721	-17.258	-0.187
Fe						
HETATM	144	S	0	14.984	-16.466	0.627
S						
HETATM	145	S	0	9.592	-14.565	3.539
S						
HETATM	146	N	0	11.583	-18.472	1.181
N						
HETATM	147	N	0	12.560	-16.469	-0.151
N						
HETATM	148	N	0	13.131	-15.406	-0.799
N						
HETATM	149	N	0	10.195	-16.075	1.263
N						
HETATM	150	C	0	11.015	-19.450	1.872
C						
HETATM	151	H	0	10.084	-19.610	1.760
H						
HETATM	152	C	0	11.726	-20.252	2.755
C						
HETATM	153	H	0	11.287	-20.958	3.215
H						
HETATM	154	C	0	13.060	-20.025	2.965
C						
HETATM	155	H	0	13.556	-20.570	3.565
H						
HETATM	156	C	0	13.670	-18.988	2.285
C						

HETATM	157	H	0	14.591	-18.795	2.417
H						
HETATM	158	C	0	12.909	-18.231	1.401
C						
HETATM	159	C	0	13.392	-17.109	0.632
C						
HETATM	160	C	0	14.395	-15.281	-0.509
C						
HETATM	161	C	0	15.289	-14.255	-1.067
C						
HETATM	162	C	0	14.764	-13.184	-1.824
C						
HETATM	163	H	0	13.825	-13.112	-1.947
H						
HETATM	164	C	0	15.580	-12.257	-2.376
C						
HETATM	165	H	0	15.206	-11.539	-2.873
H						
HETATM	166	C	0	16.992	-12.342	-2.225
C						
HETATM	167	C	0	17.879	-11.413	-2.806
C						
HETATM	168	H	0	17.532	-10.689	-3.314
H						
HETATM	169	C	0	19.236	-11.539	-2.648
C						
HETATM	170	H	0	19.817	-10.902	-3.046
H						
HETATM	171	C	0	19.774	-12.605	-1.898
C						
HETATM	172	H	0	20.715	-12.683	-1.793
H						
HETATM	173	C	0	18.944	-13.523	-1.325
C						
HETATM	174	H	0	19.314	-14.238	-0.822
H						
HETATM	175	C	0	17.532	-13.421	-1.471
C						
HETATM	176	C	0	16.655	-14.360	-0.902
C						
HETATM	177	H	0	17.009	-15.078	-0.392
H						
HETATM	178	C	0	9.954	-15.448	2.191
C						
HETATM	179	S	0	6.458	-18.049	-1.001
S						
HETATM	180	S	0	11.851	-19.950	-3.914
S						
HETATM	181	N	0	9.859	-16.043	-1.555
N						
HETATM	182	N	0	8.882	-18.046	-0.223
N						
HETATM	183	N	0	8.311	-19.109	0.425
N						
HETATM	184	N	0	11.246	-18.440	-1.637
N						

HETATM	185	C	0	10.428	-15.065	-2.247
C						
HETATM	186	H	0	11.358	-14.906	-2.134
H						
HETATM	187	C	0	9.716	-14.263	-3.129
C						
HETATM	188	H	0	10.156	-13.558	-3.589
H						
HETATM	189	C	0	8.382	-14.490	-3.340
C						
HETATM	190	H	0	7.885	-13.946	-3.940
H						
HETATM	191	C	0	7.773	-15.527	-2.659
C						
HETATM	192	H	0	6.851	-15.720	-2.791
H						
HETATM	193	C	0	8.534	-16.284	-1.776
C						
HETATM	194	C	0	8.050	-17.407	-1.007
C						
HETATM	195	C	0	7.047	-19.234	0.135
C						
HETATM	196	C	0	6.153	-20.260	0.692
C						
HETATM	197	C	0	6.679	-21.332	1.449
C						
HETATM	198	H	0	7.617	-21.403	1.572
H						
HETATM	199	C	0	5.862	-22.258	2.002
C						
HETATM	200	H	0	6.235	-22.976	2.499
H						
HETATM	201	C	0	4.451	-22.174	1.850
C						
HETATM	202	C	0	3.562	-23.102	2.431
C						
HETATM	203	H	0	3.910	-23.826	2.939
H						
HETATM	204	C	0	2.206	-22.976	2.273
C						
HETATM	205	H	0	1.624	-23.613	2.672
H						
HETATM	206	C	0	1.668	-21.910	1.524
C						
HETATM	207	H	0	0.728	-21.832	1.419
H						
HETATM	208	C	0	2.497	-20.992	0.951
C						
HETATM	209	H	0	2.128	-20.276	0.447
H						
HETATM	210	C	0	3.909	-21.094	1.097
C						
HETATM	211	C	0	4.787	-20.156	0.527
C						
HETATM	212	H	0	4.433	-19.437	0.017
H						

HETATM	213	C	0	11.488	-19.067	-2.565
C						
HETATM	214	Fe	0	11.105	8.994	0.614
Fe						
HETATM	215	S	0	15.368	9.786	1.428
S						
HETATM	216	S	0	9.975	11.687	4.340
S						
HETATM	217	N	0	11.967	7.780	1.982
N						
HETATM	218	N	0	12.943	9.782	0.650
N						
HETATM	219	N	0	13.514	10.845	0.002
N						
HETATM	220	N	0	10.580	10.177	2.063
N						
HETATM	221	C	0	11.398	6.801	2.674
C						
HETATM	222	H	0	10.468	6.642	2.561
H						
HETATM	223	C	0	12.110	6.000	3.556
C						
HETATM	224	H	0	11.670	5.295	4.015
H						
HETATM	225	C	0	13.444	6.227	3.767
C						
HETATM	226	H	0	13.940	5.682	4.367
H						
HETATM	227	C	0	14.054	7.264	3.085
C						
HETATM	228	H	0	14.974	7.456	3.218
H						
HETATM	229	C	0	13.293	8.021	2.203
C						
HETATM	230	C	0	13.776	9.144	1.433
C						
HETATM	231	C	0	14.778	10.970	0.292
C						
HETATM	232	C	0	15.673	11.996	-0.266
C						
HETATM	233	C	0	15.147	13.069	-1.023
C						
HETATM	234	H	0	14.209	13.140	-1.146
H						
HETATM	235	C	0	15.964	13.995	-1.576
C						
HETATM	236	H	0	15.590	14.712	-2.072
H						
HETATM	237	C	0	17.375	13.910	-1.423
C						
HETATM	238	C	0	18.263	14.839	-2.004
C						
HETATM	239	H	0	17.916	15.563	-2.513
H						
HETATM	240	C	0	19.620	14.713	-1.846
C						

HETATM	241	H	0	20.202	15.350	-2.245
H						
HETATM	242	C	0	20.158	13.647	-1.098
C						
HETATM	243	H	0	21.099	13.569	-0.992
H						
HETATM	244	C	0	19.328	12.729	-0.524
C						
HETATM	245	H	0	19.698	12.013	-0.021
H						
HETATM	246	C	0	17.916	12.830	-0.671
C						
HETATM	247	C	0	17.039	11.892	-0.100
C						
HETATM	248	H	0	17.393	11.173	0.410
H						
HETATM	249	C	0	10.338	10.804	2.992
C						
HETATM	250	S	0	6.842	8.202	-0.200
S						
HETATM	251	S	0	12.234	6.301	-3.112
S						
HETATM	252	N	0	10.243	10.209	-0.755
N						
HETATM	253	N	0	9.267	8.206	0.577
N						
HETATM	254	N	0	8.695	7.143	1.225
N						
HETATM	255	N	0	11.630	7.812	-0.835
N						
HETATM	256	C	0	10.811	11.187	-1.445
C						
HETATM	257	H	0	11.742	11.346	-1.332
H						
HETATM	258	C	0	10.100	11.988	-2.328
C						
HETATM	259	H	0	10.539	12.693	-2.788
H						
HETATM	260	C	0	8.766	11.761	-2.539
C						
HETATM	261	H	0	8.269	12.306	-3.139
H						
HETATM	262	C	0	8.156	10.724	-1.858
C						
HETATM	263	H	0	7.235	10.532	-1.991
H						
HETATM	264	C	0	8.917	9.967	-0.974
C						
HETATM	265	C	0	8.434	8.845	-0.205
C						
HETATM	266	C	0	7.431	7.017	0.937
C						
HETATM	267	C	0	6.537	5.992	1.494
C						
HETATM	268	C	0	7.063	4.920	2.251
C						

HETATM	269	H	0	8.001	4.848	2.374
H						
HETATM	270	C	0	6.245	3.993	2.803
C						
HETATM	271	H	0	6.620	3.276	3.300
H						
HETATM	272	C	0	4.835	4.079	2.651
C						
HETATM	273	C	0	3.946	3.149	3.233
C						
HETATM	274	H	0	4.294	2.426	3.741
H						
HETATM	275	C	0	2.590	3.276	3.075
C						
HETATM	276	H	0	2.008	2.639	3.473
H						
HETATM	277	C	0	2.052	4.341	2.325
C						
HETATM	278	H	0	1.110	4.419	2.219
H						
HETATM	279	C	0	2.881	5.259	1.751
C						
HETATM	280	H	0	2.512	5.975	1.249
H						
HETATM	281	C	0	4.293	5.158	1.898
C						
HETATM	282	C	0	5.171	6.096	1.328
C						
HETATM	283	H	0	4.817	6.815	0.818
H						
HETATM	284	C	0	11.872	7.185	-1.764
C						
HETATM	285	Fe	0	7.275	-2.754	0.142
Fe						
HETATM	286	S	0	11.538	-1.962	0.956
S						
HETATM	287	S	0	6.146	-0.062	3.868
S						
HETATM	288	N	0	8.137	-3.969	1.511
N						
HETATM	289	N	0	9.114	-1.966	0.179
N						
HETATM	290	N	0	9.685	-0.903	-0.469
N						
HETATM	291	N	0	6.750	-1.572	1.592
N						
HETATM	292	C	0	7.568	-4.947	2.201
C						
HETATM	293	H	0	6.638	-5.106	2.089
H						
HETATM	294	C	0	8.281	-5.748	3.084
C						
HETATM	295	H	0	7.841	-6.454	3.544
H						
HETATM	296	C	0	9.615	-5.522	3.295
C						

HETATM	297	H	0	10.111	-6.066	3.895
H						
HETATM	298	C	0	10.224	-4.485	2.614
C						
HETATM	299	H	0	11.145	-4.292	2.747
H						
HETATM	300	C	0	9.463	-3.727	1.730
C						
HETATM	301	C	0	9.946	-2.605	0.962
C						
HETATM	302	C	0	10.949	-0.778	-0.180
C						
HETATM	303	C	0	11.843	0.247	-0.738
C						
HETATM	304	C	0	11.318	1.320	-1.494
C						
HETATM	305	H	0	10.379	1.391	-1.617
H						
HETATM	306	C	0	12.135	2.246	-2.047
C						
HETATM	307	H	0	11.761	2.964	-2.543
H						
HETATM	308	C	0	13.545	2.161	-1.895
C						
HETATM	309	C	0	14.434	3.090	-2.477
C						
HETATM	310	H	0	14.087	3.814	-2.984
H						
HETATM	311	C	0	15.790	2.964	-2.318
C						
HETATM	312	H	0	16.372	3.601	-2.716
H						
HETATM	313	C	0	16.328	1.898	-1.569
C						
HETATM	314	H	0	17.269	1.820	-1.463
H						
HETATM	315	C	0	15.499	0.980	-0.995
C						
HETATM	316	H	0	15.868	0.264	-0.493
H						
HETATM	317	C	0	14.087	1.082	-1.142
C						
HETATM	318	C	0	13.209	0.144	-0.571
C						
HETATM	319	H	0	13.563	-0.576	-0.062
H						
HETATM	320	C	0	6.508	-0.945	2.520
C						
HETATM	321	S	0	3.013	-3.546	-0.672
S						
HETATM	322	S	0	8.404	-5.448	-3.583
S						
HETATM	323	N	0	6.413	-1.540	-1.226
N						
HETATM	324	N	0	5.436	-3.543	0.106
N						

HETATM	325	N	0	4.866	-4.606	0.754
N						
HETATM	326	N	0	7.801	-3.937	-1.307
N						
HETATM	327	C	0	6.982	-0.562	-1.917
C						
HETATM	328	H	0	7.913	-0.402	-1.805
H						
HETATM	329	C	0	6.271	0.240	-2.800
C						
HETATM	330	H	0	6.709	0.946	-3.259
H						
HETATM	331	C	0	4.937	0.013	-3.010
C						
HETATM	332	H	0	4.440	0.557	-3.611
H						
HETATM	333	C	0	4.326	-1.025	-2.329
C						
HETATM	334	H	0	3.406	-1.217	-2.462
H						
HETATM	335	C	0	5.087	-1.782	-1.447
C						
HETATM	336	C	0	4.604	-2.904	-0.677
C						
HETATM	337	C	0	3.602	-4.731	0.464
C						
HETATM	338	C	0	2.708	-5.757	1.022
C						
HETATM	339	C	0	3.232	-6.829	1.779
C						
HETATM	340	H	0	4.171	-6.901	1.902
H						
HETATM	341	C	0	2.416	-7.755	2.331
C						
HETATM	342	H	0	2.790	-8.473	2.828
H						
HETATM	343	C	0	1.004	-7.670	2.179
C						
HETATM	344	C	0	0.117	-8.599	2.761
C						
HETATM	345	H	0	0.464	-9.323	3.269
H						
HETATM	346	C	0	-1.239	-8.473	2.602
C						
HETATM	347	H	0	-1.821	-9.110	3.001
H						
HETATM	348	C	0	-1.778	-7.408	1.854
C						
HETATM	349	H	0	-2.719	-7.330	1.748
H						
HETATM	350	C	0	-0.948	-6.489	1.280
C						
HETATM	351	H	0	-1.318	-5.774	0.777
H						
HETATM	352	C	0	0.464	-6.591	1.427
C						

HETATM	353	C	0	1.342	-5.652	0.856
C						
HETATM	354	H	0	0.988	-4.933	0.346
H						
HETATM	355	C	0	8.043	-4.564	-2.235
C						
HETATM	356	Fe	0	3.446	-14.503	-0.329
Fe						
HETATM	357	S	0	7.709	-13.711	0.484
S						
HETATM	358	S	0	2.316	-11.811	3.397
S						
HETATM	359	N	0	4.308	-15.718	1.039
N						
HETATM	360	N	0	5.285	-13.714	-0.293
N						
HETATM	361	N	0	5.856	-12.652	-0.942
N						
HETATM	362	N	0	2.921	-13.321	1.120
N						
HETATM	363	C	0	3.739	-16.696	1.730
C						
HETATM	364	H	0	2.809	-16.855	1.617
H						
HETATM	365	C	0	4.451	-17.497	2.612
C						
HETATM	366	H	0	4.011	-18.203	3.073
H						
HETATM	367	C	0	5.785	-17.271	2.823
C						
HETATM	368	H	0	6.282	-17.815	3.423
H						
HETATM	369	C	0	6.395	-16.233	2.142
C						
HETATM	370	H	0	7.316	-16.041	2.274
H						
HETATM	371	C	0	5.633	-15.476	1.259
C						
HETATM	372	C	0	6.117	-14.354	0.490
C						
HETATM	373	C	0	7.120	-12.526	-0.652
C						
HETATM	374	C	0	8.013	-11.501	-1.209
C						
HETATM	375	C	0	7.489	-10.429	-1.966
C						
HETATM	376	H	0	6.550	-10.358	-2.089
H						
HETATM	377	C	0	8.305	-9.503	-2.518
C						
HETATM	378	H	0	7.932	-8.785	-3.016
H						
HETATM	379	C	0	9.716	-9.587	-2.367
C						
HETATM	380	C	0	10.604	-8.658	-2.948
C						

HETATM	381	H	0	10.257	-7.935	-3.456
H						
HETATM	382	C	0	11.960	-8.785	-2.790
C						
HETATM	383	H	0	12.542	-8.147	-3.189
H						
HETATM	384	C	0	12.499	-9.851	-2.040
C						
HETATM	385	H	0	13.440	-9.929	-1.936
H						
HETATM	386	C	0	11.670	-10.769	-1.467
C						
HETATM	387	H	0	12.039	-11.484	-0.964
H						
HETATM	388	C	0	10.258	-10.667	-1.613
C						
HETATM	389	C	0	9.379	-11.605	-1.044
C						
HETATM	390	H	0	9.734	-12.324	-0.534
H						
HETATM	391	C	0	2.679	-12.694	2.049
C						
HETATM	392	S	0	-0.817	-15.295	-1.143
S						
HETATM	393	S	0	4.575	-17.195	-4.056
S						
HETATM	394	N	0	2.584	-13.289	-1.698
N						
HETATM	395	N	0	1.607	-15.292	-0.366
N						
HETATM	396	N	0	1.036	-16.355	0.283
N						
HETATM	397	N	0	3.971	-15.685	-1.779
N						
HETATM	398	C	0	3.153	-12.311	-2.389
C						
HETATM	399	H	0	4.082	-12.151	-2.276
H						
HETATM	400	C	0	2.440	-11.509	-3.271
C						
HETATM	401	H	0	2.880	-10.803	-3.732
H						
HETATM	402	C	0	1.106	-11.736	-3.482
C						
HETATM	403	H	0	0.611	-11.191	-4.082
H						
HETATM	404	C	0	0.497	-12.772	-2.801
C						
HETATM	405	H	0	-0.424	-12.966	-2.933
H						
HETATM	406	C	0	1.258	-13.530	-1.918
C						
HETATM	407	C	0	0.775	-14.652	-1.149
C						
HETATM	408	C	0	-0.227	-16.479	-0.007
C						

HETATM	409	C	0	-1.122	-17.506	0.550
C						
HETATM	410	C	0	-0.597	-18.577	1.307
C						
HETATM	411	H	0	0.342	-18.648	1.430
H						
HETATM	412	C	0	-1.414	-19.503	1.860
C						
HETATM	413	H	0	-1.039	-20.222	2.357
H						
HETATM	414	C	0	-2.825	-19.419	1.708
C						
HETATM	415	C	0	-3.712	-20.348	2.289
C						
HETATM	416	H	0	-3.365	-21.072	2.797
H						
HETATM	417	C	0	-5.069	-20.222	2.131
C						
HETATM	418	H	0	-5.650	-20.859	2.530
H						
HETATM	419	C	0	-5.608	-19.156	1.381
C						
HETATM	420	H	0	-6.548	-19.078	1.277
H						
HETATM	421	C	0	-4.777	-18.238	0.808
C						
HETATM	422	H	0	-5.147	-17.522	0.305
H						
HETATM	423	C	0	-3.366	-18.339	0.954
C						
HETATM	424	C	0	-2.488	-17.401	0.385
C						
HETATM	425	H	0	-2.842	-16.682	-0.125
H						
HETATM	426	C	0	4.213	-16.313	-2.708
C						
HETATM	427	Fe	0	3.830	11.749	0.472
Fe						
HETATM	428	S	0	8.092	12.541	1.286
S						
HETATM	429	S	0	2.700	14.441	4.197
S						
HETATM	430	N	0	4.692	10.534	1.840
N						
HETATM	431	N	0	5.668	12.537	0.508
N						
HETATM	432	N	0	6.239	13.599	-0.140
N						
HETATM	433	N	0	3.305	12.931	1.921
N						
HETATM	434	C	0	4.123	9.555	2.531
C						
HETATM	435	H	0	3.193	9.397	2.419
H						
HETATM	436	C	0	4.835	8.755	3.414
C						

HETATM	437	H	0	4.395	8.049	3.873
H						
HETATM	438	C	0	6.169	8.981	3.625
C						
HETATM	439	H	0	6.665	8.437	4.224
H						
HETATM	440	C	0	6.778	10.018	2.943
C						
HETATM	441	H	0	7.699	10.210	3.076
H						
HETATM	442	C	0	6.017	10.776	2.060
C						
HETATM	443	C	0	6.501	11.898	1.291
C						
HETATM	444	C	0	7.503	13.725	0.150
C						
HETATM	445	C	0	8.397	14.750	-0.408
C						
HETATM	446	C	0	7.873	15.823	-1.165
C						
HETATM	447	H	0	6.933	15.894	-1.288
H						
HETATM	448	C	0	8.689	16.749	-1.718
C						
HETATM	449	H	0	8.314	17.467	-2.214
H						
HETATM	450	C	0	10.100	16.664	-1.566
C						
HETATM	451	C	0	10.988	17.594	-2.147
C						
HETATM	452	H	0	10.641	18.318	-2.655
H						
HETATM	453	C	0	12.344	17.467	-1.988
C						
HETATM	454	H	0	12.926	18.105	-2.387
H						
HETATM	455	C	0	12.883	16.401	-1.240
C						
HETATM	456	H	0	13.824	16.323	-1.134
H						
HETATM	457	C	0	12.053	15.484	-0.666
C						
HETATM	458	H	0	12.422	14.768	-0.163
H						
HETATM	459	C	0	10.641	15.584	-0.813
C						
HETATM	460	C	0	9.763	14.647	-0.242
C						
HETATM	461	H	0	10.117	13.927	0.267
H						
HETATM	462	C	0	3.062	13.559	2.849
C						
HETATM	463	S	0	-0.433	10.956	-0.342
S						
HETATM	464	S	0	4.959	9.056	-3.254
S						

HETATM	465	N	0	2.968	12.964	-0.897
N						
HETATM	466	N	0	1.991	10.960	0.435
N						
HETATM	467	N	0	1.420	9.898	1.083
N						
HETATM	468	N	0	4.355	10.567	-0.978
N						
HETATM	469	C	0	3.537	13.942	-1.587
C						
HETATM	470	H	0	4.466	14.101	-1.475
H						
HETATM	471	C	0	2.824	14.742	-2.470
C						
HETATM	472	H	0	3.264	15.448	-2.930
H						
HETATM	473	C	0	1.490	14.516	-2.681
C						
HETATM	474	H	0	0.993	15.060	-3.281
H						
HETATM	475	C	0	0.881	13.479	-2.000
C						
HETATM	476	H	0	-0.041	13.287	-2.133
H						
HETATM	477	C	0	1.642	12.721	-1.116
C						
HETATM	478	C	0	1.158	11.599	-0.348
C						
HETATM	479	C	0	0.155	9.772	0.794
C						
HETATM	480	C	0	-0.738	8.747	1.352
C						
HETATM	481	C	0	-0.213	7.675	2.109
C						
HETATM	482	H	0	0.725	7.603	2.231
H						
HETATM	483	C	0	-1.030	6.748	2.661
C						
HETATM	484	H	0	-0.656	6.030	3.157
H						
HETATM	485	C	0	-2.441	6.833	2.509
C						
HETATM	486	C	0	-3.329	5.903	3.091
C						
HETATM	487	H	0	-2.981	5.180	3.599
H						
HETATM	488	C	0	-4.685	6.030	2.932
C						
HETATM	489	H	0	-5.266	5.393	3.330
H						
HETATM	490	C	0	-5.224	7.096	2.183
C						
HETATM	491	H	0	-6.164	7.174	2.077
H						
HETATM	492	C	0	-4.394	8.014	1.609
C						

HETATM	493	H	0	-4.764	8.730	1.107
H						
HETATM	494	C	0	-2.982	7.913	1.756
C						
HETATM	495	C	0	-2.104	8.850	1.185
C						
HETATM	496	H	0	-2.459	9.570	0.676
H						
HETATM	497	C	0	4.596	9.939	-1.906
C						
HETATM	498	Fe	0	0.000	0.000	0.000
Fe						
HETATM	499	S	0	4.334	0.821	0.853
S						
HETATM	500	S	0	-1.105	2.822	3.779
S						
HETATM	501	N	0	0.869	-1.278	1.305
N						
HETATM	502	N	0	1.844	0.825	0.049
N						
HETATM	503	N	0	2.426	1.914	-0.610
N						
HETATM	504	N	0	-0.520	1.137	1.498
N						
HETATM	505	C	0	0.290	-2.340	1.920
C						
HETATM	506	H	0	-0.752	-2.523	1.664
H						
HETATM	507	C	0	0.997	-3.148	2.843
C						
HETATM	508	H	0	0.492	-3.991	3.311
H						
HETATM	509	C	0	2.344	-2.845	3.143
C						
HETATM	510	H	0	2.910	-3.449	3.852
H						
HETATM	511	C	0	2.953	-1.738	2.508
C						
HETATM	512	H	0	3.978	-1.451	2.738
H						
HETATM	513	C	0	2.179	-0.992	1.594
C						
HETATM	514	C	0	2.680	0.168	0.847
C						
HETATM	515	C	0	3.712	2.062	-0.316
C						
HETATM	516	C	0	4.605	3.096	-0.873
C						
HETATM	517	C	0	4.061	4.199	-1.632
C						
HETATM	518	H	0	2.982	4.268	-1.766
H						
HETATM	519	C	0	4.915	5.149	-2.186
C						
HETATM	520	H	0	4.519	5.989	-2.760
H						

HETATM	521	C	0	6.348	5.036	-2.032
C						
HETATM	522	C	0	7.258	5.982	-2.626
C						
HETATM	523	H	0	6.847	6.810	-3.205
H						
HETATM	524	C	0	8.637	5.847	-2.444
C						
HETATM	525	H	0	9.330	6.550	-2.908
H						
HETATM	526	C	0	9.171	4.762	-1.662
C						
HETATM	527	H	0	10.253	4.683	-1.548
H						
HETATM	528	C	0	8.315	3.826	-1.082
C						
HETATM	529	H	0	8.706	2.986	-0.507
H						
HETATM	530	C	0	6.888	3.944	-1.254
C						
HETATM	531	C	0	5.988	2.993	-0.677
C						
HETATM	532	H	0	6.413	2.176	-0.090
H						
HETATM	533	C	0	-0.745	1.826	2.438
C						
HETATM	534	S	0	-4.334	-0.820	-0.854
S						
HETATM	535	S	0	1.104	-2.822	-3.779
S						
HETATM	536	N	0	-0.869	1.279	-1.305
N						
HETATM	537	N	0	-1.844	-0.824	-0.049
N						
HETATM	538	N	0	-2.426	-1.914	0.610
N						
HETATM	539	N	0	0.520	-1.136	-1.498
N						
HETATM	540	C	0	-0.290	2.341	-1.920
C						
HETATM	541	H	0	0.751	2.524	-1.664
H						
HETATM	542	C	0	-0.998	3.148	-2.843
C						
HETATM	543	H	0	-0.492	3.992	-3.311
H						
HETATM	544	C	0	-2.344	2.845	-3.143
C						
HETATM	545	H	0	-2.910	3.449	-3.852
H						
HETATM	546	C	0	-2.953	1.737	-2.508
C						
HETATM	547	H	0	-3.977	1.450	-2.739
H						
HETATM	548	C	0	-2.178	0.992	-1.594
C						

HETATM	549	C	0	-2.680	-0.168	-0.847
C						
HETATM	550	C	0	-3.711	-2.061	0.316
C						
HETATM	551	C	0	-4.605	-3.096	0.873
C						
HETATM	552	C	0	-4.061	-4.198	1.632
C						
HETATM	553	H	0	-2.982	-4.268	1.767
H						
HETATM	554	C	0	-4.916	-5.148	2.185
C						
HETATM	555	H	0	-4.520	-5.988	2.760
H						
HETATM	556	C	0	-6.348	-5.035	2.031
C						
HETATM	557	C	0	-7.258	-5.981	2.626
C						
HETATM	558	H	0	-6.849	-6.809	3.204
H						
HETATM	559	C	0	-8.637	-5.846	2.443
C						
HETATM	560	H	0	-9.331	-6.549	2.906
H						
HETATM	561	C	0	-9.171	-4.761	1.660
C						
HETATM	562	H	0	-10.253	-4.682	1.546
H						
HETATM	563	C	0	-8.315	-3.825	1.081
C						
HETATM	564	H	0	-8.706	-2.984	0.505
H						
HETATM	565	C	0	-6.888	-3.943	1.254
C						
HETATM	566	C	0	-5.988	-2.992	0.676
C						
HETATM	567	H	0	-6.413	-2.175	0.090
H						
HETATM	568	C	0	0.745	-1.826	-2.438
C						
HETATM	569	Fe	0	-3.830	-11.749	-0.472
Fe						
HETATM	570	S	0	0.433	-10.956	0.342
S						
HETATM	571	S	0	-4.959	-9.056	3.254
S						
HETATM	572	N	0	-2.968	-12.964	0.897
N						
HETATM	573	N	0	-1.991	-10.960	-0.435
N						
HETATM	574	N	0	-1.420	-9.898	-1.083
N						
HETATM	575	N	0	-4.355	-10.567	0.978
N						
HETATM	576	C	0	-3.537	-13.942	1.587
C						

HETATM	577	H	0	-4.466	-14.101	1.475
H						
HETATM	578	C	0	-2.824	-14.742	2.470
C						
HETATM	579	H	0	-3.264	-15.448	2.930
H						
HETATM	580	C	0	-1.490	-14.516	2.681
C						
HETATM	581	H	0	-0.993	-15.060	3.281
H						
HETATM	582	C	0	-0.881	-13.479	2.000
C						
HETATM	583	H	0	0.041	-13.287	2.133
H						
HETATM	584	C	0	-1.642	-12.721	1.116
C						
HETATM	585	C	0	-1.158	-11.599	0.348
C						
HETATM	586	C	0	-0.155	-9.772	-0.794
C						
HETATM	587	C	0	0.738	-8.747	-1.352
C						
HETATM	588	C	0	0.213	-7.675	-2.108
C						
HETATM	589	H	0	-0.725	-7.603	-2.231
H						
HETATM	590	C	0	1.030	-6.748	-2.661
C						
HETATM	591	H	0	0.656	-6.030	-3.157
H						
HETATM	592	C	0	2.441	-6.833	-2.509
C						
HETATM	593	C	0	3.329	-5.903	-3.091
C						
HETATM	594	H	0	2.981	-5.180	-3.599
H						
HETATM	595	C	0	4.685	-6.030	-2.932
C						
HETATM	596	H	0	5.266	-5.393	-3.330
H						
HETATM	597	C	0	5.224	-7.096	-2.183
C						
HETATM	598	H	0	6.164	-7.174	-2.077
H						
HETATM	599	C	0	4.394	-8.014	-1.609
C						
HETATM	600	H	0	4.764	-8.730	-1.107
H						
HETATM	601	C	0	2.982	-7.913	-1.756
C						
HETATM	602	C	0	2.104	-8.850	-1.185
C						
HETATM	603	H	0	2.459	-9.570	-0.676
H						
HETATM	604	C	0	-4.596	-9.939	1.906
C						

HETATM	605	S	0	-8.092	-12.541	-1.286
S						
HETATM	606	S	0	-2.700	-14.441	-4.197
S						
HETATM	607	N	0	-4.692	-10.534	-1.840
N						
HETATM	608	N	0	-5.668	-12.537	-0.508
N						
HETATM	609	N	0	-6.239	-13.599	0.140
N						
HETATM	610	N	0	-3.305	-12.931	-1.921
N						
HETATM	611	C	0	-4.123	-9.555	-2.531
C						
HETATM	612	H	0	-3.193	-9.397	-2.419
H						
HETATM	613	C	0	-4.835	-8.755	-3.414
C						
HETATM	614	H	0	-4.395	-8.049	-3.873
H						
HETATM	615	C	0	-6.169	-8.981	-3.625
C						
HETATM	616	H	0	-6.665	-8.437	-4.224
H						
HETATM	617	C	0	-6.778	-10.018	-2.943
C						
HETATM	618	H	0	-7.699	-10.210	-3.076
H						
HETATM	619	C	0	-6.017	-10.776	-2.060
C						
HETATM	620	C	0	-6.501	-11.898	-1.291
C						
HETATM	621	C	0	-7.503	-13.725	-0.150
C						
HETATM	622	C	0	-8.397	-14.750	0.408
C						
HETATM	623	C	0	-7.873	-15.823	1.165
C						
HETATM	624	H	0	-6.933	-15.894	1.288
H						
HETATM	625	C	0	-8.689	-16.749	1.718
C						
HETATM	626	H	0	-8.314	-17.467	2.214
H						
HETATM	627	C	0	-10.100	-16.664	1.566
C						
HETATM	628	C	0	-10.988	-17.594	2.147
C						
HETATM	629	H	0	-10.641	-18.318	2.655
H						
HETATM	630	C	0	-12.344	-17.468	1.988
C						
HETATM	631	H	0	-12.926	-18.105	2.387
H						
HETATM	632	C	0	-12.883	-16.402	1.240
C						

HETATM	633	H	0	-13.824	-16.323	1.134
H						
HETATM	634	C	0	-12.053	-15.484	0.666
C						
HETATM	635	H	0	-12.422	-14.768	0.163
H						
HETATM	636	C	0	-10.641	-15.584	0.813
C						
HETATM	637	C	0	-9.763	-14.647	0.242
C						
HETATM	638	H	0	-10.117	-13.927	-0.267
H						
HETATM	639	C	0	-3.062	-13.559	-2.849
C						
HETATM	640	Fe	0	-3.446	14.503	0.330
Fe						
HETATM	641	S	0	0.817	15.295	1.143
S						
HETATM	642	S	0	-4.575	17.195	4.056
S						
HETATM	643	N	0	-2.584	13.289	1.698
N						
HETATM	644	N	0	-1.607	15.292	0.366
N						
HETATM	645	N	0	-1.036	16.354	-0.283
N						
HETATM	646	N	0	-3.971	15.685	1.779
N						
HETATM	647	C	0	-3.153	12.310	2.389
C						
HETATM	648	H	0	-4.082	12.151	2.276
H						
HETATM	649	C	0	-2.440	11.509	3.271
C						
HETATM	650	H	0	-2.880	10.803	3.732
H						
HETATM	651	C	0	-1.106	11.736	3.482
C						
HETATM	652	H	0	-0.611	11.191	4.082
H						
HETATM	653	C	0	-0.497	12.772	2.801
C						
HETATM	654	H	0	0.424	12.966	2.933
H						
HETATM	655	C	0	-1.258	13.530	1.918
C						
HETATM	656	C	0	-0.775	14.652	1.149
C						
HETATM	657	C	0	0.227	16.479	0.007
C						
HETATM	658	C	0	1.122	17.505	-0.550
C						
HETATM	659	C	0	0.597	18.577	-1.307
C						
HETATM	660	H	0	-0.342	18.648	-1.430
H						

HETATM	661	C	0	1.414	19.503	-1.859
C						
HETATM	662	H	0	1.039	20.222	-2.357
H						
HETATM	663	C	0	2.825	19.419	-1.708
C						
HETATM	664	C	0	3.712	20.348	-2.289
C						
HETATM	665	H	0	3.365	21.072	-2.797
H						
HETATM	666	C	0	5.069	20.222	-2.131
C						
HETATM	667	H	0	5.650	20.859	-2.530
H						
HETATM	668	C	0	5.608	19.156	-1.381
C						
HETATM	669	H	0	6.548	19.078	-1.277
H						
HETATM	670	C	0	4.777	18.238	-0.808
C						
HETATM	671	H	0	5.147	17.522	-0.305
H						
HETATM	672	C	0	3.366	18.339	-0.954
C						
HETATM	673	C	0	2.488	17.401	-0.385
C						
HETATM	674	H	0	2.842	16.682	0.125
H						
HETATM	675	C	0	-4.213	16.313	2.708
C						
HETATM	676	S	0	-7.709	13.711	-0.484
S						
HETATM	677	S	0	-2.316	11.811	-3.397
S						
HETATM	678	N	0	-4.308	15.718	-1.039
N						
HETATM	679	N	0	-5.285	13.714	0.293
N						
HETATM	680	N	0	-5.856	12.652	0.942
N						
HETATM	681	N	0	-2.921	13.321	-1.120
N						
HETATM	682	C	0	-3.739	16.696	-1.730
C						
HETATM	683	H	0	-2.809	16.855	-1.617
H						
HETATM	684	C	0	-4.451	17.497	-2.612
C						
HETATM	685	H	0	-4.011	18.203	-3.073
H						
HETATM	686	C	0	-5.785	17.271	-2.823
C						
HETATM	687	H	0	-6.282	17.815	-3.423
H						
HETATM	688	C	0	-6.395	16.233	-2.142
C						

HETATM	689	H	0	-7.316	16.041	-2.274
H						
HETATM	690	C	0	-5.633	15.476	-1.259
C						
HETATM	691	C	0	-6.117	14.354	-0.490
C						
HETATM	692	C	0	-7.120	12.526	0.652
C						
HETATM	693	C	0	-8.013	11.501	1.209
C						
HETATM	694	C	0	-7.488	10.429	1.966
C						
HETATM	695	H	0	-6.550	10.358	2.089
H						
HETATM	696	C	0	-8.305	9.503	2.519
C						
HETATM	697	H	0	-7.932	8.785	3.016
H						
HETATM	698	C	0	-9.716	9.587	2.367
C						
HETATM	699	C	0	-10.604	8.658	2.948
C						
HETATM	700	H	0	-10.257	7.935	3.456
H						
HETATM	701	C	0	-11.960	8.785	2.790
C						
HETATM	702	H	0	-12.542	8.147	3.189
H						
HETATM	703	C	0	-12.499	9.851	2.040
C						
HETATM	704	H	0	-13.440	9.929	1.936
H						
HETATM	705	C	0	-11.670	10.769	1.467
C						
HETATM	706	H	0	-12.039	11.484	0.964
H						
HETATM	707	C	0	-10.258	10.667	1.613
C						
HETATM	708	C	0	-9.379	11.605	1.044
C						
HETATM	709	H	0	-9.734	12.324	0.534
H						
HETATM	710	C	0	-2.679	12.693	-2.049
C						
HETATM	711	Fe	0	-7.275	2.754	-0.142
Fe						
HETATM	712	S	0	-3.013	3.546	0.672
S						
HETATM	713	S	0	-8.404	5.448	3.584
S						
HETATM	714	N	0	-6.413	1.540	1.226
N						
HETATM	715	N	0	-5.436	3.543	-0.106
N						
HETATM	716	N	0	-4.866	4.606	-0.754
N						

HETATM	717	N	0	-7.801	3.937	1.307
N						
HETATM	718	C	0	-6.982	0.562	1.917
C						
HETATM	719	H	0	-7.913	0.402	1.805
H						
HETATM	720	C	0	-6.271	-0.240	2.800
C						
HETATM	721	H	0	-6.709	-0.946	3.259
H						
HETATM	722	C	0	-4.937	-0.013	3.010
C						
HETATM	723	H	0	-4.440	-0.557	3.611
H						
HETATM	724	C	0	-4.326	1.025	2.329
C						
HETATM	725	H	0	-3.406	1.217	2.462
H						
HETATM	726	C	0	-5.087	1.782	1.447
C						
HETATM	727	C	0	-4.604	2.904	0.677
C						
HETATM	728	C	0	-3.602	4.731	-0.464
C						
HETATM	729	C	0	-2.707	5.757	-1.022
C						
HETATM	730	C	0	-3.232	6.829	-1.779
C						
HETATM	731	H	0	-4.171	6.900	-1.902
H						
HETATM	732	C	0	-2.416	7.755	-2.331
C						
HETATM	733	H	0	-2.790	8.473	-2.828
H						
HETATM	734	C	0	-1.004	7.670	-2.179
C						
HETATM	735	C	0	-0.117	8.599	-2.761
C						
HETATM	736	H	0	-0.464	9.323	-3.269
H						
HETATM	737	C	0	1.239	8.473	-2.602
C						
HETATM	738	H	0	1.821	9.110	-3.001
H						
HETATM	739	C	0	1.778	7.408	-1.854
C						
HETATM	740	H	0	2.719	7.330	-1.748
H						
HETATM	741	C	0	0.948	6.489	-1.280
C						
HETATM	742	H	0	1.318	5.774	-0.777
H						
HETATM	743	C	0	-0.464	6.591	-1.427
C						
HETATM	744	C	0	-1.342	5.652	-0.856
C						

HETATM	745	H	0	-0.988	4.933	-0.346
H						
HETATM	746	C	0	-8.043	4.564	2.235
C						
HETATM	747	S	0	-11.538	1.962	-0.956
S						
HETATM	748	S	0	-6.146	0.062	-3.868
S						
HETATM	749	N	0	-8.137	3.969	-1.511
N						
HETATM	750	N	0	-9.114	1.966	-0.179
N						
HETATM	751	N	0	-9.685	0.903	0.469
N						
HETATM	752	N	0	-6.750	1.572	-1.592
N						
HETATM	753	C	0	-7.568	4.947	-2.201
C						
HETATM	754	H	0	-6.638	5.106	-2.089
H						
HETATM	755	C	0	-8.281	5.748	-3.084
C						
HETATM	756	H	0	-7.841	6.454	-3.544
H						
HETATM	757	C	0	-9.615	5.522	-3.295
C						
HETATM	758	H	0	-10.111	6.066	-3.895
H						
HETATM	759	C	0	-10.224	4.485	-2.614
C						
HETATM	760	H	0	-11.145	4.292	-2.747
H						
HETATM	761	C	0	-9.463	3.727	-1.730
C						
HETATM	762	C	0	-9.946	2.605	-0.962
C						
HETATM	763	C	0	-10.949	0.778	0.180
C						
HETATM	764	C	0	-11.843	-0.247	0.738
C						
HETATM	765	C	0	-11.318	-1.320	1.494
C						
HETATM	766	H	0	-10.379	-1.391	1.617
H						
HETATM	767	C	0	-12.135	-2.246	2.047
C						
HETATM	768	H	0	-11.761	-2.964	2.543
H						
HETATM	769	C	0	-13.545	-2.161	1.895
C						
HETATM	770	C	0	-14.434	-3.091	2.477
C						
HETATM	771	H	0	-14.087	-3.814	2.984
H						
HETATM	772	C	0	-15.790	-2.964	2.318
C						

HETATM	773	H	0	-16.372	-3.601	2.716
H						
HETATM	774	C	0	-16.328	-1.898	1.569
C						
HETATM	775	H	0	-17.269	-1.820	1.463
H						
HETATM	776	C	0	-15.499	-0.980	0.995
C						
HETATM	777	H	0	-15.868	-0.264	0.493
H						
HETATM	778	C	0	-14.087	-1.082	1.142
C						
HETATM	779	C	0	-13.209	-0.144	0.571
C						
HETATM	780	H	0	-13.563	0.576	0.062
H						
HETATM	781	C	0	-6.508	0.945	-2.520
C						
HETATM	782	Fe	0	-11.105	-8.994	-0.614
Fe						
HETATM	783	S	0	-6.842	-8.202	0.200
S						
HETATM	784	S	0	-12.234	-6.301	3.112
S						
HETATM	785	N	0	-10.243	-10.209	0.755
N						
HETATM	786	N	0	-9.267	-8.206	-0.577
N						
HETATM	787	N	0	-8.695	-7.143	-1.225
N						
HETATM	788	N	0	-11.630	-7.812	0.835
N						
HETATM	789	C	0	-10.811	-11.187	1.445
C						
HETATM	790	H	0	-11.742	-11.347	1.332
H						
HETATM	791	C	0	-10.100	-11.988	2.328
C						
HETATM	792	H	0	-10.539	-12.693	2.788
H						
HETATM	793	C	0	-8.766	-11.761	2.539
C						
HETATM	794	H	0	-8.269	-12.306	3.139
H						
HETATM	795	C	0	-8.156	-10.724	1.858
C						
HETATM	796	H	0	-7.235	-10.532	1.991
H						
HETATM	797	C	0	-8.917	-9.967	0.974
C						
HETATM	798	C	0	-8.434	-8.845	0.205
C						
HETATM	799	C	0	-7.431	-7.017	-0.937
C						
HETATM	800	C	0	-6.537	-5.992	-1.494
C						

HETATM	801	C	0	-7.063	-4.920	-2.251
C						
HETATM	802	H	0	-8.001	-4.848	-2.374
H						
HETATM	803	C	0	-6.245	-3.993	-2.803
C						
HETATM	804	H	0	-6.620	-3.276	-3.300
H						
HETATM	805	C	0	-4.835	-4.079	-2.651
C						
HETATM	806	C	0	-3.946	-3.149	-3.233
C						
HETATM	807	H	0	-4.294	-2.426	-3.741
H						
HETATM	808	C	0	-2.590	-3.276	-3.075
C						
HETATM	809	H	0	-2.008	-2.639	-3.472
H						
HETATM	810	C	0	-2.052	-4.341	-2.325
C						
HETATM	811	H	0	-1.110	-4.419	-2.219
H						
HETATM	812	C	0	-2.881	-5.259	-1.751
C						
HETATM	813	H	0	-2.512	-5.975	-1.249
H						
HETATM	814	C	0	-4.293	-5.158	-1.898
C						
HETATM	815	C	0	-5.171	-6.096	-1.328
C						
HETATM	816	H	0	-4.817	-6.816	-0.818
H						
HETATM	817	C	0	-11.872	-7.185	1.764
C						
HETATM	818	S	0	-15.368	-9.786	-1.428
S						
HETATM	819	S	0	-9.975	-11.687	-4.340
S						
HETATM	820	N	0	-11.967	-7.780	-1.982
N						
HETATM	821	N	0	-12.943	-9.782	-0.650
N						
HETATM	822	N	0	-13.514	-10.845	-0.002
N						
HETATM	823	N	0	-10.580	-10.177	-2.063
N						
HETATM	824	C	0	-11.398	-6.801	-2.674
C						
HETATM	825	H	0	-10.468	-6.642	-2.561
H						
HETATM	826	C	0	-12.110	-6.000	-3.556
C						
HETATM	827	H	0	-11.670	-5.295	-4.015
H						
HETATM	828	C	0	-13.444	-6.227	-3.767
C						

HETATM	829	H	0	-13.940	-5.682	-4.367
H						
HETATM	830	C	0	-14.054	-7.264	-3.085
C						
HETATM	831	H	0	-14.974	-7.456	-3.218
H						
HETATM	832	C	0	-13.293	-8.021	-2.203
C						
HETATM	833	C	0	-13.776	-9.144	-1.433
C						
HETATM	834	C	0	-14.778	-10.971	-0.292
C						
HETATM	835	C	0	-15.673	-11.996	0.266
C						
HETATM	836	C	0	-15.147	-13.069	1.023
C						
HETATM	837	H	0	-14.209	-13.140	1.146
H						
HETATM	838	C	0	-15.964	-13.995	1.576
C						
HETATM	839	H	0	-15.590	-14.712	2.072
H						
HETATM	840	C	0	-17.375	-13.910	1.423
C						
HETATM	841	C	0	-18.263	-14.839	2.004
C						
HETATM	842	H	0	-17.916	-15.563	2.513
H						
HETATM	843	C	0	-19.620	-14.713	1.846
C						
HETATM	844	H	0	-20.202	-15.350	2.245
H						
HETATM	845	C	0	-20.158	-13.647	1.098
C						
HETATM	846	H	0	-21.099	-13.569	0.992
H						
HETATM	847	C	0	-19.328	-12.729	0.524
C						
HETATM	848	H	0	-19.698	-12.013	0.021
H						
HETATM	849	C	0	-17.916	-12.830	0.671
C						
HETATM	850	C	0	-17.039	-11.893	0.100
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HETATM	851	H	0	-17.393	-11.173	-0.410
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HETATM	852	C	0	-10.338	-10.804	-2.992
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HETATM	853	Fe	0	-10.721	17.258	0.187
Fe						
HETATM	854	S	0	-6.458	18.049	1.001
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HETATM	855	S	0	-11.851	19.950	3.914
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HETATM	856	N	0	-9.859	16.043	1.555
N						

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HETATM	858	N	0	-8.311	19.109	-0.425
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HETATM	859	N	0	-11.246	18.440	1.637
N						
HETATM	860	C	0	-10.428	15.065	2.247
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HETATM	861	H	0	-11.358	14.906	2.134
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HETATM	862	C	0	-9.716	14.263	3.129
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HETATM	863	H	0	-10.156	13.558	3.589
H						
HETATM	864	C	0	-8.382	14.490	3.340
C						
HETATM	865	H	0	-7.885	13.946	3.940
H						
HETATM	866	C	0	-7.773	15.527	2.659
C						
HETATM	867	H	0	-6.851	15.720	2.791
H						
HETATM	868	C	0	-8.534	16.284	1.776
C						
HETATM	869	C	0	-8.050	17.406	1.007
C						
HETATM	870	C	0	-7.047	19.234	-0.135
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HETATM	871	C	0	-6.153	20.260	-0.692
C						
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HETATM	873	H	0	-7.617	21.403	-1.572
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HETATM	875	H	0	-6.235	22.976	-2.499
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HETATM	876	C	0	-4.451	22.174	-1.850
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HETATM	877	C	0	-3.562	23.102	-2.431
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HETATM	879	C	0	-2.206	22.976	-2.273
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HETATM	880	H	0	-1.624	23.613	-2.672
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HETATM	881	C	0	-1.668	21.910	-1.524
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HETATM	882	H	0	-0.728	21.832	-1.419
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HETATM	883	C	0	-2.497	20.992	-0.951
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HETATM	884	H	0	-2.128	20.276	-0.447
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HETATM	885	C	0	-3.909	21.094	-1.097
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HETATM	886	C	0	-4.787	20.156	-0.527
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HETATM	887	H	0	-4.433	19.437	-0.017
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HETATM	888	C	0	-11.488	19.067	2.565
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HETATM	889	S	0	-14.984	16.466	-0.627
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HETATM	890	S	0	-9.592	14.565	-3.539
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HETATM	891	N	0	-11.583	18.472	-1.181
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HETATM	892	N	0	-12.560	16.469	0.151
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HETATM	893	N	0	-13.131	15.406	0.799
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HETATM	894	N	0	-10.195	16.075	-1.263
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HETATM	895	C	0	-11.015	19.450	-1.872
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HETATM	896	H	0	-10.084	19.610	-1.759
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HETATM	897	C	0	-11.726	20.252	-2.755
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HETATM	898	H	0	-11.287	20.958	-3.215
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HETATM	899	C	0	-13.060	20.025	-2.965
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HETATM	900	H	0	-13.556	20.570	-3.565
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HETATM	901	C	0	-13.670	18.988	-2.285
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HETATM	902	H	0	-14.591	18.795	-2.417
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HETATM	903	C	0	-12.909	18.231	-1.401
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HETATM	904	C	0	-13.392	17.109	-0.632
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HETATM	905	C	0	-14.395	15.281	0.510
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HETATM	906	C	0	-15.289	14.255	1.067
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HETATM	907	C	0	-14.764	13.183	1.824
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HETATM	908	H	0	-13.825	13.112	1.947
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HETATM	909	C	0	-15.580	12.257	2.376
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HETATM	910	H	0	-15.206	11.539	2.873
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HETATM	911	C	0	-16.992	12.342	2.225
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HETATM	912	C	0	-17.879	11.413	2.806
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HETATM	913	H	0	-17.532	10.689	3.314
H						
HETATM	914	C	0	-19.236	11.539	2.648
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HETATM	915	H	0	-19.817	10.902	3.046
H						
HETATM	916	C	0	-19.774	12.605	1.898
C						
HETATM	917	H	0	-20.715	12.683	1.793
H						
HETATM	918	C	0	-18.944	13.523	1.325
C						
HETATM	919	H	0	-19.314	14.238	0.822
H						
HETATM	920	C	0	-17.532	13.421	1.471
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HETATM	921	C	0	-16.655	14.359	0.902
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HETATM	922	H	0	-17.009	15.078	0.392
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HETATM	923	C	0	-9.954	15.448	-2.191
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HETATM	924	Fe	0	-14.551	5.509	-0.284
Fe						
HETATM	925	S	0	-10.288	6.301	0.530
S						
HETATM	926	S	0	-15.680	8.202	3.441
S						
HETATM	927	N	0	-13.689	4.294	1.084
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HETATM	928	N	0	-12.712	6.297	-0.248
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HETATM	929	N	0	-12.141	7.360	-0.896
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HETATM	930	N	0	-15.076	6.691	1.165
N						
HETATM	931	C	0	-14.258	3.316	1.775
C						
HETATM	932	H	0	-15.187	3.157	1.663
H						
HETATM	933	C	0	-13.545	2.514	2.658
C						
HETATM	934	H	0	-13.985	1.809	3.117
H						
HETATM	935	C	0	-12.211	2.741	2.868
C						
HETATM	936	H	0	-11.714	2.198	3.468
H						
HETATM	937	C	0	-11.602	3.779	2.187
C						
HETATM	938	H	0	-10.681	3.971	2.320
H						
HETATM	939	C	0	-12.363	4.536	1.304
C						
HETATM	940	C	0	-11.879	5.659	0.535
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HETATM	941	C	0	-10.876	7.486	-0.606
C						
HETATM	942	C	0	-9.983	8.511	-1.164
C						
HETATM	943	C	0	-10.508	9.583	-1.922
C						
HETATM	944	H	0	-11.446	9.655	-2.044
H						
HETATM	945	C	0	-9.691	10.510	-2.473
C						
HETATM	946	H	0	-10.065	11.227	-2.970
H						
HETATM	947	C	0	-8.280	10.425	-2.322
C						
HETATM	948	C	0	-7.393	11.354	-2.903
C						
HETATM	949	H	0	-7.740	12.077	-3.412
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HETATM	950	C	0	-6.036	11.227	-2.745
C						
HETATM	951	H	0	-5.455	11.865	-3.143
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HETATM	952	C	0	-5.497	10.162	-1.996
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HETATM	953	H	0	-4.557	10.084	-1.890
H						
HETATM	954	C	0	-6.327	9.243	-1.422
C						
HETATM	955	H	0	-5.957	8.528	-0.920
H						
HETATM	956	C	0	-7.739	9.345	-1.569
C						
HETATM	957	C	0	-8.617	8.407	-0.998
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HETATM	958	H	0	-8.262	7.688	-0.489
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HETATM	959	C	0	-15.317	7.319	2.093
C						
HETATM	960	S	0	-18.813	4.717	-1.098
S						
HETATM	961	S	0	-13.421	2.816	-4.010
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HETATM	962	N	0	-15.413	6.723	-1.653
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HETATM	963	N	0	-16.390	4.720	-0.321
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HETATM	964	N	0	-16.961	3.658	0.327
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HETATM	965	N	0	-14.026	4.326	-1.734
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HETATM	966	C	0	-14.844	7.701	-2.344
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HETATM	967	H	0	-13.914	7.861	-2.231
H						
HETATM	968	C	0	-15.556	8.503	-3.226
C						

HETATM	969	H	0	-15.116	9.209	-3.686
H						
HETATM	970	C	0	-16.890	8.276	-3.438
C						
HETATM	971	H	0	-17.386	8.821	-4.037
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HETATM	972	C	0	-17.499	7.239	-2.756
C						
HETATM	973	H	0	-18.420	7.046	-2.889
H						
HETATM	974	C	0	-16.738	6.482	-1.872
C						
HETATM	975	C	0	-17.222	5.360	-1.104
C						
HETATM	976	C	0	-18.224	3.533	0.038
C						
HETATM	977	C	0	-19.118	2.507	0.596
C						
HETATM	978	C	0	-18.594	1.435	1.352
C						
HETATM	979	H	0	-17.654	1.364	1.475
H						
HETATM	980	C	0	-19.410	0.509	1.905
C						
HETATM	981	H	0	-19.036	-0.210	2.401
H						
HETATM	982	C	0	-20.821	0.594	1.753
C						
HETATM	983	C	0	-21.709	-0.336	2.335
C						
HETATM	984	H	0	-21.362	-1.060	2.842
H						
HETATM	985	C	0	-23.065	-0.210	2.176
C						
HETATM	986	H	0	-23.647	-0.847	2.574
H						
HETATM	987	C	0	-23.604	0.856	1.427
C						
HETATM	988	H	0	-24.545	0.934	1.321
H						
HETATM	989	C	0	-22.774	1.774	0.853
C						
HETATM	990	H	0	-23.143	2.490	0.350
H						
HETATM	991	C	0	-21.363	1.673	1.000
C						
HETATM	992	C	0	-20.484	2.611	0.429
C						
HETATM	993	H	0	-20.838	3.331	-0.080
H						
HETATM	994	C	0	-13.783	3.699	-2.662
C						
HETATM	995	Fe	0	-18.380	-6.240	-0.757
Fe						
HETATM	996	S	0	-14.117	-5.447	0.057
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HETATM	997	S	0	-19.509	-3.547	2.970
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HETATM	998	N	0	-17.518	-7.455	0.613
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HETATM	999	N	0	-16.541	-5.451	-0.719
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HETATM	1000	N	0	-15.970	-4.389	-1.368
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HETATM	1001	N	0	-18.905	-5.058	0.693
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HETATM	1002	C	0	-18.087	-8.433	1.303
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HETATM	1003	H	0	-19.017	-8.592	1.190
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HETATM	1004	C	0	-17.374	-9.233	2.185
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HETATM	1005	H	0	-17.814	-9.939	2.646
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HETATM	1006	C	0	-16.040	-9.007	2.397
C						
HETATM	1007	H	0	-15.545	-9.551	2.997
H						
HETATM	1008	C	0	-15.431	-7.970	1.715
C						
HETATM	1009	H	0	-14.511	-7.778	1.848
H						
HETATM	1010	C	0	-16.192	-7.212	0.832
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HETATM	1011	C	0	-15.709	-6.090	0.063
C						
HETATM	1012	C	0	-14.707	-4.263	-1.079
C						
HETATM	1013	C	0	-13.813	-3.238	-1.636
C						
HETATM	1014	C	0	-14.337	-2.166	-2.393
C						
HETATM	1015	H	0	-15.277	-2.094	-2.516
H						
HETATM	1016	C	0	-13.520	-1.239	-2.945
C						
HETATM	1017	H	0	-13.895	-0.521	-3.442
H						
HETATM	1018	C	0	-12.109	-1.324	-2.793
C						
HETATM	1019	C	0	-11.222	-0.394	-3.375
C						
HETATM	1020	H	0	-11.569	0.329	-3.883
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HETATM	1021	C	0	-9.866	-0.521	-3.217
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HETATM	1022	H	0	-9.284	0.116	-3.615
H						
HETATM	1023	C	0	-9.327	-1.587	-2.467
C						
HETATM	1024	H	0	-8.386	-1.665	-2.361
H						

HETATM	1025	C	0	-10.157	-2.505	-1.893
C						
HETATM	1026	H	0	-9.788	-3.220	-1.391
H						
HETATM	1027	C	0	-11.568	-2.404	-2.040
C						
HETATM	1028	C	0	-12.446	-3.341	-1.470
C						
HETATM	1029	H	0	-12.093	-4.061	-0.960
H						
HETATM	1030	C	0	-19.148	-4.430	1.622
C						
HETATM	1031	S	0	-22.643	-7.032	-1.570
S						
HETATM	1032	S	0	-17.251	-8.933	-4.482
S						
HETATM	1033	N	0	-19.242	-5.025	-2.125
N						
HETATM	1034	N	0	-20.219	-7.028	-0.793
N						
HETATM	1035	N	0	-20.790	-8.090	-0.144
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HETATM	1036	N	0	-17.855	-7.423	-2.205
N						
HETATM	1037	C	0	-18.673	-4.046	-2.816
C						
HETATM	1038	H	0	-17.743	-3.888	-2.703
H						
HETATM	1039	C	0	-19.386	-3.246	-3.698
C						
HETATM	1040	H	0	-18.946	-2.540	-4.158
H						
HETATM	1041	C	0	-20.720	-3.472	-3.909
C						
HETATM	1042	H	0	-21.216	-2.928	-4.509
H						
HETATM	1043	C	0	-21.329	-4.509	-3.227
C						
HETATM	1044	H	0	-22.250	-4.701	-3.360
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HETATM	1045	C	0	-20.568	-5.267	-2.345
C						
HETATM	1046	C	0	-21.051	-6.389	-1.575
C						
HETATM	1047	C	0	-22.054	-8.216	-0.434
C						
HETATM	1048	C	0	-22.947	-9.241	0.123
C						
HETATM	1049	C	0	-22.423	-10.314	0.881
C						
HETATM	1050	H	0	-21.484	-10.385	1.004
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HETATM	1051	C	0	-23.240	-11.240	1.433
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HETATM	1052	H	0	-22.866	-11.958	1.930
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HETATM	1053	C	0	-24.651	-11.155	1.281
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HETATM	1054	C	0	-25.538	-12.085	1.862
C						
HETATM	1055	H	0	-25.191	-12.809	2.371
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HETATM	1056	C	0	-26.895	-11.959	1.704
C						
HETATM	1057	H	0	-27.476	-12.596	2.103
H						
HETATM	1058	C	0	-27.433	-10.893	0.955
C						
HETATM	1059	H	0	-28.374	-10.815	0.850
H						
HETATM	1060	C	0	-26.604	-9.974	0.381
C						
HETATM	1061	H	0	-26.973	-9.259	-0.121
H						
HETATM	1062	C	0	-25.192	-10.075	0.528
C						
HETATM	1063	C	0	-24.314	-9.138	-0.042
C						
HETATM	1064	H	0	-24.668	-8.418	-0.552
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HETATM	1065	C	0	-17.614	-8.050	-3.134
C						

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HETATM	171	C	0	19.774	-12.605	-1.898
C						
HETATM	172	H	0	20.715	-12.683	-1.793
H						
HETATM	173	C	0	18.944	-13.523	-1.325
C						
HETATM	174	H	0	19.314	-14.238	-0.822
H						
HETATM	175	C	0	17.532	-13.421	-1.471
C						
HETATM	176	C	0	16.655	-14.360	-0.902
C						
HETATM	177	H	0	17.009	-15.078	-0.392
H						
HETATM	178	C	0	9.954	-15.448	2.191
C						
HETATM	179	S	0	6.458	-18.049	-1.001
S						
HETATM	180	S	0	11.851	-19.950	-3.914
S						
HETATM	181	N	0	9.859	-16.043	-1.555
N						
HETATM	182	N	0	8.882	-18.046	-0.223
N						
HETATM	183	N	0	8.311	-19.109	0.425
N						
HETATM	184	N	0	11.246	-18.440	-1.637
N						
HETATM	185	C	0	10.428	-15.065	-2.247
C						
HETATM	186	H	0	11.358	-14.906	-2.134
H						
HETATM	187	C	0	9.716	-14.263	-3.129
C						
HETATM	188	H	0	10.156	-13.558	-3.589
H						
HETATM	189	C	0	8.382	-14.490	-3.340
C						
HETATM	190	H	0	7.885	-13.946	-3.940
H						

HETATM	191	C	0	7.773	-15.527	-2.659
C						
HETATM	192	H	0	6.851	-15.720	-2.791
H						
HETATM	193	C	0	8.534	-16.284	-1.776
C						
HETATM	194	C	0	8.050	-17.407	-1.007
C						
HETATM	195	C	0	7.047	-19.234	0.135
C						
HETATM	196	C	0	6.153	-20.260	0.692
C						
HETATM	197	C	0	6.679	-21.332	1.449
C						
HETATM	198	H	0	7.617	-21.403	1.572
H						
HETATM	199	C	0	5.862	-22.258	2.002
C						
HETATM	200	H	0	6.235	-22.976	2.499
H						
HETATM	201	C	0	4.451	-22.174	1.850
C						
HETATM	202	C	0	3.562	-23.102	2.431
C						
HETATM	203	H	0	3.910	-23.826	2.939
H						
HETATM	204	C	0	2.206	-22.976	2.273
C						
HETATM	205	H	0	1.624	-23.613	2.672
H						
HETATM	206	C	0	1.668	-21.910	1.524
C						
HETATM	207	H	0	0.728	-21.832	1.419
H						
HETATM	208	C	0	2.497	-20.992	0.951
C						
HETATM	209	H	0	2.128	-20.276	0.447
H						
HETATM	210	C	0	3.909	-21.094	1.097
C						
HETATM	211	C	0	4.787	-20.156	0.527
C						
HETATM	212	H	0	4.433	-19.437	0.017
H						
HETATM	213	C	0	11.488	-19.067	-2.565
C						
HETATM	214	Fe	0	11.105	8.994	0.614
Fe						
HETATM	215	S	0	15.368	9.786	1.428
S						
HETATM	216	S	0	9.975	11.687	4.340
S						
HETATM	217	N	0	11.967	7.780	1.982
N						
HETATM	218	N	0	12.943	9.782	0.650
N						

HETATM	219	N	0	13.514	10.845	0.002
N						
HETATM	220	N	0	10.580	10.177	2.063
N						
HETATM	221	C	0	11.398	6.801	2.674
C						
HETATM	222	H	0	10.468	6.642	2.561
H						
HETATM	223	C	0	12.110	6.000	3.556
C						
HETATM	224	H	0	11.670	5.295	4.015
H						
HETATM	225	C	0	13.444	6.227	3.767
C						
HETATM	226	H	0	13.940	5.682	4.367
H						
HETATM	227	C	0	14.054	7.264	3.085
C						
HETATM	228	H	0	14.974	7.456	3.218
H						
HETATM	229	C	0	13.293	8.021	2.203
C						
HETATM	230	C	0	13.776	9.144	1.433
C						
HETATM	231	C	0	14.778	10.970	0.292
C						
HETATM	232	C	0	15.673	11.996	-0.266
C						
HETATM	233	C	0	15.147	13.069	-1.023
C						
HETATM	234	H	0	14.209	13.140	-1.146
H						
HETATM	235	C	0	15.964	13.995	-1.576
C						
HETATM	236	H	0	15.590	14.712	-2.072
H						
HETATM	237	C	0	17.375	13.910	-1.423
C						
HETATM	238	C	0	18.263	14.839	-2.004
C						
HETATM	239	H	0	17.916	15.563	-2.513
H						
HETATM	240	C	0	19.620	14.713	-1.846
C						
HETATM	241	H	0	20.202	15.350	-2.245
H						
HETATM	242	C	0	20.158	13.647	-1.098
C						
HETATM	243	H	0	21.099	13.569	-0.992
H						
HETATM	244	C	0	19.328	12.729	-0.524
C						
HETATM	245	H	0	19.698	12.013	-0.021
H						
HETATM	246	C	0	17.916	12.830	-0.671
C						

HETATM	247	C	0	17.039	11.892	-0.100
C						
HETATM	248	H	0	17.393	11.173	0.410
H						
HETATM	249	C	0	10.338	10.804	2.992
C						
HETATM	250	S	0	6.842	8.202	-0.200
S						
HETATM	251	S	0	12.234	6.301	-3.112
S						
HETATM	252	N	0	10.243	10.209	-0.755
N						
HETATM	253	N	0	9.267	8.206	0.577
N						
HETATM	254	N	0	8.695	7.143	1.225
N						
HETATM	255	N	0	11.630	7.812	-0.835
N						
HETATM	256	C	0	10.811	11.187	-1.445
C						
HETATM	257	H	0	11.742	11.346	-1.332
H						
HETATM	258	C	0	10.100	11.988	-2.328
C						
HETATM	259	H	0	10.539	12.693	-2.788
H						
HETATM	260	C	0	8.766	11.761	-2.539
C						
HETATM	261	H	0	8.269	12.306	-3.139
H						
HETATM	262	C	0	8.156	10.724	-1.858
C						
HETATM	263	H	0	7.235	10.532	-1.991
H						
HETATM	264	C	0	8.917	9.967	-0.974
C						
HETATM	265	C	0	8.434	8.845	-0.205
C						
HETATM	266	C	0	7.431	7.017	0.937
C						
HETATM	267	C	0	6.537	5.992	1.494
C						
HETATM	268	C	0	7.063	4.920	2.251
C						
HETATM	269	H	0	8.001	4.848	2.374
H						
HETATM	270	C	0	6.245	3.993	2.803
C						
HETATM	271	H	0	6.620	3.276	3.300
H						
HETATM	272	C	0	4.835	4.079	2.651
C						
HETATM	273	C	0	3.946	3.149	3.233
C						
HETATM	274	H	0	4.294	2.426	3.741
H						

HETATM	275	C	0	2.590	3.276	3.075
C						
HETATM	276	H	0	2.008	2.639	3.473
H						
HETATM	277	C	0	2.052	4.341	2.325
C						
HETATM	278	H	0	1.110	4.419	2.219
H						
HETATM	279	C	0	2.881	5.259	1.751
C						
HETATM	280	H	0	2.512	5.975	1.249
H						
HETATM	281	C	0	4.293	5.158	1.898
C						
HETATM	282	C	0	5.171	6.096	1.328
C						
HETATM	283	H	0	4.817	6.815	0.818
H						
HETATM	284	C	0	11.872	7.185	-1.764
C						
HETATM	285	Fe	0	7.275	-2.754	0.142
Fe						
HETATM	286	S	0	11.538	-1.962	0.956
S						
HETATM	287	S	0	6.146	-0.062	3.868
S						
HETATM	288	N	0	8.137	-3.969	1.511
N						
HETATM	289	N	0	9.114	-1.966	0.179
N						
HETATM	290	N	0	9.685	-0.903	-0.469
N						
HETATM	291	N	0	6.750	-1.572	1.592
N						
HETATM	292	C	0	7.568	-4.947	2.201
C						
HETATM	293	H	0	6.638	-5.106	2.089
H						
HETATM	294	C	0	8.281	-5.748	3.084
C						
HETATM	295	H	0	7.841	-6.454	3.544
H						
HETATM	296	C	0	9.615	-5.522	3.295
C						
HETATM	297	H	0	10.111	-6.066	3.895
H						
HETATM	298	C	0	10.224	-4.485	2.614
C						
HETATM	299	H	0	11.145	-4.292	2.747
H						
HETATM	300	C	0	9.463	-3.727	1.730
C						
HETATM	301	C	0	9.946	-2.605	0.962
C						
HETATM	302	C	0	10.949	-0.778	-0.180
C						

HETATM	303	C	0	11.843	0.247	-0.738
C						
HETATM	304	C	0	11.318	1.320	-1.494
C						
HETATM	305	H	0	10.379	1.391	-1.617
H						
HETATM	306	C	0	12.135	2.246	-2.047
C						
HETATM	307	H	0	11.761	2.964	-2.543
H						
HETATM	308	C	0	13.545	2.161	-1.895
C						
HETATM	309	C	0	14.434	3.090	-2.477
C						
HETATM	310	H	0	14.087	3.814	-2.984
H						
HETATM	311	C	0	15.790	2.964	-2.318
C						
HETATM	312	H	0	16.372	3.601	-2.716
H						
HETATM	313	C	0	16.328	1.898	-1.569
C						
HETATM	314	H	0	17.269	1.820	-1.463
H						
HETATM	315	C	0	15.499	0.980	-0.995
C						
HETATM	316	H	0	15.868	0.264	-0.493
H						
HETATM	317	C	0	14.087	1.082	-1.142
C						
HETATM	318	C	0	13.209	0.144	-0.571
C						
HETATM	319	H	0	13.563	-0.576	-0.062
H						
HETATM	320	C	0	6.508	-0.945	2.520
C						
HETATM	321	S	0	3.013	-3.546	-0.672
S						
HETATM	322	S	0	8.404	-5.448	-3.583
S						
HETATM	323	N	0	6.413	-1.540	-1.226
N						
HETATM	324	N	0	5.436	-3.543	0.106
N						
HETATM	325	N	0	4.866	-4.606	0.754
N						
HETATM	326	N	0	7.801	-3.937	-1.307
N						
HETATM	327	C	0	6.982	-0.562	-1.917
C						
HETATM	328	H	0	7.913	-0.402	-1.805
H						
HETATM	329	C	0	6.271	0.240	-2.800
C						
HETATM	330	H	0	6.709	0.946	-3.259
H						

HETATM	331	C	0	4.937	0.013	-3.010
C						
HETATM	332	H	0	4.440	0.557	-3.611
H						
HETATM	333	C	0	4.326	-1.025	-2.329
C						
HETATM	334	H	0	3.406	-1.217	-2.462
H						
HETATM	335	C	0	5.087	-1.782	-1.447
C						
HETATM	336	C	0	4.604	-2.904	-0.677
C						
HETATM	337	C	0	3.602	-4.731	0.464
C						
HETATM	338	C	0	2.708	-5.757	1.022
C						
HETATM	339	C	0	3.232	-6.829	1.779
C						
HETATM	340	H	0	4.171	-6.901	1.902
H						
HETATM	341	C	0	2.416	-7.755	2.331
C						
HETATM	342	H	0	2.790	-8.473	2.828
H						
HETATM	343	C	0	1.004	-7.670	2.179
C						
HETATM	344	C	0	0.117	-8.599	2.761
C						
HETATM	345	H	0	0.464	-9.323	3.269
H						
HETATM	346	C	0	-1.239	-8.473	2.602
C						
HETATM	347	H	0	-1.821	-9.110	3.001
H						
HETATM	348	C	0	-1.778	-7.408	1.854
C						
HETATM	349	H	0	-2.719	-7.330	1.748
H						
HETATM	350	C	0	-0.948	-6.489	1.280
C						
HETATM	351	H	0	-1.318	-5.774	0.777
H						
HETATM	352	C	0	0.464	-6.591	1.427
C						
HETATM	353	C	0	1.342	-5.652	0.856
C						
HETATM	354	H	0	0.988	-4.933	0.346
H						
HETATM	355	C	0	8.043	-4.564	-2.235
C						
HETATM	356	Fe	0	3.446	-14.503	-0.329
Fe						
HETATM	357	S	0	7.709	-13.711	0.484
S						
HETATM	358	S	0	2.316	-11.811	3.397
S						

HETATM	359	N	0	4.308	-15.718	1.039
N						
HETATM	360	N	0	5.285	-13.714	-0.293
N						
HETATM	361	N	0	5.856	-12.652	-0.942
N						
HETATM	362	N	0	2.921	-13.321	1.120
N						
HETATM	363	C	0	3.739	-16.696	1.730
C						
HETATM	364	H	0	2.809	-16.855	1.617
H						
HETATM	365	C	0	4.451	-17.497	2.612
C						
HETATM	366	H	0	4.011	-18.203	3.073
H						
HETATM	367	C	0	5.785	-17.271	2.823
C						
HETATM	368	H	0	6.282	-17.815	3.423
H						
HETATM	369	C	0	6.395	-16.233	2.142
C						
HETATM	370	H	0	7.316	-16.041	2.274
H						
HETATM	371	C	0	5.633	-15.476	1.259
C						
HETATM	372	C	0	6.117	-14.354	0.490
C						
HETATM	373	C	0	7.120	-12.526	-0.652
C						
HETATM	374	C	0	8.013	-11.501	-1.209
C						
HETATM	375	C	0	7.489	-10.429	-1.966
C						
HETATM	376	H	0	6.550	-10.358	-2.089
H						
HETATM	377	C	0	8.305	-9.503	-2.518
C						
HETATM	378	H	0	7.932	-8.785	-3.016
H						
HETATM	379	C	0	9.716	-9.587	-2.367
C						
HETATM	380	C	0	10.604	-8.658	-2.948
C						
HETATM	381	H	0	10.257	-7.935	-3.456
H						
HETATM	382	C	0	11.960	-8.785	-2.790
C						
HETATM	383	H	0	12.542	-8.147	-3.189
H						
HETATM	384	C	0	12.499	-9.851	-2.040
C						
HETATM	385	H	0	13.440	-9.929	-1.936
H						
HETATM	386	C	0	11.670	-10.769	-1.467
C						

HETATM	387	H	0	12.039	-11.484	-0.964
H						
HETATM	388	C	0	10.258	-10.667	-1.613
C						
HETATM	389	C	0	9.379	-11.605	-1.044
C						
HETATM	390	H	0	9.734	-12.324	-0.534
H						
HETATM	391	C	0	2.679	-12.694	2.049
C						
HETATM	392	S	0	-0.817	-15.295	-1.143
S						
HETATM	393	S	0	4.575	-17.195	-4.056
S						
HETATM	394	N	0	2.584	-13.289	-1.698
N						
HETATM	395	N	0	1.607	-15.292	-0.366
N						
HETATM	396	N	0	1.036	-16.355	0.283
N						
HETATM	397	N	0	3.971	-15.685	-1.779
N						
HETATM	398	C	0	3.153	-12.311	-2.389
C						
HETATM	399	H	0	4.082	-12.151	-2.276
H						
HETATM	400	C	0	2.440	-11.509	-3.271
C						
HETATM	401	H	0	2.880	-10.803	-3.732
H						
HETATM	402	C	0	1.106	-11.736	-3.482
C						
HETATM	403	H	0	0.611	-11.191	-4.082
H						
HETATM	404	C	0	0.497	-12.772	-2.801
C						
HETATM	405	H	0	-0.424	-12.966	-2.933
H						
HETATM	406	C	0	1.258	-13.530	-1.918
C						
HETATM	407	C	0	0.775	-14.652	-1.149
C						
HETATM	408	C	0	-0.227	-16.479	-0.007
C						
HETATM	409	C	0	-1.122	-17.506	0.550
C						
HETATM	410	C	0	-0.597	-18.577	1.307
C						
HETATM	411	H	0	0.342	-18.648	1.430
H						
HETATM	412	C	0	-1.414	-19.503	1.860
C						
HETATM	413	H	0	-1.039	-20.222	2.357
H						
HETATM	414	C	0	-2.825	-19.419	1.708
C						

HETATM	415	C	0	-3.712	-20.348	2.289
C						
HETATM	416	H	0	-3.365	-21.072	2.797
H						
HETATM	417	C	0	-5.069	-20.222	2.131
C						
HETATM	418	H	0	-5.650	-20.859	2.530
H						
HETATM	419	C	0	-5.608	-19.156	1.381
C						
HETATM	420	H	0	-6.548	-19.078	1.277
H						
HETATM	421	C	0	-4.777	-18.238	0.808
C						
HETATM	422	H	0	-5.147	-17.522	0.305
H						
HETATM	423	C	0	-3.366	-18.339	0.954
C						
HETATM	424	C	0	-2.488	-17.401	0.385
C						
HETATM	425	H	0	-2.842	-16.682	-0.125
H						
HETATM	426	C	0	4.213	-16.313	-2.708
C						
HETATM	427	Fe	0	3.830	11.749	0.472
Fe						
HETATM	428	S	0	8.092	12.541	1.286
S						
HETATM	429	S	0	2.700	14.441	4.197
S						
HETATM	430	N	0	4.692	10.534	1.840
N						
HETATM	431	N	0	5.668	12.537	0.508
N						
HETATM	432	N	0	6.239	13.599	-0.140
N						
HETATM	433	N	0	3.305	12.931	1.921
N						
HETATM	434	C	0	4.123	9.555	2.531
C						
HETATM	435	H	0	3.193	9.397	2.419
H						
HETATM	436	C	0	4.835	8.755	3.414
C						
HETATM	437	H	0	4.395	8.049	3.873
H						
HETATM	438	C	0	6.169	8.981	3.625
C						
HETATM	439	H	0	6.665	8.437	4.224
H						
HETATM	440	C	0	6.778	10.018	2.943
C						
HETATM	441	H	0	7.699	10.210	3.076
H						
HETATM	442	C	0	6.017	10.776	2.060
C						

HETATM	443	C	0	6.501	11.898	1.291
C						
HETATM	444	C	0	7.503	13.725	0.150
C						
HETATM	445	C	0	8.397	14.750	-0.408
C						
HETATM	446	C	0	7.873	15.823	-1.165
C						
HETATM	447	H	0	6.933	15.894	-1.288
H						
HETATM	448	C	0	8.689	16.749	-1.718
C						
HETATM	449	H	0	8.314	17.467	-2.214
H						
HETATM	450	C	0	10.100	16.664	-1.566
C						
HETATM	451	C	0	10.988	17.594	-2.147
C						
HETATM	452	H	0	10.641	18.318	-2.655
H						
HETATM	453	C	0	12.344	17.467	-1.988
C						
HETATM	454	H	0	12.926	18.105	-2.387
H						
HETATM	455	C	0	12.883	16.401	-1.240
C						
HETATM	456	H	0	13.824	16.323	-1.134
H						
HETATM	457	C	0	12.053	15.484	-0.666
C						
HETATM	458	H	0	12.422	14.768	-0.163
H						
HETATM	459	C	0	10.641	15.584	-0.813
C						
HETATM	460	C	0	9.763	14.647	-0.242
C						
HETATM	461	H	0	10.117	13.927	0.267
H						
HETATM	462	C	0	3.062	13.559	2.849
C						
HETATM	463	S	0	-0.433	10.956	-0.342
S						
HETATM	464	S	0	4.959	9.056	-3.254
S						
HETATM	465	N	0	2.968	12.964	-0.897
N						
HETATM	466	N	0	1.991	10.960	0.435
N						
HETATM	467	N	0	1.420	9.898	1.083
N						
HETATM	468	N	0	4.355	10.567	-0.978
N						
HETATM	469	C	0	3.537	13.942	-1.587
C						
HETATM	470	H	0	4.466	14.101	-1.475
H						

HETATM	471	C	0	2.824	14.742	-2.470
C						
HETATM	472	H	0	3.264	15.448	-2.930
H						
HETATM	473	C	0	1.490	14.516	-2.681
C						
HETATM	474	H	0	0.993	15.060	-3.281
H						
HETATM	475	C	0	0.881	13.479	-2.000
C						
HETATM	476	H	0	-0.041	13.287	-2.133
H						
HETATM	477	C	0	1.642	12.721	-1.116
C						
HETATM	478	C	0	1.158	11.599	-0.348
C						
HETATM	479	C	0	0.155	9.772	0.794
C						
HETATM	480	C	0	-0.738	8.747	1.352
C						
HETATM	481	C	0	-0.213	7.675	2.109
C						
HETATM	482	H	0	0.725	7.603	2.231
H						
HETATM	483	C	0	-1.030	6.748	2.661
C						
HETATM	484	H	0	-0.656	6.030	3.157
H						
HETATM	485	C	0	-2.441	6.833	2.509
C						
HETATM	486	C	0	-3.329	5.903	3.091
C						
HETATM	487	H	0	-2.981	5.180	3.599
H						
HETATM	488	C	0	-4.685	6.030	2.932
C						
HETATM	489	H	0	-5.266	5.393	3.330
H						
HETATM	490	C	0	-5.224	7.096	2.183
C						
HETATM	491	H	0	-6.164	7.174	2.077
H						
HETATM	492	C	0	-4.394	8.014	1.609
C						
HETATM	493	H	0	-4.764	8.730	1.107
H						
HETATM	494	C	0	-2.982	7.913	1.756
C						
HETATM	495	C	0	-2.104	8.850	1.185
C						
HETATM	496	H	0	-2.459	9.570	0.676
H						
HETATM	497	C	0	4.596	9.939	-1.906
C						
HETATM	498	Fe	0	0.000	0.000	0.000
Fe						

HETATM	499	S	0	4.334	0.821	0.853
S						
HETATM	500	S	0	-1.105	2.822	3.779
S						
HETATM	501	N	0	0.869	-1.278	1.305
N						
HETATM	502	N	0	1.844	0.825	0.049
N						
HETATM	503	N	0	2.426	1.914	-0.610
N						
HETATM	504	N	0	-0.520	1.137	1.498
N						
HETATM	505	C	0	0.290	-2.340	1.920
C						
HETATM	506	H	0	-0.752	-2.523	1.664
H						
HETATM	507	C	0	0.997	-3.148	2.843
C						
HETATM	508	H	0	0.492	-3.991	3.311
H						
HETATM	509	C	0	2.344	-2.845	3.143
C						
HETATM	510	H	0	2.910	-3.449	3.852
H						
HETATM	511	C	0	2.953	-1.738	2.508
C						
HETATM	512	H	0	3.978	-1.451	2.738
H						
HETATM	513	C	0	2.179	-0.992	1.594
C						
HETATM	514	C	0	2.680	0.168	0.847
C						
HETATM	515	C	0	3.712	2.062	-0.316
C						
HETATM	516	C	0	4.605	3.096	-0.873
C						
HETATM	517	C	0	4.061	4.199	-1.632
C						
HETATM	518	H	0	2.982	4.268	-1.766
H						
HETATM	519	C	0	4.915	5.149	-2.186
C						
HETATM	520	H	0	4.519	5.989	-2.760
H						
HETATM	521	C	0	6.348	5.036	-2.032
C						
HETATM	522	C	0	7.258	5.982	-2.626
C						
HETATM	523	H	0	6.847	6.810	-3.205
H						
HETATM	524	C	0	8.637	5.847	-2.444
C						
HETATM	525	H	0	9.330	6.550	-2.908
H						
HETATM	526	C	0	9.171	4.762	-1.662
C						

HETATM	527	H	0	10.253	4.683	-1.548
H						
HETATM	528	C	0	8.315	3.826	-1.082
C						
HETATM	529	H	0	8.706	2.986	-0.507
H						
HETATM	530	C	0	6.888	3.944	-1.254
C						
HETATM	531	C	0	5.988	2.993	-0.677
C						
HETATM	532	H	0	6.413	2.176	-0.090
H						
HETATM	533	C	0	-0.745	1.826	2.438
C						
HETATM	534	S	0	-4.334	-0.820	-0.854
S						
HETATM	535	S	0	1.104	-2.822	-3.779
S						
HETATM	536	N	0	-0.869	1.279	-1.305
N						
HETATM	537	N	0	-1.844	-0.824	-0.049
N						
HETATM	538	N	0	-2.426	-1.914	0.610
N						
HETATM	539	N	0	0.520	-1.136	-1.498
N						
HETATM	540	C	0	-0.290	2.341	-1.920
C						
HETATM	541	H	0	0.751	2.524	-1.664
H						
HETATM	542	C	0	-0.998	3.148	-2.843
C						
HETATM	543	H	0	-0.492	3.992	-3.311
H						
HETATM	544	C	0	-2.344	2.845	-3.143
C						
HETATM	545	H	0	-2.910	3.449	-3.852
H						
HETATM	546	C	0	-2.953	1.737	-2.508
C						
HETATM	547	H	0	-3.977	1.450	-2.739
H						
HETATM	548	C	0	-2.178	0.992	-1.594
C						
HETATM	549	C	0	-2.680	-0.168	-0.847
C						
HETATM	550	C	0	-3.711	-2.061	0.316
C						
HETATM	551	C	0	-4.605	-3.096	0.873
C						
HETATM	552	C	0	-4.061	-4.198	1.632
C						
HETATM	553	H	0	-2.982	-4.268	1.767
H						
HETATM	554	C	0	-4.916	-5.148	2.185
C						

HETATM	555	H	0	-4.520	-5.988	2.760
H						
HETATM	556	C	0	-6.348	-5.035	2.031
C						
HETATM	557	C	0	-7.258	-5.981	2.626
C						
HETATM	558	H	0	-6.849	-6.809	3.204
H						
HETATM	559	C	0	-8.637	-5.846	2.443
C						
HETATM	560	H	0	-9.331	-6.549	2.906
H						
HETATM	561	C	0	-9.171	-4.761	1.660
C						
HETATM	562	H	0	-10.253	-4.682	1.546
H						
HETATM	563	C	0	-8.315	-3.825	1.081
C						
HETATM	564	H	0	-8.706	-2.984	0.505
H						
HETATM	565	C	0	-6.888	-3.943	1.254
C						
HETATM	566	C	0	-5.988	-2.992	0.676
C						
HETATM	567	H	0	-6.413	-2.175	0.090
H						
HETATM	568	C	0	0.745	-1.826	-2.438
C						
HETATM	569	Fe	0	-3.830	-11.749	-0.472
Fe						
HETATM	570	S	0	0.433	-10.956	0.342
S						
HETATM	571	S	0	-4.959	-9.056	3.254
S						
HETATM	572	N	0	-2.968	-12.964	0.897
N						
HETATM	573	N	0	-1.991	-10.960	-0.435
N						
HETATM	574	N	0	-1.420	-9.898	-1.083
N						
HETATM	575	N	0	-4.355	-10.567	0.978
N						
HETATM	576	C	0	-3.537	-13.942	1.587
C						
HETATM	577	H	0	-4.466	-14.101	1.475
H						
HETATM	578	C	0	-2.824	-14.742	2.470
C						
HETATM	579	H	0	-3.264	-15.448	2.930
H						
HETATM	580	C	0	-1.490	-14.516	2.681
C						
HETATM	581	H	0	-0.993	-15.060	3.281
H						
HETATM	582	C	0	-0.881	-13.479	2.000
C						

HETATM	583	H	0	0.041	-13.287	2.133
H						
HETATM	584	C	0	-1.642	-12.721	1.116
C						
HETATM	585	C	0	-1.158	-11.599	0.348
C						
HETATM	586	C	0	-0.155	-9.772	-0.794
C						
HETATM	587	C	0	0.738	-8.747	-1.352
C						
HETATM	588	C	0	0.213	-7.675	-2.108
C						
HETATM	589	H	0	-0.725	-7.603	-2.231
H						
HETATM	590	C	0	1.030	-6.748	-2.661
C						
HETATM	591	H	0	0.656	-6.030	-3.157
H						
HETATM	592	C	0	2.441	-6.833	-2.509
C						
HETATM	593	C	0	3.329	-5.903	-3.091
C						
HETATM	594	H	0	2.981	-5.180	-3.599
H						
HETATM	595	C	0	4.685	-6.030	-2.932
C						
HETATM	596	H	0	5.266	-5.393	-3.330
H						
HETATM	597	C	0	5.224	-7.096	-2.183
C						
HETATM	598	H	0	6.164	-7.174	-2.077
H						
HETATM	599	C	0	4.394	-8.014	-1.609
C						
HETATM	600	H	0	4.764	-8.730	-1.107
H						
HETATM	601	C	0	2.982	-7.913	-1.756
C						
HETATM	602	C	0	2.104	-8.850	-1.185
C						
HETATM	603	H	0	2.459	-9.570	-0.676
H						
HETATM	604	C	0	-4.596	-9.939	1.906
C						
HETATM	605	S	0	-8.092	-12.541	-1.286
S						
HETATM	606	S	0	-2.700	-14.441	-4.197
S						
HETATM	607	N	0	-4.692	-10.534	-1.840
N						
HETATM	608	N	0	-5.668	-12.537	-0.508
N						
HETATM	609	N	0	-6.239	-13.599	0.140
N						
HETATM	610	N	0	-3.305	-12.931	-1.921
N						

HETATM	611	C	0	-4.123	-9.555	-2.531
C						
HETATM	612	H	0	-3.193	-9.397	-2.419
H						
HETATM	613	C	0	-4.835	-8.755	-3.414
C						
HETATM	614	H	0	-4.395	-8.049	-3.873
H						
HETATM	615	C	0	-6.169	-8.981	-3.625
C						
HETATM	616	H	0	-6.665	-8.437	-4.224
H						
HETATM	617	C	0	-6.778	-10.018	-2.943
C						
HETATM	618	H	0	-7.699	-10.210	-3.076
H						
HETATM	619	C	0	-6.017	-10.776	-2.060
C						
HETATM	620	C	0	-6.501	-11.898	-1.291
C						
HETATM	621	C	0	-7.503	-13.725	-0.150
C						
HETATM	622	C	0	-8.397	-14.750	0.408
C						
HETATM	623	C	0	-7.873	-15.823	1.165
C						
HETATM	624	H	0	-6.933	-15.894	1.288
H						
HETATM	625	C	0	-8.689	-16.749	1.718
C						
HETATM	626	H	0	-8.314	-17.467	2.214
H						
HETATM	627	C	0	-10.100	-16.664	1.566
C						
HETATM	628	C	0	-10.988	-17.594	2.147
C						
HETATM	629	H	0	-10.641	-18.318	2.655
H						
HETATM	630	C	0	-12.344	-17.468	1.988
C						
HETATM	631	H	0	-12.926	-18.105	2.387
H						
HETATM	632	C	0	-12.883	-16.402	1.240
C						
HETATM	633	H	0	-13.824	-16.323	1.134
H						
HETATM	634	C	0	-12.053	-15.484	0.666
C						
HETATM	635	H	0	-12.422	-14.768	0.163
H						
HETATM	636	C	0	-10.641	-15.584	0.813
C						
HETATM	637	C	0	-9.763	-14.647	0.242
C						
HETATM	638	H	0	-10.117	-13.927	-0.267
H						

HETATM	639	C	0	-3.062	-13.559	-2.849
C						
HETATM	640	Fe	0	-3.446	14.503	0.330
Fe						
HETATM	641	S	0	0.817	15.295	1.143
S						
HETATM	642	S	0	-4.575	17.195	4.056
S						
HETATM	643	N	0	-2.584	13.289	1.698
N						
HETATM	644	N	0	-1.607	15.292	0.366
N						
HETATM	645	N	0	-1.036	16.354	-0.283
N						
HETATM	646	N	0	-3.971	15.685	1.779
N						
HETATM	647	C	0	-3.153	12.310	2.389
C						
HETATM	648	H	0	-4.082	12.151	2.276
H						
HETATM	649	C	0	-2.440	11.509	3.271
C						
HETATM	650	H	0	-2.880	10.803	3.732
H						
HETATM	651	C	0	-1.106	11.736	3.482
C						
HETATM	652	H	0	-0.611	11.191	4.082
H						
HETATM	653	C	0	-0.497	12.772	2.801
C						
HETATM	654	H	0	0.424	12.966	2.933
H						
HETATM	655	C	0	-1.258	13.530	1.918
C						
HETATM	656	C	0	-0.775	14.652	1.149
C						
HETATM	657	C	0	0.227	16.479	0.007
C						
HETATM	658	C	0	1.122	17.505	-0.550
C						
HETATM	659	C	0	0.597	18.577	-1.307
C						
HETATM	660	H	0	-0.342	18.648	-1.430
H						
HETATM	661	C	0	1.414	19.503	-1.859
C						
HETATM	662	H	0	1.039	20.222	-2.357
H						
HETATM	663	C	0	2.825	19.419	-1.708
C						
HETATM	664	C	0	3.712	20.348	-2.289
C						
HETATM	665	H	0	3.365	21.072	-2.797
H						
HETATM	666	C	0	5.069	20.222	-2.131
C						

HETATM	667	H	0	5.650	20.859	-2.530
H						
HETATM	668	C	0	5.608	19.156	-1.381
C						
HETATM	669	H	0	6.548	19.078	-1.277
H						
HETATM	670	C	0	4.777	18.238	-0.808
C						
HETATM	671	H	0	5.147	17.522	-0.305
H						
HETATM	672	C	0	3.366	18.339	-0.954
C						
HETATM	673	C	0	2.488	17.401	-0.385
C						
HETATM	674	H	0	2.842	16.682	0.125
H						
HETATM	675	C	0	-4.213	16.313	2.708
C						
HETATM	676	S	0	-7.709	13.711	-0.484
S						
HETATM	677	S	0	-2.316	11.811	-3.397
S						
HETATM	678	N	0	-4.308	15.718	-1.039
N						
HETATM	679	N	0	-5.285	13.714	0.293
N						
HETATM	680	N	0	-5.856	12.652	0.942
N						
HETATM	681	N	0	-2.921	13.321	-1.120
N						
HETATM	682	C	0	-3.739	16.696	-1.730
C						
HETATM	683	H	0	-2.809	16.855	-1.617
H						
HETATM	684	C	0	-4.451	17.497	-2.612
C						
HETATM	685	H	0	-4.011	18.203	-3.073
H						
HETATM	686	C	0	-5.785	17.271	-2.823
C						
HETATM	687	H	0	-6.282	17.815	-3.423
H						
HETATM	688	C	0	-6.395	16.233	-2.142
C						
HETATM	689	H	0	-7.316	16.041	-2.274
H						
HETATM	690	C	0	-5.633	15.476	-1.259
C						
HETATM	691	C	0	-6.117	14.354	-0.490
C						
HETATM	692	C	0	-7.120	12.526	0.652
C						
HETATM	693	C	0	-8.013	11.501	1.209
C						
HETATM	694	C	0	-7.488	10.429	1.966
C						

HETATM	695	H	0	-6.550	10.358	2.089
H						
HETATM	696	C	0	-8.305	9.503	2.519
C						
HETATM	697	H	0	-7.932	8.785	3.016
H						
HETATM	698	C	0	-9.716	9.587	2.367
C						
HETATM	699	C	0	-10.604	8.658	2.948
C						
HETATM	700	H	0	-10.257	7.935	3.456
H						
HETATM	701	C	0	-11.960	8.785	2.790
C						
HETATM	702	H	0	-12.542	8.147	3.189
H						
HETATM	703	C	0	-12.499	9.851	2.040
C						
HETATM	704	H	0	-13.440	9.929	1.936
H						
HETATM	705	C	0	-11.670	10.769	1.467
C						
HETATM	706	H	0	-12.039	11.484	0.964
H						
HETATM	707	C	0	-10.258	10.667	1.613
C						
HETATM	708	C	0	-9.379	11.605	1.044
C						
HETATM	709	H	0	-9.734	12.324	0.534
H						
HETATM	710	C	0	-2.679	12.693	-2.049
C						
HETATM	711	Fe	0	-7.275	2.754	-0.142
Fe						
HETATM	712	S	0	-3.013	3.546	0.672
S						
HETATM	713	S	0	-8.404	5.448	3.584
S						
HETATM	714	N	0	-6.413	1.540	1.226
N						
HETATM	715	N	0	-5.436	3.543	-0.106
N						
HETATM	716	N	0	-4.866	4.606	-0.754
N						
HETATM	717	N	0	-7.801	3.937	1.307
N						
HETATM	718	C	0	-6.982	0.562	1.917
C						
HETATM	719	H	0	-7.913	0.402	1.805
H						
HETATM	720	C	0	-6.271	-0.240	2.800
C						
HETATM	721	H	0	-6.709	-0.946	3.259
H						
HETATM	722	C	0	-4.937	-0.013	3.010
C						

HETATM	723	H	0	-4.440	-0.557	3.611
H						
HETATM	724	C	0	-4.326	1.025	2.329
C						
HETATM	725	H	0	-3.406	1.217	2.462
H						
HETATM	726	C	0	-5.087	1.782	1.447
C						
HETATM	727	C	0	-4.604	2.904	0.677
C						
HETATM	728	C	0	-3.602	4.731	-0.464
C						
HETATM	729	C	0	-2.707	5.757	-1.022
C						
HETATM	730	C	0	-3.232	6.829	-1.779
C						
HETATM	731	H	0	-4.171	6.900	-1.902
H						
HETATM	732	C	0	-2.416	7.755	-2.331
C						
HETATM	733	H	0	-2.790	8.473	-2.828
H						
HETATM	734	C	0	-1.004	7.670	-2.179
C						
HETATM	735	C	0	-0.117	8.599	-2.761
C						
HETATM	736	H	0	-0.464	9.323	-3.269
H						
HETATM	737	C	0	1.239	8.473	-2.602
C						
HETATM	738	H	0	1.821	9.110	-3.001
H						
HETATM	739	C	0	1.778	7.408	-1.854
C						
HETATM	740	H	0	2.719	7.330	-1.748
H						
HETATM	741	C	0	0.948	6.489	-1.280
C						
HETATM	742	H	0	1.318	5.774	-0.777
H						
HETATM	743	C	0	-0.464	6.591	-1.427
C						
HETATM	744	C	0	-1.342	5.652	-0.856
C						
HETATM	745	H	0	-0.988	4.933	-0.346
H						
HETATM	746	C	0	-8.043	4.564	2.235
C						
HETATM	747	S	0	-11.538	1.962	-0.956
S						
HETATM	748	S	0	-6.146	0.062	-3.868
S						
HETATM	749	N	0	-8.137	3.969	-1.511
N						
HETATM	750	N	0	-9.114	1.966	-0.179
N						

HETATM	751	N	0	-9.685	0.903	0.469
N						
HETATM	752	N	0	-6.750	1.572	-1.592
N						
HETATM	753	C	0	-7.568	4.947	-2.201
C						
HETATM	754	H	0	-6.638	5.106	-2.089
H						
HETATM	755	C	0	-8.281	5.748	-3.084
C						
HETATM	756	H	0	-7.841	6.454	-3.544
H						
HETATM	757	C	0	-9.615	5.522	-3.295
C						
HETATM	758	H	0	-10.111	6.066	-3.895
H						
HETATM	759	C	0	-10.224	4.485	-2.614
C						
HETATM	760	H	0	-11.145	4.292	-2.747
H						
HETATM	761	C	0	-9.463	3.727	-1.730
C						
HETATM	762	C	0	-9.946	2.605	-0.962
C						
HETATM	763	C	0	-10.949	0.778	0.180
C						
HETATM	764	C	0	-11.843	-0.247	0.738
C						
HETATM	765	C	0	-11.318	-1.320	1.494
C						
HETATM	766	H	0	-10.379	-1.391	1.617
H						
HETATM	767	C	0	-12.135	-2.246	2.047
C						
HETATM	768	H	0	-11.761	-2.964	2.543
H						
HETATM	769	C	0	-13.545	-2.161	1.895
C						
HETATM	770	C	0	-14.434	-3.091	2.477
C						
HETATM	771	H	0	-14.087	-3.814	2.984
H						
HETATM	772	C	0	-15.790	-2.964	2.318
C						
HETATM	773	H	0	-16.372	-3.601	2.716
H						
HETATM	774	C	0	-16.328	-1.898	1.569
C						
HETATM	775	H	0	-17.269	-1.820	1.463
H						
HETATM	776	C	0	-15.499	-0.980	0.995
C						
HETATM	777	H	0	-15.868	-0.264	0.493
H						
HETATM	778	C	0	-14.087	-1.082	1.142
C						

HETATM	779	C	0	-13.209	-0.144	0.571
C						
HETATM	780	H	0	-13.563	0.576	0.062
H						
HETATM	781	C	0	-6.508	0.945	-2.520
C						
HETATM	782	Fe	0	-11.105	-8.994	-0.614
Fe						
HETATM	783	S	0	-6.842	-8.202	0.200
S						
HETATM	784	S	0	-12.234	-6.301	3.112
S						
HETATM	785	N	0	-10.243	-10.209	0.755
N						
HETATM	786	N	0	-9.267	-8.206	-0.577
N						
HETATM	787	N	0	-8.695	-7.143	-1.225
N						
HETATM	788	N	0	-11.630	-7.812	0.835
N						
HETATM	789	C	0	-10.811	-11.187	1.445
C						
HETATM	790	H	0	-11.742	-11.347	1.332
H						
HETATM	791	C	0	-10.100	-11.988	2.328
C						
HETATM	792	H	0	-10.539	-12.693	2.788
H						
HETATM	793	C	0	-8.766	-11.761	2.539
C						
HETATM	794	H	0	-8.269	-12.306	3.139
H						
HETATM	795	C	0	-8.156	-10.724	1.858
C						
HETATM	796	H	0	-7.235	-10.532	1.991
H						
HETATM	797	C	0	-8.917	-9.967	0.974
C						
HETATM	798	C	0	-8.434	-8.845	0.205
C						
HETATM	799	C	0	-7.431	-7.017	-0.937
C						
HETATM	800	C	0	-6.537	-5.992	-1.494
C						
HETATM	801	C	0	-7.063	-4.920	-2.251
C						
HETATM	802	H	0	-8.001	-4.848	-2.374
H						
HETATM	803	C	0	-6.245	-3.993	-2.803
C						
HETATM	804	H	0	-6.620	-3.276	-3.300
H						
HETATM	805	C	0	-4.835	-4.079	-2.651
C						
HETATM	806	C	0	-3.946	-3.149	-3.233
C						

HETATM	807	H	0	-4.294	-2.426	-3.741
H						
HETATM	808	C	0	-2.590	-3.276	-3.075
C						
HETATM	809	H	0	-2.008	-2.639	-3.472
H						
HETATM	810	C	0	-2.052	-4.341	-2.325
C						
HETATM	811	H	0	-1.110	-4.419	-2.219
H						
HETATM	812	C	0	-2.881	-5.259	-1.751
C						
HETATM	813	H	0	-2.512	-5.975	-1.249
H						
HETATM	814	C	0	-4.293	-5.158	-1.898
C						
HETATM	815	C	0	-5.171	-6.096	-1.328
C						
HETATM	816	H	0	-4.817	-6.816	-0.818
H						
HETATM	817	C	0	-11.872	-7.185	1.764
C						
HETATM	818	S	0	-15.368	-9.786	-1.428
S						
HETATM	819	S	0	-9.975	-11.687	-4.340
S						
HETATM	820	N	0	-11.967	-7.780	-1.982
N						
HETATM	821	N	0	-12.943	-9.782	-0.650
N						
HETATM	822	N	0	-13.514	-10.845	-0.002
N						
HETATM	823	N	0	-10.580	-10.177	-2.063
N						
HETATM	824	C	0	-11.398	-6.801	-2.674
C						
HETATM	825	H	0	-10.468	-6.642	-2.561
H						
HETATM	826	C	0	-12.110	-6.000	-3.556
C						
HETATM	827	H	0	-11.670	-5.295	-4.015
H						
HETATM	828	C	0	-13.444	-6.227	-3.767
C						
HETATM	829	H	0	-13.940	-5.682	-4.367
H						
HETATM	830	C	0	-14.054	-7.264	-3.085
C						
HETATM	831	H	0	-14.974	-7.456	-3.218
H						
HETATM	832	C	0	-13.293	-8.021	-2.203
C						
HETATM	833	C	0	-13.776	-9.144	-1.433
C						
HETATM	834	C	0	-14.778	-10.971	-0.292
C						

HETATM	835	C	0	-15.673	-11.996	0.266
C						
HETATM	836	C	0	-15.147	-13.069	1.023
C						
HETATM	837	H	0	-14.209	-13.140	1.146
H						
HETATM	838	C	0	-15.964	-13.995	1.576
C						
HETATM	839	H	0	-15.590	-14.712	2.072
H						
HETATM	840	C	0	-17.375	-13.910	1.423
C						
HETATM	841	C	0	-18.263	-14.839	2.004
C						
HETATM	842	H	0	-17.916	-15.563	2.513
H						
HETATM	843	C	0	-19.620	-14.713	1.846
C						
HETATM	844	H	0	-20.202	-15.350	2.245
H						
HETATM	845	C	0	-20.158	-13.647	1.098
C						
HETATM	846	H	0	-21.099	-13.569	0.992
H						
HETATM	847	C	0	-19.328	-12.729	0.524
C						
HETATM	848	H	0	-19.698	-12.013	0.021
H						
HETATM	849	C	0	-17.916	-12.830	0.671
C						
HETATM	850	C	0	-17.039	-11.893	0.100
C						
HETATM	851	H	0	-17.393	-11.173	-0.410
H						
HETATM	852	C	0	-10.338	-10.804	-2.992
C						
HETATM	853	Fe	0	-10.721	17.258	0.187
Fe						
HETATM	854	S	0	-6.458	18.049	1.001
S						
HETATM	855	S	0	-11.851	19.950	3.914
S						
HETATM	856	N	0	-9.859	16.043	1.555
N						
HETATM	857	N	0	-8.882	18.046	0.223
N						
HETATM	858	N	0	-8.311	19.109	-0.425
N						
HETATM	859	N	0	-11.246	18.440	1.637
N						
HETATM	860	C	0	-10.428	15.065	2.247
C						
HETATM	861	H	0	-11.358	14.906	2.134
H						
HETATM	862	C	0	-9.716	14.263	3.129
C						

HETATM	863	H	0	-10.156	13.558	3.589
H						
HETATM	864	C	0	-8.382	14.490	3.340
C						
HETATM	865	H	0	-7.885	13.946	3.940
H						
HETATM	866	C	0	-7.773	15.527	2.659
C						
HETATM	867	H	0	-6.851	15.720	2.791
H						
HETATM	868	C	0	-8.534	16.284	1.776
C						
HETATM	869	C	0	-8.050	17.406	1.007
C						
HETATM	870	C	0	-7.047	19.234	-0.135
C						
HETATM	871	C	0	-6.153	20.260	-0.692
C						
HETATM	872	C	0	-6.679	21.332	-1.449
C						
HETATM	873	H	0	-7.617	21.403	-1.572
H						
HETATM	874	C	0	-5.862	22.258	-2.002
C						
HETATM	875	H	0	-6.235	22.976	-2.499
H						
HETATM	876	C	0	-4.451	22.174	-1.850
C						
HETATM	877	C	0	-3.562	23.102	-2.431
C						
HETATM	878	H	0	-3.910	23.826	-2.939
H						
HETATM	879	C	0	-2.206	22.976	-2.273
C						
HETATM	880	H	0	-1.624	23.613	-2.672
H						
HETATM	881	C	0	-1.668	21.910	-1.524
C						
HETATM	882	H	0	-0.728	21.832	-1.419
H						
HETATM	883	C	0	-2.497	20.992	-0.951
C						
HETATM	884	H	0	-2.128	20.276	-0.447
H						
HETATM	885	C	0	-3.909	21.094	-1.097
C						
HETATM	886	C	0	-4.787	20.156	-0.527
C						
HETATM	887	H	0	-4.433	19.437	-0.017
H						
HETATM	888	C	0	-11.488	19.067	2.565
C						
HETATM	889	S	0	-14.984	16.466	-0.627
S						
HETATM	890	S	0	-9.592	14.565	-3.539
S						

HETATM	891	N	0	-11.583	18.472	-1.181
N						
HETATM	892	N	0	-12.560	16.469	0.151
N						
HETATM	893	N	0	-13.131	15.406	0.799
N						
HETATM	894	N	0	-10.195	16.075	-1.263
N						
HETATM	895	C	0	-11.015	19.450	-1.872
C						
HETATM	896	H	0	-10.084	19.610	-1.759
H						
HETATM	897	C	0	-11.726	20.252	-2.755
C						
HETATM	898	H	0	-11.287	20.958	-3.215
H						
HETATM	899	C	0	-13.060	20.025	-2.965
C						
HETATM	900	H	0	-13.556	20.570	-3.565
H						
HETATM	901	C	0	-13.670	18.988	-2.285
C						
HETATM	902	H	0	-14.591	18.795	-2.417
H						
HETATM	903	C	0	-12.909	18.231	-1.401
C						
HETATM	904	C	0	-13.392	17.109	-0.632
C						
HETATM	905	C	0	-14.395	15.281	0.510
C						
HETATM	906	C	0	-15.289	14.255	1.067
C						
HETATM	907	C	0	-14.764	13.183	1.824
C						
HETATM	908	H	0	-13.825	13.112	1.947
H						
HETATM	909	C	0	-15.580	12.257	2.376
C						
HETATM	910	H	0	-15.206	11.539	2.873
H						
HETATM	911	C	0	-16.992	12.342	2.225
C						
HETATM	912	C	0	-17.879	11.413	2.806
C						
HETATM	913	H	0	-17.532	10.689	3.314
H						
HETATM	914	C	0	-19.236	11.539	2.648
C						
HETATM	915	H	0	-19.817	10.902	3.046
H						
HETATM	916	C	0	-19.774	12.605	1.898
C						
HETATM	917	H	0	-20.715	12.683	1.793
H						
HETATM	918	C	0	-18.944	13.523	1.325
C						

HETATM	919	H	0	-19.314	14.238	0.822
H						
HETATM	920	C	0	-17.532	13.421	1.471
C						
HETATM	921	C	0	-16.655	14.359	0.902
C						
HETATM	922	H	0	-17.009	15.078	0.392
H						
HETATM	923	C	0	-9.954	15.448	-2.191
C						
HETATM	924	Fe	0	-14.551	5.509	-0.284
Fe						
HETATM	925	S	0	-10.288	6.301	0.530
S						
HETATM	926	S	0	-15.680	8.202	3.441
S						
HETATM	927	N	0	-13.689	4.294	1.084
N						
HETATM	928	N	0	-12.712	6.297	-0.248
N						
HETATM	929	N	0	-12.141	7.360	-0.896
N						
HETATM	930	N	0	-15.076	6.691	1.165
N						
HETATM	931	C	0	-14.258	3.316	1.775
C						
HETATM	932	H	0	-15.187	3.157	1.663
H						
HETATM	933	C	0	-13.545	2.514	2.658
C						
HETATM	934	H	0	-13.985	1.809	3.117
H						
HETATM	935	C	0	-12.211	2.741	2.868
C						
HETATM	936	H	0	-11.714	2.198	3.468
H						
HETATM	937	C	0	-11.602	3.779	2.187
C						
HETATM	938	H	0	-10.681	3.971	2.320
H						
HETATM	939	C	0	-12.363	4.536	1.304
C						
HETATM	940	C	0	-11.879	5.659	0.535
C						
HETATM	941	C	0	-10.876	7.486	-0.606
C						
HETATM	942	C	0	-9.983	8.511	-1.164
C						
HETATM	943	C	0	-10.508	9.583	-1.922
C						
HETATM	944	H	0	-11.446	9.655	-2.044
H						
HETATM	945	C	0	-9.691	10.510	-2.473
C						
HETATM	946	H	0	-10.065	11.227	-2.970
H						

HETATM	947	C	0	-8.280	10.425	-2.322
C						
HETATM	948	C	0	-7.393	11.354	-2.903
C						
HETATM	949	H	0	-7.740	12.077	-3.412
H						
HETATM	950	C	0	-6.036	11.227	-2.745
C						
HETATM	951	H	0	-5.455	11.865	-3.143
H						
HETATM	952	C	0	-5.497	10.162	-1.996
C						
HETATM	953	H	0	-4.557	10.084	-1.890
H						
HETATM	954	C	0	-6.327	9.243	-1.422
C						
HETATM	955	H	0	-5.957	8.528	-0.920
H						
HETATM	956	C	0	-7.739	9.345	-1.569
C						
HETATM	957	C	0	-8.617	8.407	-0.998
C						
HETATM	958	H	0	-8.262	7.688	-0.489
H						
HETATM	959	C	0	-15.317	7.319	2.093
C						
HETATM	960	S	0	-18.813	4.717	-1.098
S						
HETATM	961	S	0	-13.421	2.816	-4.010
S						
HETATM	962	N	0	-15.413	6.723	-1.653
N						
HETATM	963	N	0	-16.390	4.720	-0.321
N						
HETATM	964	N	0	-16.961	3.658	0.327
N						
HETATM	965	N	0	-14.026	4.326	-1.734
N						
HETATM	966	C	0	-14.844	7.701	-2.344
C						
HETATM	967	H	0	-13.914	7.861	-2.231
H						
HETATM	968	C	0	-15.556	8.503	-3.226
C						
HETATM	969	H	0	-15.116	9.209	-3.686
H						
HETATM	970	C	0	-16.890	8.276	-3.438
C						
HETATM	971	H	0	-17.386	8.821	-4.037
H						
HETATM	972	C	0	-17.499	7.239	-2.756
C						
HETATM	973	H	0	-18.420	7.046	-2.889
H						
HETATM	974	C	0	-16.738	6.482	-1.872
C						

HETATM	975	C	0	-17.222	5.360	-1.104
C						
HETATM	976	C	0	-18.224	3.533	0.038
C						
HETATM	977	C	0	-19.118	2.507	0.596
C						
HETATM	978	C	0	-18.594	1.435	1.352
C						
HETATM	979	H	0	-17.654	1.364	1.475
H						
HETATM	980	C	0	-19.410	0.509	1.905
C						
HETATM	981	H	0	-19.036	-0.210	2.401
H						
HETATM	982	C	0	-20.821	0.594	1.753
C						
HETATM	983	C	0	-21.709	-0.336	2.335
C						
HETATM	984	H	0	-21.362	-1.060	2.842
H						
HETATM	985	C	0	-23.065	-0.210	2.176
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HETATM	68	C	0	11.568	2.404	2.040
C						
HETATM	69	C	0	12.446	3.341	1.470
C						
HETATM	70	H	0	12.093	4.061	0.960
H						
HETATM	71	C	0	19.148	4.430	-1.622
C						
HETATM	72	Fe	0	14.551	-5.509	0.284
Fe						
HETATM	73	S	0	18.813	-4.717	1.098
S						
HETATM	74	S	0	13.422	-2.816	4.010
S						
HETATM	75	N	0	15.413	-6.724	1.653
N						
HETATM	76	N	0	16.390	-4.720	0.321
N						
HETATM	77	N	0	16.961	-3.658	-0.327
N						
HETATM	78	N	0	14.026	-4.326	1.734
N						
HETATM	79	C	0	14.844	-7.701	2.344
C						
HETATM	80	H	0	13.914	-7.861	2.231
H						
HETATM	81	C	0	15.556	-8.503	3.226
C						
HETATM	82	H	0	15.116	-9.209	3.686
H						
HETATM	83	C	0	16.890	-8.277	3.438
C						
HETATM	84	H	0	17.386	-8.821	4.037
H						

HETATM	85	C	0	17.499	-7.240	2.756
C						
HETATM	86	H	0	18.420	-7.047	2.889
H						
HETATM	87	C	0	16.738	-6.482	1.873
C						
HETATM	88	C	0	17.222	-5.360	1.104
C						
HETATM	89	C	0	18.224	-3.533	-0.038
C						
HETATM	90	C	0	19.118	-2.507	-0.596
C						
HETATM	91	C	0	18.594	-1.435	-1.352
C						
HETATM	92	H	0	17.654	-1.364	-1.475
H						
HETATM	93	C	0	19.410	-0.509	-1.905
C						
HETATM	94	H	0	19.036	0.210	-2.401
H						
HETATM	95	C	0	20.821	-0.594	-1.753
C						
HETATM	96	C	0	21.709	0.336	-2.335
C						
HETATM	97	H	0	21.362	1.060	-2.842
H						
HETATM	98	C	0	23.065	0.210	-2.176
C						
HETATM	99	H	0	23.647	0.847	-2.574
H						
HETATM	100	C	0	23.604	-0.856	-1.427
C						
HETATM	101	H	0	24.545	-0.934	-1.321
H						
HETATM	102	C	0	22.774	-1.774	-0.853
C						
HETATM	103	H	0	23.143	-2.490	-0.350
H						
HETATM	104	C	0	21.363	-1.673	-1.000
C						
HETATM	105	C	0	20.484	-2.611	-0.429
C						
HETATM	106	H	0	20.838	-3.331	0.081
H						
HETATM	107	C	0	13.783	-3.699	2.662
C						
HETATM	108	S	0	10.288	-6.301	-0.530
S						
HETATM	109	S	0	15.680	-8.202	-3.441
S						
HETATM	110	N	0	13.689	-4.294	-1.084
N						
HETATM	111	N	0	12.712	-6.297	0.248
N						
HETATM	112	N	0	12.141	-7.360	0.896
N						

HETATM	113	N	0	15.076	-6.691	-1.165
N						
HETATM	114	C	0	14.258	-3.316	-1.775
C						
HETATM	115	H	0	15.187	-3.157	-1.663
H						
HETATM	116	C	0	13.545	-2.515	-2.658
C						
HETATM	117	H	0	13.985	-1.809	-3.117
H						
HETATM	118	C	0	12.211	-2.741	-2.868
C						
HETATM	119	H	0	11.714	-2.198	-3.468
H						
HETATM	120	C	0	11.602	-3.779	-2.187
C						
HETATM	121	H	0	10.681	-3.971	-2.320
H						
HETATM	122	C	0	12.363	-4.536	-1.304
C						
HETATM	123	C	0	11.879	-5.659	-0.535
C						
HETATM	124	C	0	10.876	-7.486	0.606
C						
HETATM	125	C	0	9.983	-8.511	1.164
C						
HETATM	126	C	0	10.508	-9.583	1.922
C						
HETATM	127	H	0	11.446	-9.655	2.044
H						
HETATM	128	C	0	9.691	-10.510	2.473
C						
HETATM	129	H	0	10.065	-11.227	2.970
H						
HETATM	130	C	0	8.280	-10.425	2.322
C						
HETATM	131	C	0	7.393	-11.354	2.903
C						
HETATM	132	H	0	7.740	-12.078	3.412
H						
HETATM	133	C	0	6.036	-11.227	2.745
C						
HETATM	134	H	0	5.455	-11.865	3.143
H						
HETATM	135	C	0	5.497	-10.162	1.996
C						
HETATM	136	H	0	4.557	-10.084	1.890
H						
HETATM	137	C	0	6.327	-9.243	1.422
C						
HETATM	138	H	0	5.957	-8.528	0.920
H						
HETATM	139	C	0	7.739	-9.345	1.569
C						
HETATM	140	C	0	8.617	-8.407	0.998
C						

HETATM	141	H	0	8.262	-7.688	0.489
H						
HETATM	142	C	0	15.317	-7.319	-2.093
C						
HETATM	143	Fe	0	10.721	-17.258	-0.187
Fe						
HETATM	144	S	0	14.984	-16.466	0.627
S						
HETATM	145	S	0	9.592	-14.565	3.539
S						
HETATM	146	N	0	11.583	-18.472	1.181
N						
HETATM	147	N	0	12.560	-16.469	-0.151
N						
HETATM	148	N	0	13.131	-15.406	-0.799
N						
HETATM	149	N	0	10.195	-16.075	1.263
N						
HETATM	150	C	0	11.015	-19.450	1.872
C						
HETATM	151	H	0	10.084	-19.610	1.760
H						
HETATM	152	C	0	11.726	-20.252	2.755
C						
HETATM	153	H	0	11.287	-20.958	3.215
H						
HETATM	154	C	0	13.060	-20.025	2.965
C						
HETATM	155	H	0	13.556	-20.570	3.565
H						
HETATM	156	C	0	13.670	-18.988	2.285
C						
HETATM	157	H	0	14.591	-18.795	2.417
H						
HETATM	158	C	0	12.909	-18.231	1.401
C						
HETATM	159	C	0	13.392	-17.109	0.632
C						
HETATM	160	C	0	14.395	-15.281	-0.509
C						
HETATM	161	C	0	15.289	-14.255	-1.067
C						
HETATM	162	C	0	14.764	-13.184	-1.824
C						
HETATM	163	H	0	13.825	-13.112	-1.947
H						
HETATM	164	C	0	15.580	-12.257	-2.376
C						
HETATM	165	H	0	15.206	-11.539	-2.873
H						
HETATM	166	C	0	16.992	-12.342	-2.225
C						
HETATM	167	C	0	17.879	-11.413	-2.806
C						
HETATM	168	H	0	17.532	-10.689	-3.314
H						

HETATM	169	C	0	19.236	-11.539	-2.648
C						
HETATM	170	H	0	19.817	-10.902	-3.046
H						
HETATM	171	C	0	19.774	-12.605	-1.898
C						
HETATM	172	H	0	20.715	-12.683	-1.793
H						
HETATM	173	C	0	18.944	-13.523	-1.325
C						
HETATM	174	H	0	19.314	-14.238	-0.822
H						
HETATM	175	C	0	17.532	-13.421	-1.471
C						
HETATM	176	C	0	16.655	-14.360	-0.902
C						
HETATM	177	H	0	17.009	-15.078	-0.392
H						
HETATM	178	C	0	9.954	-15.448	2.191
C						
HETATM	179	S	0	6.458	-18.049	-1.001
S						
HETATM	180	S	0	11.851	-19.950	-3.914
S						
HETATM	181	N	0	9.859	-16.043	-1.555
N						
HETATM	182	N	0	8.882	-18.046	-0.223
N						
HETATM	183	N	0	8.311	-19.109	0.425
N						
HETATM	184	N	0	11.246	-18.440	-1.637
N						
HETATM	185	C	0	10.428	-15.065	-2.247
C						
HETATM	186	H	0	11.358	-14.906	-2.134
H						
HETATM	187	C	0	9.716	-14.263	-3.129
C						
HETATM	188	H	0	10.156	-13.558	-3.589
H						
HETATM	189	C	0	8.382	-14.490	-3.340
C						
HETATM	190	H	0	7.885	-13.946	-3.940
H						
HETATM	191	C	0	7.773	-15.527	-2.659
C						
HETATM	192	H	0	6.851	-15.720	-2.791
H						
HETATM	193	C	0	8.534	-16.284	-1.776
C						
HETATM	194	C	0	8.050	-17.407	-1.007
C						
HETATM	195	C	0	7.047	-19.234	0.135
C						
HETATM	196	C	0	6.153	-20.260	0.692
C						

HETATM	197	C	0	6.679	-21.332	1.449
C						
HETATM	198	H	0	7.617	-21.403	1.572
H						
HETATM	199	C	0	5.862	-22.258	2.002
C						
HETATM	200	H	0	6.235	-22.976	2.499
H						
HETATM	201	C	0	4.451	-22.174	1.850
C						
HETATM	202	C	0	3.562	-23.102	2.431
C						
HETATM	203	H	0	3.910	-23.826	2.939
H						
HETATM	204	C	0	2.206	-22.976	2.273
C						
HETATM	205	H	0	1.624	-23.613	2.672
H						
HETATM	206	C	0	1.668	-21.910	1.524
C						
HETATM	207	H	0	0.728	-21.832	1.419
H						
HETATM	208	C	0	2.497	-20.992	0.951
C						
HETATM	209	H	0	2.128	-20.276	0.447
H						
HETATM	210	C	0	3.909	-21.094	1.097
C						
HETATM	211	C	0	4.787	-20.156	0.527
C						
HETATM	212	H	0	4.433	-19.437	0.017
H						
HETATM	213	C	0	11.488	-19.067	-2.565
C						
HETATM	214	Fe	0	11.105	8.994	0.614
Fe						
HETATM	215	S	0	15.368	9.786	1.428
S						
HETATM	216	S	0	9.975	11.687	4.340
S						
HETATM	217	N	0	11.967	7.780	1.982
N						
HETATM	218	N	0	12.943	9.782	0.650
N						
HETATM	219	N	0	13.514	10.845	0.002
N						
HETATM	220	N	0	10.580	10.177	2.063
N						
HETATM	221	C	0	11.398	6.801	2.674
C						
HETATM	222	H	0	10.468	6.642	2.561
H						
HETATM	223	C	0	12.110	6.000	3.556
C						
HETATM	224	H	0	11.670	5.295	4.015
H						

HETATM	225	C	0	13.444	6.227	3.767
C						
HETATM	226	H	0	13.940	5.682	4.367
H						
HETATM	227	C	0	14.054	7.264	3.085
C						
HETATM	228	H	0	14.974	7.456	3.218
H						
HETATM	229	C	0	13.293	8.021	2.203
C						
HETATM	230	C	0	13.776	9.144	1.433
C						
HETATM	231	C	0	14.778	10.970	0.292
C						
HETATM	232	C	0	15.673	11.996	-0.266
C						
HETATM	233	C	0	15.147	13.069	-1.023
C						
HETATM	234	H	0	14.209	13.140	-1.146
H						
HETATM	235	C	0	15.964	13.995	-1.576
C						
HETATM	236	H	0	15.590	14.712	-2.072
H						
HETATM	237	C	0	17.375	13.910	-1.423
C						
HETATM	238	C	0	18.263	14.839	-2.004
C						
HETATM	239	H	0	17.916	15.563	-2.513
H						
HETATM	240	C	0	19.620	14.713	-1.846
C						
HETATM	241	H	0	20.202	15.350	-2.245
H						
HETATM	242	C	0	20.158	13.647	-1.098
C						
HETATM	243	H	0	21.099	13.569	-0.992
H						
HETATM	244	C	0	19.328	12.729	-0.524
C						
HETATM	245	H	0	19.698	12.013	-0.021
H						
HETATM	246	C	0	17.916	12.830	-0.671
C						
HETATM	247	C	0	17.039	11.892	-0.100
C						
HETATM	248	H	0	17.393	11.173	0.410
H						
HETATM	249	C	0	10.338	10.804	2.992
C						
HETATM	250	S	0	6.842	8.202	-0.200
S						
HETATM	251	S	0	12.234	6.301	-3.112
S						
HETATM	252	N	0	10.243	10.209	-0.755
N						

HETATM	253	N	0	9.267	8.206	0.577
N						
HETATM	254	N	0	8.695	7.143	1.225
N						
HETATM	255	N	0	11.630	7.812	-0.835
N						
HETATM	256	C	0	10.811	11.187	-1.445
C						
HETATM	257	H	0	11.742	11.346	-1.332
H						
HETATM	258	C	0	10.100	11.988	-2.328
C						
HETATM	259	H	0	10.539	12.693	-2.788
H						
HETATM	260	C	0	8.766	11.761	-2.539
C						
HETATM	261	H	0	8.269	12.306	-3.139
H						
HETATM	262	C	0	8.156	10.724	-1.858
C						
HETATM	263	H	0	7.235	10.532	-1.991
H						
HETATM	264	C	0	8.917	9.967	-0.974
C						
HETATM	265	C	0	8.434	8.845	-0.205
C						
HETATM	266	C	0	7.431	7.017	0.937
C						
HETATM	267	C	0	6.537	5.992	1.494
C						
HETATM	268	C	0	7.063	4.920	2.251
C						
HETATM	269	H	0	8.001	4.848	2.374
H						
HETATM	270	C	0	6.245	3.993	2.803
C						
HETATM	271	H	0	6.620	3.276	3.300
H						
HETATM	272	C	0	4.835	4.079	2.651
C						
HETATM	273	C	0	3.946	3.149	3.233
C						
HETATM	274	H	0	4.294	2.426	3.741
H						
HETATM	275	C	0	2.590	3.276	3.075
C						
HETATM	276	H	0	2.008	2.639	3.473
H						
HETATM	277	C	0	2.052	4.341	2.325
C						
HETATM	278	H	0	1.110	4.419	2.219
H						
HETATM	279	C	0	2.881	5.259	1.751
C						
HETATM	280	H	0	2.512	5.975	1.249
H						

HETATM	281	C	0	4.293	5.158	1.898
C						
HETATM	282	C	0	5.171	6.096	1.328
C						
HETATM	283	H	0	4.817	6.815	0.818
H						
HETATM	284	C	0	11.872	7.185	-1.764
C						
HETATM	285	Fe	0	7.275	-2.754	0.142
Fe						
HETATM	286	S	0	11.538	-1.962	0.956
S						
HETATM	287	S	0	6.146	-0.062	3.868
S						
HETATM	288	N	0	8.137	-3.969	1.511
N						
HETATM	289	N	0	9.114	-1.966	0.179
N						
HETATM	290	N	0	9.685	-0.903	-0.469
N						
HETATM	291	N	0	6.750	-1.572	1.592
N						
HETATM	292	C	0	7.568	-4.947	2.201
C						
HETATM	293	H	0	6.638	-5.106	2.089
H						
HETATM	294	C	0	8.281	-5.748	3.084
C						
HETATM	295	H	0	7.841	-6.454	3.544
H						
HETATM	296	C	0	9.615	-5.522	3.295
C						
HETATM	297	H	0	10.111	-6.066	3.895
H						
HETATM	298	C	0	10.224	-4.485	2.614
C						
HETATM	299	H	0	11.145	-4.292	2.747
H						
HETATM	300	C	0	9.463	-3.727	1.730
C						
HETATM	301	C	0	9.946	-2.605	0.962
C						
HETATM	302	C	0	10.949	-0.778	-0.180
C						
HETATM	303	C	0	11.843	0.247	-0.738
C						
HETATM	304	C	0	11.318	1.320	-1.494
C						
HETATM	305	H	0	10.379	1.391	-1.617
H						
HETATM	306	C	0	12.135	2.246	-2.047
C						
HETATM	307	H	0	11.761	2.964	-2.543
H						
HETATM	308	C	0	13.545	2.161	-1.895
C						

HETATM	309	C	0	14.434	3.090	-2.477
C						
HETATM	310	H	0	14.087	3.814	-2.984
H						
HETATM	311	C	0	15.790	2.964	-2.318
C						
HETATM	312	H	0	16.372	3.601	-2.716
H						
HETATM	313	C	0	16.328	1.898	-1.569
C						
HETATM	314	H	0	17.269	1.820	-1.463
H						
HETATM	315	C	0	15.499	0.980	-0.995
C						
HETATM	316	H	0	15.868	0.264	-0.493
H						
HETATM	317	C	0	14.087	1.082	-1.142
C						
HETATM	318	C	0	13.209	0.144	-0.571
C						
HETATM	319	H	0	13.563	-0.576	-0.062
H						
HETATM	320	C	0	6.508	-0.945	2.520
C						
HETATM	321	S	0	3.013	-3.546	-0.672
S						
HETATM	322	S	0	8.404	-5.448	-3.583
S						
HETATM	323	N	0	6.413	-1.540	-1.226
N						
HETATM	324	N	0	5.436	-3.543	0.106
N						
HETATM	325	N	0	4.866	-4.606	0.754
N						
HETATM	326	N	0	7.801	-3.937	-1.307
N						
HETATM	327	C	0	6.982	-0.562	-1.917
C						
HETATM	328	H	0	7.913	-0.402	-1.805
H						
HETATM	329	C	0	6.271	0.240	-2.800
C						
HETATM	330	H	0	6.709	0.946	-3.259
H						
HETATM	331	C	0	4.937	0.013	-3.010
C						
HETATM	332	H	0	4.440	0.557	-3.611
H						
HETATM	333	C	0	4.326	-1.025	-2.329
C						
HETATM	334	H	0	3.406	-1.217	-2.462
H						
HETATM	335	C	0	5.087	-1.782	-1.447
C						
HETATM	336	C	0	4.604	-2.904	-0.677
C						

HETATM	337	C	0	3.602	-4.731	0.464
C						
HETATM	338	C	0	2.708	-5.757	1.022
C						
HETATM	339	C	0	3.232	-6.829	1.779
C						
HETATM	340	H	0	4.171	-6.901	1.902
H						
HETATM	341	C	0	2.416	-7.755	2.331
C						
HETATM	342	H	0	2.790	-8.473	2.828
H						
HETATM	343	C	0	1.004	-7.670	2.179
C						
HETATM	344	C	0	0.117	-8.599	2.761
C						
HETATM	345	H	0	0.464	-9.323	3.269
H						
HETATM	346	C	0	-1.239	-8.473	2.602
C						
HETATM	347	H	0	-1.821	-9.110	3.001
H						
HETATM	348	C	0	-1.778	-7.408	1.854
C						
HETATM	349	H	0	-2.719	-7.330	1.748
H						
HETATM	350	C	0	-0.948	-6.489	1.280
C						
HETATM	351	H	0	-1.318	-5.774	0.777
H						
HETATM	352	C	0	0.464	-6.591	1.427
C						
HETATM	353	C	0	1.342	-5.652	0.856
C						
HETATM	354	H	0	0.988	-4.933	0.346
H						
HETATM	355	C	0	8.043	-4.564	-2.235
C						
HETATM	356	Fe	0	3.446	-14.503	-0.329
Fe						
HETATM	357	S	0	7.709	-13.711	0.484
S						
HETATM	358	S	0	2.316	-11.811	3.397
S						
HETATM	359	N	0	4.308	-15.718	1.039
N						
HETATM	360	N	0	5.285	-13.714	-0.293
N						
HETATM	361	N	0	5.856	-12.652	-0.942
N						
HETATM	362	N	0	2.921	-13.321	1.120
N						
HETATM	363	C	0	3.739	-16.696	1.730
C						
HETATM	364	H	0	2.809	-16.855	1.617
H						

HETATM	365	C	0	4.451	-17.497	2.612
C						
HETATM	366	H	0	4.011	-18.203	3.073
H						
HETATM	367	C	0	5.785	-17.271	2.823
C						
HETATM	368	H	0	6.282	-17.815	3.423
H						
HETATM	369	C	0	6.395	-16.233	2.142
C						
HETATM	370	H	0	7.316	-16.041	2.274
H						
HETATM	371	C	0	5.633	-15.476	1.259
C						
HETATM	372	C	0	6.117	-14.354	0.490
C						
HETATM	373	C	0	7.120	-12.526	-0.652
C						
HETATM	374	C	0	8.013	-11.501	-1.209
C						
HETATM	375	C	0	7.489	-10.429	-1.966
C						
HETATM	376	H	0	6.550	-10.358	-2.089
H						
HETATM	377	C	0	8.305	-9.503	-2.518
C						
HETATM	378	H	0	7.932	-8.785	-3.016
H						
HETATM	379	C	0	9.716	-9.587	-2.367
C						
HETATM	380	C	0	10.604	-8.658	-2.948
C						
HETATM	381	H	0	10.257	-7.935	-3.456
H						
HETATM	382	C	0	11.960	-8.785	-2.790
C						
HETATM	383	H	0	12.542	-8.147	-3.189
H						
HETATM	384	C	0	12.499	-9.851	-2.040
C						
HETATM	385	H	0	13.440	-9.929	-1.936
H						
HETATM	386	C	0	11.670	-10.769	-1.467
C						
HETATM	387	H	0	12.039	-11.484	-0.964
H						
HETATM	388	C	0	10.258	-10.667	-1.613
C						
HETATM	389	C	0	9.379	-11.605	-1.044
C						
HETATM	390	H	0	9.734	-12.324	-0.534
H						
HETATM	391	C	0	2.679	-12.694	2.049
C						
HETATM	392	S	0	-0.817	-15.295	-1.143
S						

HETATM	393	S	0	4.575	-17.195	-4.056
S						
HETATM	394	N	0	2.584	-13.289	-1.698
N						
HETATM	395	N	0	1.607	-15.292	-0.366
N						
HETATM	396	N	0	1.036	-16.355	0.283
N						
HETATM	397	N	0	3.971	-15.685	-1.779
N						
HETATM	398	C	0	3.153	-12.311	-2.389
C						
HETATM	399	H	0	4.082	-12.151	-2.276
H						
HETATM	400	C	0	2.440	-11.509	-3.271
C						
HETATM	401	H	0	2.880	-10.803	-3.732
H						
HETATM	402	C	0	1.106	-11.736	-3.482
C						
HETATM	403	H	0	0.611	-11.191	-4.082
H						
HETATM	404	C	0	0.497	-12.772	-2.801
C						
HETATM	405	H	0	-0.424	-12.966	-2.933
H						
HETATM	406	C	0	1.258	-13.530	-1.918
C						
HETATM	407	C	0	0.775	-14.652	-1.149
C						
HETATM	408	C	0	-0.227	-16.479	-0.007
C						
HETATM	409	C	0	-1.122	-17.506	0.550
C						
HETATM	410	C	0	-0.597	-18.577	1.307
C						
HETATM	411	H	0	0.342	-18.648	1.430
H						
HETATM	412	C	0	-1.414	-19.503	1.860
C						
HETATM	413	H	0	-1.039	-20.222	2.357
H						
HETATM	414	C	0	-2.825	-19.419	1.708
C						
HETATM	415	C	0	-3.712	-20.348	2.289
C						
HETATM	416	H	0	-3.365	-21.072	2.797
H						
HETATM	417	C	0	-5.069	-20.222	2.131
C						
HETATM	418	H	0	-5.650	-20.859	2.530
H						
HETATM	419	C	0	-5.608	-19.156	1.381
C						
HETATM	420	H	0	-6.548	-19.078	1.277
H						

HETATM	421	C	0	-4.777	-18.238	0.808
C						
HETATM	422	H	0	-5.147	-17.522	0.305
H						
HETATM	423	C	0	-3.366	-18.339	0.954
C						
HETATM	424	C	0	-2.488	-17.401	0.385
C						
HETATM	425	H	0	-2.842	-16.682	-0.125
H						
HETATM	426	C	0	4.213	-16.313	-2.708
C						
HETATM	427	Fe	0	3.830	11.749	0.472
Fe						
HETATM	428	S	0	8.092	12.541	1.286
S						
HETATM	429	S	0	2.700	14.441	4.197
S						
HETATM	430	N	0	4.692	10.534	1.840
N						
HETATM	431	N	0	5.668	12.537	0.508
N						
HETATM	432	N	0	6.239	13.599	-0.140
N						
HETATM	433	N	0	3.305	12.931	1.921
N						
HETATM	434	C	0	4.123	9.555	2.531
C						
HETATM	435	H	0	3.193	9.397	2.419
H						
HETATM	436	C	0	4.835	8.755	3.414
C						
HETATM	437	H	0	4.395	8.049	3.873
H						
HETATM	438	C	0	6.169	8.981	3.625
C						
HETATM	439	H	0	6.665	8.437	4.224
H						
HETATM	440	C	0	6.778	10.018	2.943
C						
HETATM	441	H	0	7.699	10.210	3.076
H						
HETATM	442	C	0	6.017	10.776	2.060
C						
HETATM	443	C	0	6.501	11.898	1.291
C						
HETATM	444	C	0	7.503	13.725	0.150
C						
HETATM	445	C	0	8.397	14.750	-0.408
C						
HETATM	446	C	0	7.873	15.823	-1.165
C						
HETATM	447	H	0	6.933	15.894	-1.288
H						
HETATM	448	C	0	8.689	16.749	-1.718
C						

HETATM	449	H	0	8.314	17.467	-2.214
H						
HETATM	450	C	0	10.100	16.664	-1.566
C						
HETATM	451	C	0	10.988	17.594	-2.147
C						
HETATM	452	H	0	10.641	18.318	-2.655
H						
HETATM	453	C	0	12.344	17.467	-1.988
C						
HETATM	454	H	0	12.926	18.105	-2.387
H						
HETATM	455	C	0	12.883	16.401	-1.240
C						
HETATM	456	H	0	13.824	16.323	-1.134
H						
HETATM	457	C	0	12.053	15.484	-0.666
C						
HETATM	458	H	0	12.422	14.768	-0.163
H						
HETATM	459	C	0	10.641	15.584	-0.813
C						
HETATM	460	C	0	9.763	14.647	-0.242
C						
HETATM	461	H	0	10.117	13.927	0.267
H						
HETATM	462	C	0	3.062	13.559	2.849
C						
HETATM	463	S	0	-0.433	10.956	-0.342
S						
HETATM	464	S	0	4.959	9.056	-3.254
S						
HETATM	465	N	0	2.968	12.964	-0.897
N						
HETATM	466	N	0	1.991	10.960	0.435
N						
HETATM	467	N	0	1.420	9.898	1.083
N						
HETATM	468	N	0	4.355	10.567	-0.978
N						
HETATM	469	C	0	3.537	13.942	-1.587
C						
HETATM	470	H	0	4.466	14.101	-1.475
H						
HETATM	471	C	0	2.824	14.742	-2.470
C						
HETATM	472	H	0	3.264	15.448	-2.930
H						
HETATM	473	C	0	1.490	14.516	-2.681
C						
HETATM	474	H	0	0.993	15.060	-3.281
H						
HETATM	475	C	0	0.881	13.479	-2.000
C						
HETATM	476	H	0	-0.041	13.287	-2.133
H						

HETATM	477	C	0	1.642	12.721	-1.116
C						
HETATM	478	C	0	1.158	11.599	-0.348
C						
HETATM	479	C	0	0.155	9.772	0.794
C						
HETATM	480	C	0	-0.738	8.747	1.352
C						
HETATM	481	C	0	-0.213	7.675	2.109
C						
HETATM	482	H	0	0.725	7.603	2.231
H						
HETATM	483	C	0	-1.030	6.748	2.661
C						
HETATM	484	H	0	-0.656	6.030	3.157
H						
HETATM	485	C	0	-2.441	6.833	2.509
C						
HETATM	486	C	0	-3.329	5.903	3.091
C						
HETATM	487	H	0	-2.981	5.180	3.599
H						
HETATM	488	C	0	-4.685	6.030	2.932
C						
HETATM	489	H	0	-5.266	5.393	3.330
H						
HETATM	490	C	0	-5.224	7.096	2.183
C						
HETATM	491	H	0	-6.164	7.174	2.077
H						
HETATM	492	C	0	-4.394	8.014	1.609
C						
HETATM	493	H	0	-4.764	8.730	1.107
H						
HETATM	494	C	0	-2.982	7.913	1.756
C						
HETATM	495	C	0	-2.104	8.850	1.185
C						
HETATM	496	H	0	-2.459	9.570	0.676
H						
HETATM	497	C	0	4.596	9.939	-1.906
C						
HETATM	498	Fe	0	0.000	0.000	0.000
Fe						
HETATM	499	S	0	4.334	0.821	0.853
S						
HETATM	500	S	0	-1.105	2.822	3.779
S						
HETATM	501	N	0	0.869	-1.278	1.305
N						
HETATM	502	N	0	1.844	0.825	0.049
N						
HETATM	503	N	0	2.426	1.914	-0.610
N						
HETATM	504	N	0	-0.520	1.137	1.498
N						

HETATM	505	C	0	0.290	-2.340	1.920
C						
HETATM	506	H	0	-0.752	-2.523	1.664
H						
HETATM	507	C	0	0.997	-3.148	2.843
C						
HETATM	508	H	0	0.492	-3.991	3.311
H						
HETATM	509	C	0	2.344	-2.845	3.143
C						
HETATM	510	H	0	2.910	-3.449	3.852
H						
HETATM	511	C	0	2.953	-1.738	2.508
C						
HETATM	512	H	0	3.978	-1.451	2.738
H						
HETATM	513	C	0	2.179	-0.992	1.594
C						
HETATM	514	C	0	2.680	0.168	0.847
C						
HETATM	515	C	0	3.712	2.062	-0.316
C						
HETATM	516	C	0	4.605	3.096	-0.873
C						
HETATM	517	C	0	4.061	4.199	-1.632
C						
HETATM	518	H	0	2.982	4.268	-1.766
H						
HETATM	519	C	0	4.915	5.149	-2.186
C						
HETATM	520	H	0	4.519	5.989	-2.760
H						
HETATM	521	C	0	6.348	5.036	-2.032
C						
HETATM	522	C	0	7.258	5.982	-2.626
C						
HETATM	523	H	0	6.847	6.810	-3.205
H						
HETATM	524	C	0	8.637	5.847	-2.444
C						
HETATM	525	H	0	9.330	6.550	-2.908
H						
HETATM	526	C	0	9.171	4.762	-1.662
C						
HETATM	527	H	0	10.253	4.683	-1.548
H						
HETATM	528	C	0	8.315	3.826	-1.082
C						
HETATM	529	H	0	8.706	2.986	-0.507
H						
HETATM	530	C	0	6.888	3.944	-1.254
C						
HETATM	531	C	0	5.988	2.993	-0.677
C						
HETATM	532	H	0	6.413	2.176	-0.090
H						

HETATM	533	C	0	-0.745	1.826	2.438
C						
HETATM	534	S	0	-4.334	-0.820	-0.854
S						
HETATM	535	S	0	1.104	-2.822	-3.779
S						
HETATM	536	N	0	-0.869	1.279	-1.305
N						
HETATM	537	N	0	-1.844	-0.824	-0.049
N						
HETATM	538	N	0	-2.426	-1.914	0.610
N						
HETATM	539	N	0	0.520	-1.136	-1.498
N						
HETATM	540	C	0	-0.290	2.341	-1.920
C						
HETATM	541	H	0	0.751	2.524	-1.664
H						
HETATM	542	C	0	-0.998	3.148	-2.843
C						
HETATM	543	H	0	-0.492	3.992	-3.311
H						
HETATM	544	C	0	-2.344	2.845	-3.143
C						
HETATM	545	H	0	-2.910	3.449	-3.852
H						
HETATM	546	C	0	-2.953	1.737	-2.508
C						
HETATM	547	H	0	-3.977	1.450	-2.739
H						
HETATM	548	C	0	-2.178	0.992	-1.594
C						
HETATM	549	C	0	-2.680	-0.168	-0.847
C						
HETATM	550	C	0	-3.711	-2.061	0.316
C						
HETATM	551	C	0	-4.605	-3.096	0.873
C						
HETATM	552	C	0	-4.061	-4.198	1.632
C						
HETATM	553	H	0	-2.982	-4.268	1.767
H						
HETATM	554	C	0	-4.916	-5.148	2.185
C						
HETATM	555	H	0	-4.520	-5.988	2.760
H						
HETATM	556	C	0	-6.348	-5.035	2.031
C						
HETATM	557	C	0	-7.258	-5.981	2.626
C						
HETATM	558	H	0	-6.849	-6.809	3.204
H						
HETATM	559	C	0	-8.637	-5.846	2.443
C						
HETATM	560	H	0	-9.331	-6.549	2.906
H						

HETATM	561	C	0	-9.171	-4.761	1.660
C						
HETATM	562	H	0	-10.253	-4.682	1.546
H						
HETATM	563	C	0	-8.315	-3.825	1.081
C						
HETATM	564	H	0	-8.706	-2.984	0.505
H						
HETATM	565	C	0	-6.888	-3.943	1.254
C						
HETATM	566	C	0	-5.988	-2.992	0.676
C						
HETATM	567	H	0	-6.413	-2.175	0.090
H						
HETATM	568	C	0	0.745	-1.826	-2.438
C						
HETATM	569	Fe	0	-3.830	-11.749	-0.472
Fe						
HETATM	570	S	0	0.433	-10.956	0.342
S						
HETATM	571	S	0	-4.959	-9.056	3.254
S						
HETATM	572	N	0	-2.968	-12.964	0.897
N						
HETATM	573	N	0	-1.991	-10.960	-0.435
N						
HETATM	574	N	0	-1.420	-9.898	-1.083
N						
HETATM	575	N	0	-4.355	-10.567	0.978
N						
HETATM	576	C	0	-3.537	-13.942	1.587
C						
HETATM	577	H	0	-4.466	-14.101	1.475
H						
HETATM	578	C	0	-2.824	-14.742	2.470
C						
HETATM	579	H	0	-3.264	-15.448	2.930
H						
HETATM	580	C	0	-1.490	-14.516	2.681
C						
HETATM	581	H	0	-0.993	-15.060	3.281
H						
HETATM	582	C	0	-0.881	-13.479	2.000
C						
HETATM	583	H	0	0.041	-13.287	2.133
H						
HETATM	584	C	0	-1.642	-12.721	1.116
C						
HETATM	585	C	0	-1.158	-11.599	0.348
C						
HETATM	586	C	0	-0.155	-9.772	-0.794
C						
HETATM	587	C	0	0.738	-8.747	-1.352
C						
HETATM	588	C	0	0.213	-7.675	-2.108
C						

HETATM	589	H	0	-0.725	-7.603	-2.231
H						
HETATM	590	C	0	1.030	-6.748	-2.661
C						
HETATM	591	H	0	0.656	-6.030	-3.157
H						
HETATM	592	C	0	2.441	-6.833	-2.509
C						
HETATM	593	C	0	3.329	-5.903	-3.091
C						
HETATM	594	H	0	2.981	-5.180	-3.599
H						
HETATM	595	C	0	4.685	-6.030	-2.932
C						
HETATM	596	H	0	5.266	-5.393	-3.330
H						
HETATM	597	C	0	5.224	-7.096	-2.183
C						
HETATM	598	H	0	6.164	-7.174	-2.077
H						
HETATM	599	C	0	4.394	-8.014	-1.609
C						
HETATM	600	H	0	4.764	-8.730	-1.107
H						
HETATM	601	C	0	2.982	-7.913	-1.756
C						
HETATM	602	C	0	2.104	-8.850	-1.185
C						
HETATM	603	H	0	2.459	-9.570	-0.676
H						
HETATM	604	C	0	-4.596	-9.939	1.906
C						
HETATM	605	S	0	-8.092	-12.541	-1.286
S						
HETATM	606	S	0	-2.700	-14.441	-4.197
S						
HETATM	607	N	0	-4.692	-10.534	-1.840
N						
HETATM	608	N	0	-5.668	-12.537	-0.508
N						
HETATM	609	N	0	-6.239	-13.599	0.140
N						
HETATM	610	N	0	-3.305	-12.931	-1.921
N						
HETATM	611	C	0	-4.123	-9.555	-2.531
C						
HETATM	612	H	0	-3.193	-9.397	-2.419
H						
HETATM	613	C	0	-4.835	-8.755	-3.414
C						
HETATM	614	H	0	-4.395	-8.049	-3.873
H						
HETATM	615	C	0	-6.169	-8.981	-3.625
C						
HETATM	616	H	0	-6.665	-8.437	-4.224
H						

HETATM	617	C	0	-6.778	-10.018	-2.943
C						
HETATM	618	H	0	-7.699	-10.210	-3.076
H						
HETATM	619	C	0	-6.017	-10.776	-2.060
C						
HETATM	620	C	0	-6.501	-11.898	-1.291
C						
HETATM	621	C	0	-7.503	-13.725	-0.150
C						
HETATM	622	C	0	-8.397	-14.750	0.408
C						
HETATM	623	C	0	-7.873	-15.823	1.165
C						
HETATM	624	H	0	-6.933	-15.894	1.288
H						
HETATM	625	C	0	-8.689	-16.749	1.718
C						
HETATM	626	H	0	-8.314	-17.467	2.214
H						
HETATM	627	C	0	-10.100	-16.664	1.566
C						
HETATM	628	C	0	-10.988	-17.594	2.147
C						
HETATM	629	H	0	-10.641	-18.318	2.655
H						
HETATM	630	C	0	-12.344	-17.468	1.988
C						
HETATM	631	H	0	-12.926	-18.105	2.387
H						
HETATM	632	C	0	-12.883	-16.402	1.240
C						
HETATM	633	H	0	-13.824	-16.323	1.134
H						
HETATM	634	C	0	-12.053	-15.484	0.666
C						
HETATM	635	H	0	-12.422	-14.768	0.163
H						
HETATM	636	C	0	-10.641	-15.584	0.813
C						
HETATM	637	C	0	-9.763	-14.647	0.242
C						
HETATM	638	H	0	-10.117	-13.927	-0.267
H						
HETATM	639	C	0	-3.062	-13.559	-2.849
C						
HETATM	640	Fe	0	-3.446	14.503	0.330
Fe						
HETATM	641	S	0	0.817	15.295	1.143
S						
HETATM	642	S	0	-4.575	17.195	4.056
S						
HETATM	643	N	0	-2.584	13.289	1.698
N						
HETATM	644	N	0	-1.607	15.292	0.366
N						

HETATM	645	N	0	-1.036	16.354	-0.283
N						
HETATM	646	N	0	-3.971	15.685	1.779
N						
HETATM	647	C	0	-3.153	12.310	2.389
C						
HETATM	648	H	0	-4.082	12.151	2.276
H						
HETATM	649	C	0	-2.440	11.509	3.271
C						
HETATM	650	H	0	-2.880	10.803	3.732
H						
HETATM	651	C	0	-1.106	11.736	3.482
C						
HETATM	652	H	0	-0.611	11.191	4.082
H						
HETATM	653	C	0	-0.497	12.772	2.801
C						
HETATM	654	H	0	0.424	12.966	2.933
H						
HETATM	655	C	0	-1.258	13.530	1.918
C						
HETATM	656	C	0	-0.775	14.652	1.149
C						
HETATM	657	C	0	0.227	16.479	0.007
C						
HETATM	658	C	0	1.122	17.505	-0.550
C						
HETATM	659	C	0	0.597	18.577	-1.307
C						
HETATM	660	H	0	-0.342	18.648	-1.430
H						
HETATM	661	C	0	1.414	19.503	-1.859
C						
HETATM	662	H	0	1.039	20.222	-2.357
H						
HETATM	663	C	0	2.825	19.419	-1.708
C						
HETATM	664	C	0	3.712	20.348	-2.289
C						
HETATM	665	H	0	3.365	21.072	-2.797
H						
HETATM	666	C	0	5.069	20.222	-2.131
C						
HETATM	667	H	0	5.650	20.859	-2.530
H						
HETATM	668	C	0	5.608	19.156	-1.381
C						
HETATM	669	H	0	6.548	19.078	-1.277
H						
HETATM	670	C	0	4.777	18.238	-0.808
C						
HETATM	671	H	0	5.147	17.522	-0.305
H						
HETATM	672	C	0	3.366	18.339	-0.954
C						

HETATM	673	C	0	2.488	17.401	-0.385
C						
HETATM	674	H	0	2.842	16.682	0.125
H						
HETATM	675	C	0	-4.213	16.313	2.708
C						
HETATM	676	S	0	-7.709	13.711	-0.484
S						
HETATM	677	S	0	-2.316	11.811	-3.397
S						
HETATM	678	N	0	-4.308	15.718	-1.039
N						
HETATM	679	N	0	-5.285	13.714	0.293
N						
HETATM	680	N	0	-5.856	12.652	0.942
N						
HETATM	681	N	0	-2.921	13.321	-1.120
N						
HETATM	682	C	0	-3.739	16.696	-1.730
C						
HETATM	683	H	0	-2.809	16.855	-1.617
H						
HETATM	684	C	0	-4.451	17.497	-2.612
C						
HETATM	685	H	0	-4.011	18.203	-3.073
H						
HETATM	686	C	0	-5.785	17.271	-2.823
C						
HETATM	687	H	0	-6.282	17.815	-3.423
H						
HETATM	688	C	0	-6.395	16.233	-2.142
C						
HETATM	689	H	0	-7.316	16.041	-2.274
H						
HETATM	690	C	0	-5.633	15.476	-1.259
C						
HETATM	691	C	0	-6.117	14.354	-0.490
C						
HETATM	692	C	0	-7.120	12.526	0.652
C						
HETATM	693	C	0	-8.013	11.501	1.209
C						
HETATM	694	C	0	-7.488	10.429	1.966
C						
HETATM	695	H	0	-6.550	10.358	2.089
H						
HETATM	696	C	0	-8.305	9.503	2.519
C						
HETATM	697	H	0	-7.932	8.785	3.016
H						
HETATM	698	C	0	-9.716	9.587	2.367
C						
HETATM	699	C	0	-10.604	8.658	2.948
C						
HETATM	700	H	0	-10.257	7.935	3.456
H						

HETATM	701	C	0	-11.960	8.785	2.790
C						
HETATM	702	H	0	-12.542	8.147	3.189
H						
HETATM	703	C	0	-12.499	9.851	2.040
C						
HETATM	704	H	0	-13.440	9.929	1.936
H						
HETATM	705	C	0	-11.670	10.769	1.467
C						
HETATM	706	H	0	-12.039	11.484	0.964
H						
HETATM	707	C	0	-10.258	10.667	1.613
C						
HETATM	708	C	0	-9.379	11.605	1.044
C						
HETATM	709	H	0	-9.734	12.324	0.534
H						
HETATM	710	C	0	-2.679	12.693	-2.049
C						
HETATM	711	Fe	0	-7.275	2.754	-0.142
Fe						
HETATM	712	S	0	-3.013	3.546	0.672
S						
HETATM	713	S	0	-8.404	5.448	3.584
S						
HETATM	714	N	0	-6.413	1.540	1.226
N						
HETATM	715	N	0	-5.436	3.543	-0.106
N						
HETATM	716	N	0	-4.866	4.606	-0.754
N						
HETATM	717	N	0	-7.801	3.937	1.307
N						
HETATM	718	C	0	-6.982	0.562	1.917
C						
HETATM	719	H	0	-7.913	0.402	1.805
H						
HETATM	720	C	0	-6.271	-0.240	2.800
C						
HETATM	721	H	0	-6.709	-0.946	3.259
H						
HETATM	722	C	0	-4.937	-0.013	3.010
C						
HETATM	723	H	0	-4.440	-0.557	3.611
H						
HETATM	724	C	0	-4.326	1.025	2.329
C						
HETATM	725	H	0	-3.406	1.217	2.462
H						
HETATM	726	C	0	-5.087	1.782	1.447
C						
HETATM	727	C	0	-4.604	2.904	0.677
C						
HETATM	728	C	0	-3.602	4.731	-0.464
C						

HETATM	729	C	0	-2.707	5.757	-1.022
C						
HETATM	730	C	0	-3.232	6.829	-1.779
C						
HETATM	731	H	0	-4.171	6.900	-1.902
H						
HETATM	732	C	0	-2.416	7.755	-2.331
C						
HETATM	733	H	0	-2.790	8.473	-2.828
H						
HETATM	734	C	0	-1.004	7.670	-2.179
C						
HETATM	735	C	0	-0.117	8.599	-2.761
C						
HETATM	736	H	0	-0.464	9.323	-3.269
H						
HETATM	737	C	0	1.239	8.473	-2.602
C						
HETATM	738	H	0	1.821	9.110	-3.001
H						
HETATM	739	C	0	1.778	7.408	-1.854
C						
HETATM	740	H	0	2.719	7.330	-1.748
H						
HETATM	741	C	0	0.948	6.489	-1.280
C						
HETATM	742	H	0	1.318	5.774	-0.777
H						
HETATM	743	C	0	-0.464	6.591	-1.427
C						
HETATM	744	C	0	-1.342	5.652	-0.856
C						
HETATM	745	H	0	-0.988	4.933	-0.346
H						
HETATM	746	C	0	-8.043	4.564	2.235
C						
HETATM	747	S	0	-11.538	1.962	-0.956
S						
HETATM	748	S	0	-6.146	0.062	-3.868
S						
HETATM	749	N	0	-8.137	3.969	-1.511
N						
HETATM	750	N	0	-9.114	1.966	-0.179
N						
HETATM	751	N	0	-9.685	0.903	0.469
N						
HETATM	752	N	0	-6.750	1.572	-1.592
N						
HETATM	753	C	0	-7.568	4.947	-2.201
C						
HETATM	754	H	0	-6.638	5.106	-2.089
H						
HETATM	755	C	0	-8.281	5.748	-3.084
C						
HETATM	756	H	0	-7.841	6.454	-3.544
H						

HETATM	757	C	0	-9.615	5.522	-3.295
C						
HETATM	758	H	0	-10.111	6.066	-3.895
H						
HETATM	759	C	0	-10.224	4.485	-2.614
C						
HETATM	760	H	0	-11.145	4.292	-2.747
H						
HETATM	761	C	0	-9.463	3.727	-1.730
C						
HETATM	762	C	0	-9.946	2.605	-0.962
C						
HETATM	763	C	0	-10.949	0.778	0.180
C						
HETATM	764	C	0	-11.843	-0.247	0.738
C						
HETATM	765	C	0	-11.318	-1.320	1.494
C						
HETATM	766	H	0	-10.379	-1.391	1.617
H						
HETATM	767	C	0	-12.135	-2.246	2.047
C						
HETATM	768	H	0	-11.761	-2.964	2.543
H						
HETATM	769	C	0	-13.545	-2.161	1.895
C						
HETATM	770	C	0	-14.434	-3.091	2.477
C						
HETATM	771	H	0	-14.087	-3.814	2.984
H						
HETATM	772	C	0	-15.790	-2.964	2.318
C						
HETATM	773	H	0	-16.372	-3.601	2.716
H						
HETATM	774	C	0	-16.328	-1.898	1.569
C						
HETATM	775	H	0	-17.269	-1.820	1.463
H						
HETATM	776	C	0	-15.499	-0.980	0.995
C						
HETATM	777	H	0	-15.868	-0.264	0.493
H						
HETATM	778	C	0	-14.087	-1.082	1.142
C						
HETATM	779	C	0	-13.209	-0.144	0.571
C						
HETATM	780	H	0	-13.563	0.576	0.062
H						
HETATM	781	C	0	-6.508	0.945	-2.520
C						
HETATM	782	Fe	0	-11.105	-8.994	-0.614
Fe						
HETATM	783	S	0	-6.842	-8.202	0.200
S						
HETATM	784	S	0	-12.234	-6.301	3.112
S						

HETATM	785	N	0	-10.243	-10.209	0.755
N						
HETATM	786	N	0	-9.267	-8.206	-0.577
N						
HETATM	787	N	0	-8.695	-7.143	-1.225
N						
HETATM	788	N	0	-11.630	-7.812	0.835
N						
HETATM	789	C	0	-10.811	-11.187	1.445
C						
HETATM	790	H	0	-11.742	-11.347	1.332
H						
HETATM	791	C	0	-10.100	-11.988	2.328
C						
HETATM	792	H	0	-10.539	-12.693	2.788
H						
HETATM	793	C	0	-8.766	-11.761	2.539
C						
HETATM	794	H	0	-8.269	-12.306	3.139
H						
HETATM	795	C	0	-8.156	-10.724	1.858
C						
HETATM	796	H	0	-7.235	-10.532	1.991
H						
HETATM	797	C	0	-8.917	-9.967	0.974
C						
HETATM	798	C	0	-8.434	-8.845	0.205
C						
HETATM	799	C	0	-7.431	-7.017	-0.937
C						
HETATM	800	C	0	-6.537	-5.992	-1.494
C						
HETATM	801	C	0	-7.063	-4.920	-2.251
C						
HETATM	802	H	0	-8.001	-4.848	-2.374
H						
HETATM	803	C	0	-6.245	-3.993	-2.803
C						
HETATM	804	H	0	-6.620	-3.276	-3.300
H						
HETATM	805	C	0	-4.835	-4.079	-2.651
C						
HETATM	806	C	0	-3.946	-3.149	-3.233
C						
HETATM	807	H	0	-4.294	-2.426	-3.741
H						
HETATM	808	C	0	-2.590	-3.276	-3.075
C						
HETATM	809	H	0	-2.008	-2.639	-3.472
H						
HETATM	810	C	0	-2.052	-4.341	-2.325
C						
HETATM	811	H	0	-1.110	-4.419	-2.219
H						
HETATM	812	C	0	-2.881	-5.259	-1.751
C						

HETATM	813	H	0	-2.512	-5.975	-1.249
H						
HETATM	814	C	0	-4.293	-5.158	-1.898
C						
HETATM	815	C	0	-5.171	-6.096	-1.328
C						
HETATM	816	H	0	-4.817	-6.816	-0.818
H						
HETATM	817	C	0	-11.872	-7.185	1.764
C						
HETATM	818	S	0	-15.368	-9.786	-1.428
S						
HETATM	819	S	0	-9.975	-11.687	-4.340
S						
HETATM	820	N	0	-11.967	-7.780	-1.982
N						
HETATM	821	N	0	-12.943	-9.782	-0.650
N						
HETATM	822	N	0	-13.514	-10.845	-0.002
N						
HETATM	823	N	0	-10.580	-10.177	-2.063
N						
HETATM	824	C	0	-11.398	-6.801	-2.674
C						
HETATM	825	H	0	-10.468	-6.642	-2.561
H						
HETATM	826	C	0	-12.110	-6.000	-3.556
C						
HETATM	827	H	0	-11.670	-5.295	-4.015
H						
HETATM	828	C	0	-13.444	-6.227	-3.767
C						
HETATM	829	H	0	-13.940	-5.682	-4.367
H						
HETATM	830	C	0	-14.054	-7.264	-3.085
C						
HETATM	831	H	0	-14.974	-7.456	-3.218
H						
HETATM	832	C	0	-13.293	-8.021	-2.203
C						
HETATM	833	C	0	-13.776	-9.144	-1.433
C						
HETATM	834	C	0	-14.778	-10.971	-0.292
C						
HETATM	835	C	0	-15.673	-11.996	0.266
C						
HETATM	836	C	0	-15.147	-13.069	1.023
C						
HETATM	837	H	0	-14.209	-13.140	1.146
H						
HETATM	838	C	0	-15.964	-13.995	1.576
C						
HETATM	839	H	0	-15.590	-14.712	2.072
H						
HETATM	840	C	0	-17.375	-13.910	1.423
C						

HETATM	841	C	0	-18.263	-14.839	2.004
C						
HETATM	842	H	0	-17.916	-15.563	2.513
H						
HETATM	843	C	0	-19.620	-14.713	1.846
C						
HETATM	844	H	0	-20.202	-15.350	2.245
H						
HETATM	845	C	0	-20.158	-13.647	1.098
C						
HETATM	846	H	0	-21.099	-13.569	0.992
H						
HETATM	847	C	0	-19.328	-12.729	0.524
C						
HETATM	848	H	0	-19.698	-12.013	0.021
H						
HETATM	849	C	0	-17.916	-12.830	0.671
C						
HETATM	850	C	0	-17.039	-11.893	0.100
C						
HETATM	851	H	0	-17.393	-11.173	-0.410
H						
HETATM	852	C	0	-10.338	-10.804	-2.992
C						
HETATM	853	Fe	0	-10.721	17.258	0.187
Fe						
HETATM	854	S	0	-6.458	18.049	1.001
S						
HETATM	855	S	0	-11.851	19.950	3.914
S						
HETATM	856	N	0	-9.859	16.043	1.555
N						
HETATM	857	N	0	-8.882	18.046	0.223
N						
HETATM	858	N	0	-8.311	19.109	-0.425
N						
HETATM	859	N	0	-11.246	18.440	1.637
N						
HETATM	860	C	0	-10.428	15.065	2.247
C						
HETATM	861	H	0	-11.358	14.906	2.134
H						
HETATM	862	C	0	-9.716	14.263	3.129
C						
HETATM	863	H	0	-10.156	13.558	3.589
H						
HETATM	864	C	0	-8.382	14.490	3.340
C						
HETATM	865	H	0	-7.885	13.946	3.940
H						
HETATM	866	C	0	-7.773	15.527	2.659
C						
HETATM	867	H	0	-6.851	15.720	2.791
H						
HETATM	868	C	0	-8.534	16.284	1.776
C						

HETATM	869	C	0	-8.050	17.406	1.007
C						
HETATM	870	C	0	-7.047	19.234	-0.135
C						
HETATM	871	C	0	-6.153	20.260	-0.692
C						
HETATM	872	C	0	-6.679	21.332	-1.449
C						
HETATM	873	H	0	-7.617	21.403	-1.572
H						
HETATM	874	C	0	-5.862	22.258	-2.002
C						
HETATM	875	H	0	-6.235	22.976	-2.499
H						
HETATM	876	C	0	-4.451	22.174	-1.850
C						
HETATM	877	C	0	-3.562	23.102	-2.431
C						
HETATM	878	H	0	-3.910	23.826	-2.939
H						
HETATM	879	C	0	-2.206	22.976	-2.273
C						
HETATM	880	H	0	-1.624	23.613	-2.672
H						
HETATM	881	C	0	-1.668	21.910	-1.524
C						
HETATM	882	H	0	-0.728	21.832	-1.419
H						
HETATM	883	C	0	-2.497	20.992	-0.951
C						
HETATM	884	H	0	-2.128	20.276	-0.447
H						
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HETATM	976	C	0	-18.224	3.533	0.038
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HETATM	984	H	0	-21.362	-1.060	2.842
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HETATM	985	C	0	-23.065	-0.210	2.176
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HETATM	993	H	0	-20.838	3.331	-0.080
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HETATM	997	S	0	-19.509	-3.547	2.970
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HETATM	1007	H	0	-15.545	-9.551	2.997
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HETATM	1008	C	0	-15.431	-7.970	1.715
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HETATM 1016	C	0	-13.520	-1.239	-2.945
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HETATM 1017	H	0	-13.895	-0.521	-3.442
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HETATM 1024	H	0	-8.386	-1.665	-2.361
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HETATM 1025	C	0	-10.157	-2.505	-1.893
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HETATM 1026	H	0	-9.788	-3.220	-1.391
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HETATM 1027	C	0	-11.568	-2.404	-2.040
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HETATM 1028	C	0	-12.446	-3.341	-1.470
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HETATM 1029	H	0	-12.093	-4.061	-0.960
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HETATM 1030	C	0	-19.148	-4.430	1.622
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CONNECT 54   53   55   69

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CONNECT 975 974 960 963
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CONNECT 994 961 965
CONNECT 995 1001 1036
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CONNECT 997 1030
CONNECT 998 1002 1010
CONNECT 999 1000 1011
CONNECT 1000 999 1012
CONNECT 1001 995 1030
CONNECT 1002 998 1003 1004
CONNECT 1003 1002
CONNECT 1004 1002 1005 1006
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CONNECT 1006 1004 1007 1008
CONNECT 1007 1006
CONNECT 1008 1006 1009 1010
CONNECT 1009 1008
CONNECT 1010 998 1008 1011
CONNECT 1011 996 999 1010
CONNECT 1012 996 1000 1013
CONNECT 1013 1012 1014 1028
CONNECT 1014 1013 1015 1016
CONNECT 1015 1014
CONNECT 1016 1014 1017 1018
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CONNECT 1019 1018 1020 1021
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CONNECT 1024 1023
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CONNECT 1036 995 1065
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CONNECT 1060 1058 1061 1062
CONNECT 1061 1060
CONNECT 1062 1060 1053 1063
CONNECT 1063 1048 1062 1064
CONNECT 1064 1063
CONNECT 1065 1032 1036

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Table 2. PDB file of the optimised structure of the 15-nuclear model of the HS centre in LS matrix

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TITLE          CSD ENTRY jmk-126-9-90kslow
REMARK        1 File created by GaussView 6.0.16
HETATM        1 Fe          0      -18.386   6.224  -0.757
Fe
HETATM        2 S          0      -22.650   7.012  -1.570
S
HETATM        3 S          0      -17.259   8.917  -4.482
S
HETATM        4 N          0      -19.247   5.009  -2.125
N

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HETATM	5	N	0	-20.225	7.010	-0.793
N						
HETATM	6	N	0	-20.797	8.072	-0.144
N						
HETATM	7	N	0	-17.862	7.407	-2.205
N						
HETATM	8	C	0	-18.677	4.030	-2.816
C						
HETATM	9	H	0	-17.747	3.872	-2.703
H						
HETATM	10	C	0	-19.388	3.229	-3.698
C						
HETATM	11	H	0	-18.948	2.524	-4.158
H						
HETATM	12	C	0	-20.723	3.454	-3.909
C						
HETATM	13	H	0	-21.219	2.909	-4.509
H						
HETATM	14	C	0	-21.333	4.491	-3.227
C						
HETATM	15	H	0	-22.254	4.682	-3.360
H						
HETATM	16	C	0	-20.572	5.249	-2.345
C						
HETATM	17	C	0	-21.057	6.370	-1.575
C						
HETATM	18	C	0	-22.061	8.197	-0.434
C						
HETATM	19	C	0	-22.956	9.221	0.123
C						
HETATM	20	C	0	-22.432	10.295	0.881
C						
HETATM	21	H	0	-21.493	10.366	1.004
H						
HETATM	22	C	0	-23.250	11.220	1.433
C						
HETATM	23	H	0	-22.876	11.938	1.930
H						
HETATM	24	C	0	-24.660	11.133	1.281
C						
HETATM	25	C	0	-25.549	12.063	1.862
C						
HETATM	26	H	0	-25.202	12.787	2.371
H						
HETATM	27	C	0	-26.905	11.935	1.704
C						
HETATM	28	H	0	-27.487	12.572	2.103
H						
HETATM	29	C	0	-27.443	10.869	0.955
C						
HETATM	30	H	0	-28.383	10.790	0.849
H						
HETATM	31	C	0	-26.613	9.951	0.381
C						
HETATM	32	H	0	-26.982	9.235	-0.121
H						

HETATM	33	C	0	-25.201	10.053	0.528
C						
HETATM	34	C	0	-24.322	9.117	-0.042
C						
HETATM	35	H	0	-24.676	8.396	-0.552
H						
HETATM	36	C	0	-17.621	8.034	-3.134
C						
HETATM	37	S	0	-14.122	5.435	0.057
S						
HETATM	38	S	0	-19.512	3.530	2.970
S						
HETATM	39	N	0	-17.525	7.439	0.613
N						
HETATM	40	N	0	-16.546	5.437	-0.719
N						
HETATM	41	N	0	-15.974	4.375	-1.368
N						
HETATM	42	N	0	-18.910	5.041	0.693
N						
HETATM	43	C	0	-18.094	8.417	1.303
C						
HETATM	44	H	0	-19.024	8.576	1.190
H						
HETATM	45	C	0	-17.382	9.218	2.185
C						
HETATM	46	H	0	-17.823	9.923	2.646
H						
HETATM	47	C	0	-16.048	8.993	2.397
C						
HETATM	48	H	0	-15.553	9.537	2.997
H						
HETATM	49	C	0	-15.438	7.956	1.715
C						
HETATM	50	H	0	-14.518	7.765	1.848
H						
HETATM	51	C	0	-16.199	7.198	0.832
C						
HETATM	52	C	0	-15.714	6.077	0.063
C						
HETATM	53	C	0	-14.711	4.250	-1.079
C						
HETATM	54	C	0	-13.815	3.226	-1.636
C						
HETATM	55	C	0	-14.339	2.153	-2.393
C						
HETATM	56	H	0	-15.278	2.080	-2.516
H						
HETATM	57	C	0	-13.521	1.227	-2.945
C						
HETATM	58	H	0	-13.896	0.509	-3.442
H						
HETATM	59	C	0	-12.111	1.314	-2.793
C						
HETATM	60	C	0	-11.222	0.384	-3.375
C						

HETATM	61	H	0	-11.569	-0.339	-3.883
H						
HETATM	62	C	0	-9.866	0.513	-3.217
C						
HETATM	63	H	0	-9.284	-0.124	-3.615
H						
HETATM	64	C	0	-9.328	1.578	-2.467
C						
HETATM	65	H	0	-8.388	1.657	-2.361
H						
HETATM	66	C	0	-10.159	2.496	-1.893
C						
HETATM	67	H	0	-9.790	3.212	-1.391
H						
HETATM	68	C	0	-11.570	2.394	-2.040
C						
HETATM	69	C	0	-12.449	3.330	-1.470
C						
HETATM	70	H	0	-12.096	4.050	-0.960
H						
HETATM	71	C	0	-19.152	4.413	1.622
C						
HETATM	72	Fe	0	-14.546	-5.522	-0.284
Fe						
HETATM	73	S	0	-18.809	-4.733	-1.098
S						
HETATM	74	S	0	-13.419	-2.828	-4.010
S						
HETATM	75	N	0	-15.407	-6.737	-1.653
N						
HETATM	76	N	0	-16.386	-4.735	-0.321
N						
HETATM	77	N	0	-16.958	-3.672	0.327
N						
HETATM	78	N	0	-14.022	-4.339	-1.734
N						
HETATM	79	C	0	-14.837	-7.714	-2.344
C						
HETATM	80	H	0	-13.907	-7.873	-2.231
H						
HETATM	81	C	0	-15.549	-8.517	-3.226
C						
HETATM	82	H	0	-15.108	-9.222	-3.686
H						
HETATM	83	C	0	-16.883	-8.291	-3.438
C						
HETATM	84	H	0	-17.378	-8.836	-4.037
H						
HETATM	85	C	0	-17.493	-7.255	-2.756
C						
HETATM	86	H	0	-18.414	-7.063	-2.889
H						
HETATM	87	C	0	-16.733	-6.497	-1.873
C						
HETATM	88	C	0	-17.217	-5.375	-1.104
C						

HETATM	89	C	0	-18.221	-3.549	0.038
C						
HETATM	90	C	0	-19.116	-2.524	0.596
C						
HETATM	91	C	0	-18.592	-1.451	1.352
C						
HETATM	92	H	0	-17.653	-1.379	1.475
H						
HETATM	93	C	0	-19.410	-0.526	1.905
C						
HETATM	94	H	0	-19.036	0.193	2.401
H						
HETATM	95	C	0	-20.821	-0.612	1.752
C						
HETATM	96	C	0	-21.709	0.317	2.335
C						
HETATM	97	H	0	-21.363	1.041	2.842
H						
HETATM	98	C	0	-23.065	0.190	2.176
C						
HETATM	99	H	0	-23.648	0.826	2.574
H						
HETATM	100	C	0	-23.603	-0.877	1.427
C						
HETATM	101	H	0	-24.544	-0.956	1.321
H						
HETATM	102	C	0	-22.772	-1.794	0.853
C						
HETATM	103	H	0	-23.141	-2.510	0.350
H						
HETATM	104	C	0	-21.361	-1.691	1.000
C						
HETATM	105	C	0	-20.482	-2.629	0.429
C						
HETATM	106	H	0	-20.835	-3.349	-0.081
H						
HETATM	107	C	0	-13.780	-3.711	-2.662
C						
HETATM	108	S	0	-10.283	-6.310	0.530
S						
HETATM	109	S	0	-15.672	-8.216	3.441
S						
HETATM	110	N	0	-13.685	-4.306	1.084
N						
HETATM	111	N	0	-12.706	-6.309	-0.248
N						
HETATM	112	N	0	-12.134	-7.371	-0.896
N						
HETATM	113	N	0	-15.070	-6.705	1.165
N						
HETATM	114	C	0	-14.255	-3.329	1.775
C						
HETATM	115	H	0	-15.185	-3.170	1.663
H						
HETATM	116	C	0	-13.543	-2.526	2.658
C						

HETATM	117	H	0	-13.983	-1.821	3.117
H						
HETATM	118	C	0	-12.209	-2.752	2.868
C						
HETATM	119	H	0	-11.713	-2.208	3.468
H						
HETATM	120	C	0	-11.598	-3.789	2.187
C						
HETATM	121	H	0	-10.677	-3.980	2.320
H						
HETATM	122	C	0	-12.359	-4.547	1.304
C						
HETATM	123	C	0	-11.874	-5.669	0.535
C						
HETATM	124	C	0	-10.870	-7.495	-0.606
C						
HETATM	125	C	0	-9.976	-8.520	-1.164
C						
HETATM	126	C	0	-10.499	-9.592	-1.922
C						
HETATM	127	H	0	-11.438	-9.665	-2.044
H						
HETATM	128	C	0	-9.682	-10.518	-2.473
C						
HETATM	129	H	0	-10.055	-11.236	-2.970
H						
HETATM	130	C	0	-8.271	-10.432	-2.322
C						
HETATM	131	C	0	-7.383	-11.360	-2.903
C						
HETATM	132	H	0	-7.729	-12.084	-3.412
H						
HETATM	133	C	0	-6.027	-11.233	-2.745
C						
HETATM	134	H	0	-5.444	-11.870	-3.143
H						
HETATM	135	C	0	-5.488	-10.167	-1.996
C						
HETATM	136	H	0	-4.548	-10.088	-1.890
H						
HETATM	137	C	0	-6.319	-9.249	-1.422
C						
HETATM	138	H	0	-5.950	-8.534	-0.920
H						
HETATM	139	C	0	-7.731	-9.352	-1.569
C						
HETATM	140	C	0	-8.610	-8.415	-0.998
C						
HETATM	141	H	0	-8.256	-7.695	-0.489
H						
HETATM	142	C	0	-15.311	-7.332	2.093
C						
HETATM	143	Fe	0	-10.706	-17.267	0.187
Fe						
HETATM	144	S	0	-14.969	-16.479	-0.627
S						

HETATM	145	S	0	-9.579	-14.574	-3.539
S						
HETATM	146	N	0	-11.567	-18.482	-1.181
N						
HETATM	147	N	0	-12.546	-16.480	0.151
N						
HETATM	148	N	0	-13.117	-15.418	0.799
N						
HETATM	149	N	0	-10.181	-16.084	-1.263
N						
HETATM	150	C	0	-10.997	-19.460	-1.872
C						
HETATM	151	H	0	-10.067	-19.618	-1.760
H						
HETATM	152	C	0	-11.708	-20.262	-2.755
C						
HETATM	153	H	0	-11.269	-20.968	-3.215
H						
HETATM	154	C	0	-13.042	-20.036	-2.965
C						
HETATM	155	H	0	-13.538	-20.581	-3.565
H						
HETATM	156	C	0	-13.654	-19.000	-2.285
C						
HETATM	157	H	0	-14.574	-18.808	-2.417
H						
HETATM	158	C	0	-12.893	-18.242	-1.401
C						
HETATM	159	C	0	-13.377	-17.120	-0.632
C						
HETATM	160	C	0	-14.381	-15.293	0.509
C						
HETATM	161	C	0	-15.276	-14.269	1.067
C						
HETATM	162	C	0	-14.753	-13.196	1.824
C						
HETATM	163	H	0	-13.813	-13.125	1.947
H						
HETATM	164	C	0	-15.569	-12.271	2.376
C						
HETATM	165	H	0	-15.196	-11.552	2.873
H						
HETATM	166	C	0	-16.981	-12.357	2.225
C						
HETATM	167	C	0	-17.869	-11.428	2.806
C						
HETATM	168	H	0	-17.523	-10.705	3.314
H						
HETATM	169	C	0	-19.226	-11.556	2.648
C						
HETATM	170	H	0	-19.808	-10.919	3.046
H						
HETATM	171	C	0	-19.763	-12.622	1.898
C						
HETATM	172	H	0	-20.704	-12.701	1.793
H						

HETATM	173	C	0	-18.932	-13.540	1.325
C						
HETATM	174	H	0	-19.302	-14.255	0.822
H						
HETATM	175	C	0	-17.521	-13.437	1.471
C						
HETATM	176	C	0	-16.642	-14.374	0.902
C						
HETATM	177	H	0	-16.996	-15.093	0.392
H						
HETATM	178	C	0	-9.940	-15.457	-2.191
C						
HETATM	179	S	0	-6.442	-18.055	1.001
S						
HETATM	180	S	0	-11.833	-19.960	3.914
S						
HETATM	181	N	0	-9.845	-16.052	1.555
N						
HETATM	182	N	0	-8.867	-18.054	0.223
N						
HETATM	183	N	0	-8.294	-19.116	-0.425
N						
HETATM	184	N	0	-11.230	-18.450	1.637
N						
HETATM	185	C	0	-10.415	-15.074	2.247
C						
HETATM	186	H	0	-11.345	-14.915	2.134
H						
HETATM	187	C	0	-9.703	-14.272	3.129
C						
HETATM	188	H	0	-10.144	-13.567	3.589
H						
HETATM	189	C	0	-8.369	-14.498	3.340
C						
HETATM	190	H	0	-7.873	-13.952	3.940
H						
HETATM	191	C	0	-7.759	-15.534	2.659
C						
HETATM	192	H	0	-6.837	-15.726	2.791
H						
HETATM	193	C	0	-8.520	-16.292	1.776
C						
HETATM	194	C	0	-8.035	-17.414	1.007
C						
HETATM	195	C	0	-7.031	-19.240	-0.135
C						
HETATM	196	C	0	-6.135	-20.265	-0.692
C						
HETATM	197	C	0	-6.660	-21.338	-1.449
C						
HETATM	198	H	0	-7.598	-21.409	-1.572
H						
HETATM	199	C	0	-5.842	-22.263	-2.002
C						
HETATM	200	H	0	-6.215	-22.982	-2.499
H						

HETATM	201	C	0	-4.431	-22.177	-1.850
C						
HETATM	202	C	0	-3.542	-23.106	-2.431
C						
HETATM	203	H	0	-3.889	-23.829	-2.939
H						
HETATM	204	C	0	-2.186	-22.978	-2.273
C						
HETATM	205	H	0	-1.604	-23.615	-2.672
H						
HETATM	206	C	0	-1.649	-21.912	-1.524
C						
HETATM	207	H	0	-0.708	-21.833	-1.419
H						
HETATM	208	C	0	-2.479	-20.994	-0.951
C						
HETATM	209	H	0	-2.110	-20.278	-0.447
H						
HETATM	210	C	0	-3.891	-21.097	-1.097
C						
HETATM	211	C	0	-4.769	-20.160	-0.527
C						
HETATM	212	H	0	-4.416	-19.441	-0.017
H						
HETATM	213	C	0	-11.471	-19.077	2.565
C						
HETATM	214	Fe	0	-11.113	8.985	-0.614
Fe						
HETATM	215	S	0	-15.376	9.773	-1.428
S						
HETATM	216	S	0	-9.985	11.678	-4.340
S						
HETATM	217	N	0	-11.974	7.769	-1.982
N						
HETATM	218	N	0	-12.952	9.771	-0.650
N						
HETATM	219	N	0	-13.524	10.833	-0.002
N						
HETATM	220	N	0	-10.588	10.168	-2.063
N						
HETATM	221	C	0	-11.404	6.791	-2.674
C						
HETATM	222	H	0	-10.474	6.633	-2.561
H						
HETATM	223	C	0	-12.115	5.990	-3.556
C						
HETATM	224	H	0	-11.675	5.285	-4.015
H						
HETATM	225	C	0	-13.449	6.215	-3.767
C						
HETATM	226	H	0	-13.945	5.670	-4.367
H						
HETATM	227	C	0	-14.060	7.251	-3.085
C						
HETATM	228	H	0	-14.981	7.443	-3.218
H						

HETATM	229	C	0	-13.300	8.009	-2.203
C						
HETATM	230	C	0	-13.784	9.131	-1.433
C						
HETATM	231	C	0	-14.788	10.958	-0.292
C						
HETATM	232	C	0	-15.683	11.982	0.266
C						
HETATM	233	C	0	-15.159	13.056	1.023
C						
HETATM	234	H	0	-14.220	13.127	1.146
H						
HETATM	235	C	0	-15.977	13.981	1.576
C						
HETATM	236	H	0	-15.603	14.699	2.072
H						
HETATM	237	C	0	-17.387	13.894	1.423
C						
HETATM	238	C	0	-18.276	14.823	2.004
C						
HETATM	239	H	0	-17.930	15.547	2.513
H						
HETATM	240	C	0	-19.633	14.696	1.846
C						
HETATM	241	H	0	-20.215	15.332	2.245
H						
HETATM	242	C	0	-20.170	13.630	1.098
C						
HETATM	243	H	0	-21.111	13.550	0.992
H						
HETATM	244	C	0	-19.340	12.712	0.524
C						
HETATM	245	H	0	-19.708	11.996	0.021
H						
HETATM	246	C	0	-17.927	12.814	0.671
C						
HETATM	247	C	0	-17.049	11.878	0.100
C						
HETATM	248	H	0	-17.402	11.157	-0.410
H						
HETATM	249	C	0	-10.347	10.795	-2.992
C						
HETATM	250	S	0	-6.849	8.196	0.200
S						
HETATM	251	S	0	-12.240	6.290	3.112
S						
HETATM	252	N	0	-10.252	10.200	0.755
N						
HETATM	253	N	0	-9.274	8.198	-0.577
N						
HETATM	254	N	0	-8.702	7.135	-1.225
N						
HETATM	255	N	0	-11.637	7.802	0.835
N						
HETATM	256	C	0	-10.821	11.178	1.445
C						

HETATM	257	H	0	-11.752	11.336	1.332
H						
HETATM	258	C	0	-10.110	11.979	2.328
C						
HETATM	259	H	0	-10.551	12.684	2.788
H						
HETATM	260	C	0	-8.776	11.753	2.539
C						
HETATM	261	H	0	-8.280	12.298	3.139
H						
HETATM	262	C	0	-8.165	10.717	1.858
C						
HETATM	263	H	0	-7.244	10.526	1.991
H						
HETATM	264	C	0	-8.925	9.959	0.974
C						
HETATM	265	C	0	-8.442	8.837	0.205
C						
HETATM	266	C	0	-7.437	7.011	-0.937
C						
HETATM	267	C	0	-6.542	5.987	-1.494
C						
HETATM	268	C	0	-7.067	4.914	-2.251
C						
HETATM	269	H	0	-8.005	4.841	-2.374
H						
HETATM	270	C	0	-6.249	3.988	-2.803
C						
HETATM	271	H	0	-6.622	3.270	-3.300
H						
HETATM	272	C	0	-4.838	4.074	-2.651
C						
HETATM	273	C	0	-3.949	3.145	-3.233
C						
HETATM	274	H	0	-4.296	2.422	-3.741
H						
HETATM	275	C	0	-2.593	3.274	-3.075
C						
HETATM	276	H	0	-2.011	2.637	-3.472
H						
HETATM	277	C	0	-2.056	4.339	-2.325
C						
HETATM	278	H	0	-1.114	4.418	-2.219
H						
HETATM	279	C	0	-2.886	5.257	-1.751
C						
HETATM	280	H	0	-2.517	5.973	-1.249
H						
HETATM	281	C	0	-4.298	5.154	-1.898
C						
HETATM	282	C	0	-5.176	6.091	-1.327
C						
HETATM	283	H	0	-4.823	6.811	-0.818
H						
HETATM	284	C	0	-11.878	7.174	1.764
C						

HETATM	285	Fe	0	-7.273	-2.761	-0.142
Fe						
HETATM	286	S	0	-11.537	-1.973	-0.956
S						
HETATM	287	S	0	-6.146	-0.067	-3.868
S						
HETATM	288	N	0	-8.134	-3.976	-1.511
N						
HETATM	289	N	0	-9.112	-1.974	-0.179
N						
HETATM	290	N	0	-9.684	-0.911	0.469
N						
HETATM	291	N	0	-6.749	-1.578	-1.592
N						
HETATM	292	C	0	-7.564	-4.953	-2.201
C						
HETATM	293	H	0	-6.634	-5.112	-2.089
H						
HETATM	294	C	0	-8.276	-5.756	-3.084
C						
HETATM	295	H	0	-7.835	-6.461	-3.544
H						
HETATM	296	C	0	-9.610	-5.530	-3.295
C						
HETATM	297	H	0	-10.106	-6.075	-3.895
H						
HETATM	298	C	0	-10.220	-4.494	-2.614
C						
HETATM	299	H	0	-11.142	-4.302	-2.747
H						
HETATM	300	C	0	-9.459	-3.736	-1.730
C						
HETATM	301	C	0	-9.944	-2.614	-0.962
C						
HETATM	302	C	0	-10.948	-0.788	0.180
C						
HETATM	303	C	0	-11.844	0.237	0.738
C						
HETATM	304	C	0	-11.319	1.310	1.494
C						
HETATM	305	H	0	-10.380	1.382	1.617
H						
HETATM	306	C	0	-12.137	2.235	2.047
C						
HETATM	307	H	0	-11.764	2.954	2.543
H						
HETATM	308	C	0	-13.547	2.149	1.895
C						
HETATM	309	C	0	-14.437	3.078	2.477
C						
HETATM	310	H	0	-14.090	3.802	2.984
H						
HETATM	311	C	0	-15.793	2.950	2.318
C						
HETATM	312	H	0	-16.375	3.587	2.716
H						

HETATM	313	C	0	-16.330	1.884	1.569
C						
HETATM	314	H	0	-17.270	1.805	1.463
H						
HETATM	315	C	0	-15.500	0.966	0.995
C						
HETATM	316	H	0	-15.869	0.250	0.493
H						
HETATM	317	C	0	-14.088	1.070	1.142
C						
HETATM	318	C	0	-13.210	0.132	0.571
C						
HETATM	319	H	0	-13.563	-0.588	0.062
H						
HETATM	320	C	0	-6.508	-0.950	-2.520
C						
HETATM	321	S	0	-3.010	-3.549	0.672
S						
HETATM	322	S	0	-8.399	-5.455	3.584
S						
HETATM	323	N	0	-6.412	-1.545	1.226
N						
HETATM	324	N	0	-5.433	-3.548	-0.106
N						
HETATM	325	N	0	-4.862	-4.610	-0.754
N						
HETATM	326	N	0	-7.798	-3.944	1.307
N						
HETATM	327	C	0	-6.981	-0.568	1.917
C						
HETATM	328	H	0	-7.912	-0.409	1.805
H						
HETATM	329	C	0	-6.271	0.234	2.800
C						
HETATM	330	H	0	-6.710	0.940	3.259
H						
HETATM	331	C	0	-4.937	0.009	3.010
C						
HETATM	332	H	0	-4.440	0.553	3.611
H						
HETATM	333	C	0	-4.325	-1.028	2.329
C						
HETATM	334	H	0	-3.405	-1.220	2.462
H						
HETATM	335	C	0	-5.086	-1.786	1.447
C						
HETATM	336	C	0	-4.602	-2.908	0.677
C						
HETATM	337	C	0	-3.598	-4.734	-0.464
C						
HETATM	338	C	0	-2.702	-5.759	-1.022
C						
HETATM	339	C	0	-3.226	-6.831	-1.779
C						
HETATM	340	H	0	-4.165	-6.904	-1.902
H						

HETATM	341	C	0	-2.409	-7.757	-2.331
C						
HETATM	342	H	0	-2.783	-8.476	-2.828
H						
HETATM	343	C	0	-0.998	-7.671	-2.179
C						
HETATM	344	C	0	-0.110	-8.599	-2.761
C						
HETATM	345	H	0	-0.456	-9.323	-3.269
H						
HETATM	346	C	0	1.247	-8.472	-2.602
C						
HETATM	347	H	0	1.829	-9.109	-3.001
H						
HETATM	348	C	0	1.784	-7.406	-1.854
C						
HETATM	349	H	0	2.726	-7.327	-1.748
H						
HETATM	350	C	0	0.954	-6.488	-1.280
C						
HETATM	351	H	0	1.323	-5.773	-0.777
H						
HETATM	352	C	0	-0.458	-6.591	-1.427
C						
HETATM	353	C	0	-1.337	-5.654	-0.856
C						
HETATM	354	H	0	-0.983	-4.934	-0.346
H						
HETATM	355	C	0	-8.039	-4.571	2.235
C						
HETATM	356	Fe	0	-3.433	-14.506	0.330
Fe						
HETATM	357	S	0	-7.697	-13.718	-0.484
S						
HETATM	358	S	0	-2.306	-11.813	-3.397
S						
HETATM	359	N	0	-4.294	-15.721	-1.039
N						
HETATM	360	N	0	-5.273	-13.719	0.293
N						
HETATM	361	N	0	-5.845	-12.657	0.942
N						
HETATM	362	N	0	-2.909	-13.323	-1.120
N						
HETATM	363	C	0	-3.724	-16.699	-1.730
C						
HETATM	364	H	0	-2.794	-16.858	-1.617
H						
HETATM	365	C	0	-4.436	-17.501	-2.612
C						
HETATM	366	H	0	-3.995	-18.207	-3.073
H						
HETATM	367	C	0	-5.770	-17.276	-2.823
C						
HETATM	368	H	0	-6.266	-17.821	-3.423
H						

HETATM	369	C	0	-6.380	-16.238	-2.142
C						
HETATM	370	H	0	-7.302	-16.047	-2.274
H						
HETATM	371	C	0	-5.620	-15.481	-1.259
C						
HETATM	372	C	0	-6.104	-14.360	-0.490
C						
HETATM	373	C	0	-7.109	-12.533	0.652
C						
HETATM	374	C	0	-8.003	-11.508	1.209
C						
HETATM	375	C	0	-7.479	-10.435	1.966
C						
HETATM	376	H	0	-6.541	-10.364	2.089
H						
HETATM	377	C	0	-8.297	-9.510	2.518
C						
HETATM	378	H	0	-7.924	-8.791	3.016
H						
HETATM	379	C	0	-9.708	-9.596	2.367
C						
HETATM	380	C	0	-10.596	-8.667	2.948
C						
HETATM	381	H	0	-10.250	-7.944	3.456
H						
HETATM	382	C	0	-11.952	-8.795	2.790
C						
HETATM	383	H	0	-12.535	-8.158	3.189
H						
HETATM	384	C	0	-12.490	-9.862	2.040
C						
HETATM	385	H	0	-13.431	-9.940	1.936
H						
HETATM	386	C	0	-11.660	-10.779	1.467
C						
HETATM	387	H	0	-12.029	-11.494	0.964
H						
HETATM	388	C	0	-10.248	-10.676	1.613
C						
HETATM	389	C	0	-9.369	-11.613	1.044
C						
HETATM	390	H	0	-9.723	-12.333	0.534
H						
HETATM	391	C	0	-2.668	-12.696	-2.049
C						
HETATM	392	S	0	0.830	-15.294	1.143
S						
HETATM	393	S	0	-4.560	-17.199	4.056
S						
HETATM	394	N	0	-2.572	-13.291	1.698
N						
HETATM	395	N	0	-1.593	-15.293	0.366
N						
HETATM	396	N	0	-1.021	-16.355	-0.283
N						

HETATM	397	N	0	-3.957	-15.689	1.779
N						
HETATM	398	C	0	-3.142	-12.313	2.389
C						
HETATM	399	H	0	-4.072	-12.154	2.276
H						
HETATM	400	C	0	-2.430	-11.511	3.271
C						
HETATM	401	H	0	-2.871	-10.806	3.732
H						
HETATM	402	C	0	-1.096	-11.736	3.482
C						
HETATM	403	H	0	-0.601	-11.192	4.082
H						
HETATM	404	C	0	-0.486	-12.773	2.801
C						
HETATM	405	H	0	0.435	-12.965	2.933
H						
HETATM	406	C	0	-1.246	-13.531	1.918
C						
HETATM	407	C	0	-0.762	-14.653	1.149
C						
HETATM	408	C	0	0.242	-16.479	0.007
C						
HETATM	409	C	0	1.137	-17.504	-0.550
C						
HETATM	410	C	0	0.613	-18.577	-1.307
C						
HETATM	411	H	0	-0.326	-18.649	-1.430
H						
HETATM	412	C	0	1.431	-19.502	-1.859
C						
HETATM	413	H	0	1.057	-20.221	-2.357
H						
HETATM	414	C	0	2.842	-19.416	-1.708
C						
HETATM	415	C	0	3.730	-20.345	-2.289
C						
HETATM	416	H	0	3.384	-21.069	-2.797
H						
HETATM	417	C	0	5.086	-20.217	-2.131
C						
HETATM	418	H	0	5.669	-20.854	-2.530
H						
HETATM	419	C	0	5.624	-19.151	-1.381
C						
HETATM	420	H	0	6.565	-19.072	-1.277
H						
HETATM	421	C	0	4.793	-18.234	-0.808
C						
HETATM	422	H	0	5.162	-17.517	-0.305
H						
HETATM	423	C	0	3.382	-18.336	-0.954
C						
HETATM	424	C	0	2.503	-17.399	-0.385
C						

HETATM	425	H	0	2.857	-16.680	0.125
H						
HETATM	426	C	0	-4.199	-16.317	2.708
C						
HETATM	427	Fe	0	-3.840	11.746	-0.472
Fe						
HETATM	428	S	0	-8.103	12.534	-1.286
S						
HETATM	429	S	0	-2.713	14.439	-4.197
S						
HETATM	430	N	0	-4.701	10.530	-1.840
N						
HETATM	431	N	0	-5.679	12.532	-0.508
N						
HETATM	432	N	0	-6.251	13.594	0.140
N						
HETATM	433	N	0	-3.316	12.929	-1.921
N						
HETATM	434	C	0	-4.131	9.552	-2.531
C						
HETATM	435	H	0	-3.201	9.394	-2.419
H						
HETATM	436	C	0	-4.843	8.750	-3.414
C						
HETATM	437	H	0	-4.403	8.045	-3.873
H						
HETATM	438	C	0	-6.177	8.976	-3.625
C						
HETATM	439	H	0	-6.672	8.431	-4.224
H						
HETATM	440	C	0	-6.787	10.012	-2.943
C						
HETATM	441	H	0	-7.708	10.204	-3.076
H						
HETATM	442	C	0	-6.027	10.770	-2.060
C						
HETATM	443	C	0	-6.511	11.892	-1.291
C						
HETATM	444	C	0	-7.515	13.719	-0.150
C						
HETATM	445	C	0	-8.410	14.743	0.408
C						
HETATM	446	C	0	-7.887	15.816	1.165
C						
HETATM	447	H	0	-6.947	15.888	1.288
H						
HETATM	448	C	0	-8.704	16.741	1.718
C						
HETATM	449	H	0	-8.330	17.460	2.214
H						
HETATM	450	C	0	-10.115	16.655	1.566
C						
HETATM	451	C	0	-11.003	17.584	2.147
C						
HETATM	452	H	0	-10.657	18.308	2.655
H						

HETATM	453	C	0	-12.359	17.457	1.988
C						
HETATM	454	H	0	-12.942	18.094	2.387
H						
HETATM	455	C	0	-12.897	16.390	1.240
C						
HETATM	456	H	0	-13.838	16.311	1.134
H						
HETATM	457	C	0	-12.066	15.473	0.666
C						
HETATM	458	H	0	-12.435	14.757	0.163
H						
HETATM	459	C	0	-10.655	15.575	0.813
C						
HETATM	460	C	0	-9.776	14.639	0.242
C						
HETATM	461	H	0	-10.129	13.918	-0.267
H						
HETATM	462	C	0	-3.074	13.556	-2.849
C						
HETATM	463	S	0	0.423	10.956	0.342
S						
HETATM	464	S	0	-4.967	9.051	3.254
S						
HETATM	465	N	0	-2.979	12.961	0.897
N						
HETATM	466	N	0	-2.000	10.959	-0.435
N						
HETATM	467	N	0	-1.428	9.896	-1.083
N						
HETATM	468	N	0	-4.364	10.563	0.978
N						
HETATM	469	C	0	-3.549	13.938	1.587
C						
HETATM	470	H	0	-4.479	14.097	1.475
H						
HETATM	471	C	0	-2.837	14.740	2.470
C						
HETATM	472	H	0	-3.277	15.445	2.930
H						
HETATM	473	C	0	-1.503	14.514	2.681
C						
HETATM	474	H	0	-1.007	15.059	3.281
H						
HETATM	475	C	0	-0.893	13.478	2.000
C						
HETATM	476	H	0	0.029	13.287	2.133
H						
HETATM	477	C	0	-1.653	12.720	1.116
C						
HETATM	478	C	0	-1.168	11.598	0.348
C						
HETATM	479	C	0	-0.164	9.772	-0.794
C						
HETATM	480	C	0	0.730	8.747	-1.352
C						

HETATM	481	C	0	0.206	7.675	-2.108
C						
HETATM	482	H	0	-0.732	7.602	-2.231
H						
HETATM	483	C	0	1.024	6.749	-2.661
C						
HETATM	484	H	0	0.651	6.031	-3.157
H						
HETATM	485	C	0	2.435	6.835	-2.509
C						
HETATM	486	C	0	3.323	5.906	-3.091
C						
HETATM	487	H	0	2.977	5.183	-3.598
H						
HETATM	488	C	0	4.679	6.034	-2.932
C						
HETATM	489	H	0	5.262	5.398	-3.330
H						
HETATM	490	C	0	5.218	7.100	-2.183
C						
HETATM	491	H	0	6.158	7.179	-2.077
H						
HETATM	492	C	0	4.387	8.018	-1.609
C						
HETATM	493	H	0	4.756	8.734	-1.106
H						
HETATM	494	C	0	2.975	7.915	-1.756
C						
HETATM	495	C	0	2.096	8.852	-1.185
C						
HETATM	496	H	0	2.450	9.572	-0.676
H						
HETATM	497	C	0	-4.605	9.935	1.906
C						
HETATM	498	Fe	0	0.000	0.000	-0.001
Fe						
HETATM	499	S	0	-4.466	0.839	-0.841
S						
HETATM	500	S	0	1.096	2.903	-3.890
S						
HETATM	501	N	0	-1.025	-1.328	-1.377
N						
HETATM	502	N	0	-1.961	0.898	-0.118
N						
HETATM	503	N	0	-2.531	1.989	0.542
N						
HETATM	504	N	0	0.605	1.179	-1.620
N						
HETATM	505	C	0	-0.475	-2.397	-1.997
C						
HETATM	506	H	0	0.566	-2.604	-1.746
H						
HETATM	507	C	0	-1.214	-3.187	-2.914
C						
HETATM	508	H	0	-0.746	-4.044	-3.394
H						

HETATM	509	C	0	-2.554	-2.833	-3.188
C						
HETATM	510	H	0	-3.151	-3.412	-3.893
H						
HETATM	511	C	0	-3.126	-1.710	-2.542
C						
HETATM	512	H	0	-4.140	-1.396	-2.772
H						
HETATM	513	C	0	-2.323	-0.986	-1.634
C						
HETATM	514	C	0	-2.798	0.203	-0.879
C						
HETATM	515	C	0	-3.828	2.112	0.283
C						
HETATM	516	C	0	-4.711	3.145	0.855
C						
HETATM	517	C	0	-4.148	4.241	1.609
C						
HETATM	518	H	0	-3.066	4.301	1.726
H						
HETATM	519	C	0	-4.988	5.192	2.182
C						
HETATM	520	H	0	-4.579	6.027	2.754
H						
HETATM	521	C	0	-6.423	5.086	2.049
C						
HETATM	522	C	0	-7.319	6.034	2.659
C						
HETATM	523	H	0	-6.897	6.857	3.238
H						
HETATM	524	C	0	-8.700	5.911	2.490
C						
HETATM	525	H	0	-9.382	6.617	2.964
H						
HETATM	526	C	0	-9.251	4.834	1.708
C						
HETATM	527	H	0	-10.333	4.761	1.605
H						
HETATM	528	C	0	-8.408	3.894	1.116
C						
HETATM	529	H	0	-8.812	3.058	0.543
H						
HETATM	530	C	0	-6.980	4.002	1.273
C						
HETATM	531	C	0	-6.096	3.047	0.679
C						
HETATM	532	H	0	-6.532	2.236	0.095
H						
HETATM	533	C	0	0.793	1.886	-2.561
C						
HETATM	534	S	0	4.466	-0.839	0.842
S						
HETATM	535	S	0	-1.096	-2.903	3.889
S						
HETATM	536	N	0	1.026	1.328	1.377
N						

HETATM	537	N	0	1.961	-0.897	0.117
N						
HETATM	538	N	0	2.531	-1.989	-0.543
N						
HETATM	539	N	0	-0.605	-1.178	1.619
N						
HETATM	540	C	0	0.475	2.398	1.997
C						
HETATM	541	H	0	-0.566	2.605	1.744
H						
HETATM	542	C	0	1.214	3.187	2.914
C						
HETATM	543	H	0	0.746	4.045	3.394
H						
HETATM	544	C	0	2.554	2.832	3.189
C						
HETATM	545	H	0	3.150	3.411	3.894
H						
HETATM	546	C	0	3.125	1.709	2.543
C						
HETATM	547	H	0	4.139	1.394	2.774
H						
HETATM	548	C	0	2.323	0.986	1.634
C						
HETATM	549	C	0	2.798	-0.203	0.879
C						
HETATM	550	C	0	3.828	-2.112	-0.284
C						
HETATM	551	C	0	4.711	-3.145	-0.855
C						
HETATM	552	C	0	4.148	-4.241	-1.609
C						
HETATM	553	H	0	3.066	-4.300	-1.727
H						
HETATM	554	C	0	4.988	-5.192	-2.182
C						
HETATM	555	H	0	4.579	-6.027	-2.755
H						
HETATM	556	C	0	6.423	-5.086	-2.049
C						
HETATM	557	C	0	7.319	-6.034	-2.659
C						
HETATM	558	H	0	6.897	-6.856	-3.238
H						
HETATM	559	C	0	8.700	-5.911	-2.490
C						
HETATM	560	H	0	9.382	-6.617	-2.964
H						
HETATM	561	C	0	9.251	-4.834	-1.707
C						
HETATM	562	H	0	10.333	-4.761	-1.604
H						
HETATM	563	C	0	8.408	-3.894	-1.116
C						
HETATM	564	H	0	8.812	-3.058	-0.543
H						

HETATM	565	C	0	6.980	-4.002	-1.273
C						
HETATM	566	C	0	6.096	-3.047	-0.679
C						
HETATM	567	H	0	6.532	-2.236	-0.095
H						
HETATM	568	C	0	-0.793	-1.886	2.560
C						
HETATM	569	Fe	0	3.840	-11.746	0.472
Fe						
HETATM	570	S	0	-0.423	-10.956	-0.342
S						
HETATM	571	S	0	4.967	-9.051	-3.254
S						
HETATM	572	N	0	2.979	-12.961	-0.897
N						
HETATM	573	N	0	2.000	-10.959	0.435
N						
HETATM	574	N	0	1.428	-9.896	1.083
N						
HETATM	575	N	0	4.364	-10.563	-0.978
N						
HETATM	576	C	0	3.549	-13.938	-1.587
C						
HETATM	577	H	0	4.479	-14.097	-1.475
H						
HETATM	578	C	0	2.837	-14.740	-2.470
C						
HETATM	579	H	0	3.277	-15.445	-2.930
H						
HETATM	580	C	0	1.503	-14.514	-2.681
C						
HETATM	581	H	0	1.007	-15.059	-3.281
H						
HETATM	582	C	0	0.893	-13.478	-2.000
C						
HETATM	583	H	0	-0.029	-13.287	-2.133
H						
HETATM	584	C	0	1.653	-12.720	-1.116
C						
HETATM	585	C	0	1.168	-11.598	-0.348
C						
HETATM	586	C	0	0.164	-9.772	0.794
C						
HETATM	587	C	0	-0.730	-8.747	1.352
C						
HETATM	588	C	0	-0.206	-7.675	2.109
C						
HETATM	589	H	0	0.732	-7.602	2.231
H						
HETATM	590	C	0	-1.024	-6.749	2.661
C						
HETATM	591	H	0	-0.651	-6.031	3.157
H						
HETATM	592	C	0	-2.435	-6.835	2.509
C						

HETATM	593	C	0	-3.323	-5.906	3.091
C						
HETATM	594	H	0	-2.977	-5.183	3.599
H						
HETATM	595	C	0	-4.679	-6.034	2.933
C						
HETATM	596	H	0	-5.262	-5.398	3.330
H						
HETATM	597	C	0	-5.218	-7.100	2.183
C						
HETATM	598	H	0	-6.158	-7.179	2.077
H						
HETATM	599	C	0	-4.387	-8.018	1.609
C						
HETATM	600	H	0	-4.756	-8.734	1.107
H						
HETATM	601	C	0	-2.975	-7.915	1.756
C						
HETATM	602	C	0	-2.096	-8.852	1.185
C						
HETATM	603	H	0	-2.450	-9.572	0.676
H						
HETATM	604	C	0	4.605	-9.935	-1.906
C						
HETATM	605	S	0	8.103	-12.534	1.286
S						
HETATM	606	S	0	2.713	-14.439	4.197
S						
HETATM	607	N	0	4.701	-10.530	1.840
N						
HETATM	608	N	0	5.679	-12.532	0.508
N						
HETATM	609	N	0	6.251	-13.594	-0.140
N						
HETATM	610	N	0	3.316	-12.928	1.921
N						
HETATM	611	C	0	4.131	-9.552	2.531
C						
HETATM	612	H	0	3.201	-9.394	2.419
H						
HETATM	613	C	0	4.843	-8.750	3.414
C						
HETATM	614	H	0	4.403	-8.045	3.873
H						
HETATM	615	C	0	6.177	-8.976	3.625
C						
HETATM	616	H	0	6.672	-8.431	4.224
H						
HETATM	617	C	0	6.787	-10.012	2.943
C						
HETATM	618	H	0	7.708	-10.204	3.076
H						
HETATM	619	C	0	6.027	-10.770	2.061
C						
HETATM	620	C	0	6.511	-11.892	1.291
C						

HETATM	621	C	0	7.515	-13.719	0.150
C						
HETATM	622	C	0	8.410	-14.743	-0.408
C						
HETATM	623	C	0	7.886	-15.816	-1.165
C						
HETATM	624	H	0	6.947	-15.888	-1.288
H						
HETATM	625	C	0	8.704	-16.741	-1.718
C						
HETATM	626	H	0	8.330	-17.460	-2.214
H						
HETATM	627	C	0	10.115	-16.655	-1.565
C						
HETATM	628	C	0	11.003	-17.584	-2.147
C						
HETATM	629	H	0	10.657	-18.308	-2.655
H						
HETATM	630	C	0	12.359	-17.457	-1.988
C						
HETATM	631	H	0	12.942	-18.093	-2.387
H						
HETATM	632	C	0	12.897	-16.390	-1.240
C						
HETATM	633	H	0	13.838	-16.311	-1.134
H						
HETATM	634	C	0	12.066	-15.473	-0.666
C						
HETATM	635	H	0	12.435	-14.757	-0.163
H						
HETATM	636	C	0	10.655	-15.575	-0.813
C						
HETATM	637	C	0	9.776	-14.639	-0.242
C						
HETATM	638	H	0	10.129	-13.918	0.268
H						
HETATM	639	C	0	3.074	-13.556	2.849
C						
HETATM	640	Fe	0	3.433	14.506	-0.329
Fe						
HETATM	641	S	0	-0.830	15.294	-1.143
S						
HETATM	642	S	0	4.560	17.199	-4.056
S						
HETATM	643	N	0	2.572	13.291	-1.698
N						
HETATM	644	N	0	1.593	15.293	-0.366
N						
HETATM	645	N	0	1.021	16.355	0.283
N						
HETATM	646	N	0	3.957	15.689	-1.779
N						
HETATM	647	C	0	3.142	12.313	-2.389
C						
HETATM	648	H	0	4.072	12.154	-2.276
H						

HETATM	649	C	0	2.430	11.511	-3.271
C						
HETATM	650	H	0	2.871	10.806	-3.731
H						
HETATM	651	C	0	1.096	11.737	-3.482
C						
HETATM	652	H	0	0.601	11.192	-4.082
H						
HETATM	653	C	0	0.486	12.773	-2.801
C						
HETATM	654	H	0	-0.435	12.965	-2.933
H						
HETATM	655	C	0	1.246	13.531	-1.918
C						
HETATM	656	C	0	0.762	14.653	-1.149
C						
HETATM	657	C	0	-0.242	16.479	-0.007
C						
HETATM	658	C	0	-1.137	17.505	0.550
C						
HETATM	659	C	0	-0.613	18.577	1.307
C						
HETATM	660	H	0	0.326	18.649	1.430
H						
HETATM	661	C	0	-1.431	19.502	1.860
C						
HETATM	662	H	0	-1.057	20.221	2.357
H						
HETATM	663	C	0	-2.842	19.416	1.708
C						
HETATM	664	C	0	-3.730	20.345	2.289
C						
HETATM	665	H	0	-3.384	21.069	2.797
H						
HETATM	666	C	0	-5.086	20.217	2.131
C						
HETATM	667	H	0	-5.669	20.854	2.530
H						
HETATM	668	C	0	-5.624	19.151	1.381
C						
HETATM	669	H	0	-6.565	19.072	1.277
H						
HETATM	670	C	0	-4.793	18.234	0.808
C						
HETATM	671	H	0	-5.162	17.517	0.305
H						
HETATM	672	C	0	-3.382	18.336	0.954
C						
HETATM	673	C	0	-2.503	17.399	0.385
C						
HETATM	674	H	0	-2.857	16.680	-0.125
H						
HETATM	675	C	0	4.199	16.317	-2.708
C						
HETATM	676	S	0	7.697	13.718	0.484
S						

HETATM	677	S	0	2.306	11.813	3.397
S						
HETATM	678	N	0	4.294	15.721	1.039
N						
HETATM	679	N	0	5.273	13.719	-0.293
N						
HETATM	680	N	0	5.845	12.657	-0.941
N						
HETATM	681	N	0	2.909	13.323	1.120
N						
HETATM	682	C	0	3.724	16.699	1.730
C						
HETATM	683	H	0	2.794	16.858	1.617
H						
HETATM	684	C	0	4.436	17.501	2.612
C						
HETATM	685	H	0	3.995	18.207	3.073
H						
HETATM	686	C	0	5.770	17.276	2.823
C						
HETATM	687	H	0	6.266	17.821	3.423
H						
HETATM	688	C	0	6.380	16.239	2.143
C						
HETATM	689	H	0	7.302	16.047	2.274
H						
HETATM	690	C	0	5.620	15.481	1.259
C						
HETATM	691	C	0	6.104	14.360	0.490
C						
HETATM	692	C	0	7.109	12.533	-0.652
C						
HETATM	693	C	0	8.003	11.508	-1.209
C						
HETATM	694	C	0	7.479	10.435	-1.966
C						
HETATM	695	H	0	6.541	10.364	-2.089
H						
HETATM	696	C	0	8.297	9.511	-2.518
C						
HETATM	697	H	0	7.924	8.792	-3.016
H						
HETATM	698	C	0	9.708	9.596	-2.367
C						
HETATM	699	C	0	10.596	8.667	-2.948
C						
HETATM	700	H	0	10.250	7.944	-3.456
H						
HETATM	701	C	0	11.952	8.795	-2.790
C						
HETATM	702	H	0	12.535	8.158	-3.189
H						
HETATM	703	C	0	12.490	9.862	-2.040
C						
HETATM	704	H	0	13.431	9.940	-1.936
H						

HETATM	705	C	0	11.660	10.779	-1.467
C						
HETATM	706	H	0	12.029	11.494	-0.964
H						
HETATM	707	C	0	10.248	10.676	-1.613
C						
HETATM	708	C	0	9.369	11.613	-1.044
C						
HETATM	709	H	0	9.723	12.333	-0.534
H						
HETATM	710	C	0	2.668	12.696	2.049
C						
HETATM	711	Fe	0	7.273	2.761	0.142
Fe						
HETATM	712	S	0	3.010	3.549	-0.672
S						
HETATM	713	S	0	8.399	5.455	-3.583
S						
HETATM	714	N	0	6.412	1.545	-1.226
N						
HETATM	715	N	0	5.433	3.548	0.106
N						
HETATM	716	N	0	4.862	4.610	0.754
N						
HETATM	717	N	0	7.798	3.944	-1.307
N						
HETATM	718	C	0	6.981	0.568	-1.917
C						
HETATM	719	H	0	7.912	0.409	-1.805
H						
HETATM	720	C	0	6.271	-0.234	-2.800
C						
HETATM	721	H	0	6.710	-0.940	-3.259
H						
HETATM	722	C	0	4.937	-0.009	-3.010
C						
HETATM	723	H	0	4.440	-0.553	-3.610
H						
HETATM	724	C	0	4.325	1.028	-2.329
C						
HETATM	725	H	0	3.405	1.220	-2.462
H						
HETATM	726	C	0	5.086	1.786	-1.447
C						
HETATM	727	C	0	4.602	2.908	-0.677
C						
HETATM	728	C	0	3.598	4.735	0.464
C						
HETATM	729	C	0	2.702	5.759	1.022
C						
HETATM	730	C	0	3.226	6.831	1.779
C						
HETATM	731	H	0	4.165	6.904	1.902
H						
HETATM	732	C	0	2.409	7.757	2.331
C						

HETATM	733	H	0	2.783	8.476	2.828
H						
HETATM	734	C	0	0.998	7.671	2.179
C						
HETATM	735	C	0	0.110	8.599	2.761
C						
HETATM	736	H	0	0.456	9.323	3.269
H						
HETATM	737	C	0	-1.247	8.472	2.602
C						
HETATM	738	H	0	-1.829	9.109	3.001
H						
HETATM	739	C	0	-1.784	7.406	1.854
C						
HETATM	740	H	0	-2.726	7.327	1.748
H						
HETATM	741	C	0	-0.954	6.488	1.280
C						
HETATM	742	H	0	-1.323	5.773	0.777
H						
HETATM	743	C	0	0.458	6.591	1.427
C						
HETATM	744	C	0	1.337	5.654	0.856
C						
HETATM	745	H	0	0.983	4.934	0.346
H						
HETATM	746	C	0	8.039	4.571	-2.235
C						
HETATM	747	S	0	11.537	1.973	0.956
S						
HETATM	748	S	0	6.146	0.067	3.868
S						
HETATM	749	N	0	8.134	3.976	1.511
N						
HETATM	750	N	0	9.112	1.974	0.179
N						
HETATM	751	N	0	9.684	0.911	-0.469
N						
HETATM	752	N	0	6.749	1.578	1.592
N						
HETATM	753	C	0	7.564	4.953	2.201
C						
HETATM	754	H	0	6.634	5.112	2.089
H						
HETATM	755	C	0	8.276	5.756	3.084
C						
HETATM	756	H	0	7.835	6.461	3.544
H						
HETATM	757	C	0	9.610	5.530	3.295
C						
HETATM	758	H	0	10.106	6.075	3.895
H						
HETATM	759	C	0	10.220	4.494	2.614
C						
HETATM	760	H	0	11.142	4.302	2.747
H						

HETATM	761	C	0	9.459	3.736	1.730
C						
HETATM	762	C	0	9.944	2.614	0.962
C						
HETATM	763	C	0	10.948	0.788	-0.180
C						
HETATM	764	C	0	11.844	-0.237	-0.738
C						
HETATM	765	C	0	11.319	-1.310	-1.494
C						
HETATM	766	H	0	10.380	-1.382	-1.617
H						
HETATM	767	C	0	12.137	-2.235	-2.047
C						
HETATM	768	H	0	11.764	-2.954	-2.543
H						
HETATM	769	C	0	13.547	-2.149	-1.895
C						
HETATM	770	C	0	14.437	-3.078	-2.477
C						
HETATM	771	H	0	14.090	-3.802	-2.984
H						
HETATM	772	C	0	15.793	-2.950	-2.318
C						
HETATM	773	H	0	16.375	-3.587	-2.716
H						
HETATM	774	C	0	16.330	-1.884	-1.569
C						
HETATM	775	H	0	17.270	-1.805	-1.463
H						
HETATM	776	C	0	15.500	-0.966	-0.995
C						
HETATM	777	H	0	15.869	-0.250	-0.493
H						
HETATM	778	C	0	14.088	-1.070	-1.142
C						
HETATM	779	C	0	13.210	-0.132	-0.571
C						
HETATM	780	H	0	13.563	0.588	-0.062
H						
HETATM	781	C	0	6.508	0.950	2.520
C						
HETATM	782	Fe	0	11.113	-8.985	0.614
Fe						
HETATM	783	S	0	6.849	-8.196	-0.200
S						
HETATM	784	S	0	12.240	-6.290	-3.112
S						
HETATM	785	N	0	10.252	-10.200	-0.755
N						
HETATM	786	N	0	9.274	-8.198	0.577
N						
HETATM	787	N	0	8.702	-7.135	1.225
N						
HETATM	788	N	0	11.637	-7.802	-0.835
N						

HETATM	789	C	0	10.821	-11.178	-1.445
C						
HETATM	790	H	0	11.752	-11.336	-1.332
H						
HETATM	791	C	0	10.110	-11.979	-2.328
C						
HETATM	792	H	0	10.551	-12.684	-2.788
H						
HETATM	793	C	0	8.776	-11.753	-2.539
C						
HETATM	794	H	0	8.280	-12.298	-3.139
H						
HETATM	795	C	0	8.165	-10.717	-1.858
C						
HETATM	796	H	0	7.244	-10.526	-1.990
H						
HETATM	797	C	0	8.925	-9.959	-0.974
C						
HETATM	798	C	0	8.442	-8.837	-0.205
C						
HETATM	799	C	0	7.437	-7.011	0.937
C						
HETATM	800	C	0	6.542	-5.986	1.494
C						
HETATM	801	C	0	7.067	-4.914	2.251
C						
HETATM	802	H	0	8.005	-4.841	2.374
H						
HETATM	803	C	0	6.249	-3.988	2.803
C						
HETATM	804	H	0	6.622	-3.270	3.300
H						
HETATM	805	C	0	4.838	-4.074	2.651
C						
HETATM	806	C	0	3.949	-3.145	3.233
C						
HETATM	807	H	0	4.296	-2.422	3.741
H						
HETATM	808	C	0	2.593	-3.274	3.075
C						
HETATM	809	H	0	2.011	-2.637	3.473
H						
HETATM	810	C	0	2.056	-4.339	2.325
C						
HETATM	811	H	0	1.114	-4.418	2.219
H						
HETATM	812	C	0	2.886	-5.257	1.751
C						
HETATM	813	H	0	2.517	-5.973	1.249
H						
HETATM	814	C	0	4.298	-5.154	1.898
C						
HETATM	815	C	0	5.176	-6.091	1.328
C						
HETATM	816	H	0	4.823	-6.811	0.818
H						

HETATM	817	C	0	11.878	-7.174	-1.764
C						
HETATM	818	S	0	15.376	-9.773	1.428
S						
HETATM	819	S	0	9.985	-11.678	4.340
S						
HETATM	820	N	0	11.974	-7.769	1.983
N						
HETATM	821	N	0	12.952	-9.771	0.650
N						
HETATM	822	N	0	13.524	-10.833	0.002
N						
HETATM	823	N	0	10.588	-10.168	2.063
N						
HETATM	824	C	0	11.404	-6.791	2.674
C						
HETATM	825	H	0	10.474	-6.633	2.561
H						
HETATM	826	C	0	12.115	-5.990	3.556
C						
HETATM	827	H	0	11.675	-5.285	4.015
H						
HETATM	828	C	0	13.449	-6.215	3.767
C						
HETATM	829	H	0	13.945	-5.670	4.367
H						
HETATM	830	C	0	14.060	-7.251	3.085
C						
HETATM	831	H	0	14.981	-7.443	3.218
H						
HETATM	832	C	0	13.300	-8.009	2.203
C						
HETATM	833	C	0	13.784	-9.131	1.433
C						
HETATM	834	C	0	14.788	-10.958	0.292
C						
HETATM	835	C	0	15.683	-11.982	-0.265
C						
HETATM	836	C	0	15.159	-13.056	-1.023
C						
HETATM	837	H	0	14.220	-13.127	-1.146
H						
HETATM	838	C	0	15.976	-13.981	-1.576
C						
HETATM	839	H	0	15.603	-14.699	-2.072
H						
HETATM	840	C	0	17.387	-13.894	-1.423
C						
HETATM	841	C	0	18.276	-14.823	-2.004
C						
HETATM	842	H	0	17.930	-15.547	-2.513
H						
HETATM	843	C	0	19.633	-14.696	-1.846
C						
HETATM	844	H	0	20.215	-15.332	-2.245
H						

HETATM	845	C	0	20.170	-13.630	-1.098
C						
HETATM	846	H	0	21.111	-13.550	-0.992
H						
HETATM	847	C	0	19.340	-12.712	-0.523
C						
HETATM	848	H	0	19.708	-11.996	-0.021
H						
HETATM	849	C	0	17.927	-12.814	-0.671
C						
HETATM	850	C	0	17.049	-11.878	-0.100
C						
HETATM	851	H	0	17.402	-11.157	0.410
H						
HETATM	852	C	0	10.347	-10.795	2.992
C						
HETATM	853	Fe	0	10.706	17.267	-0.187
Fe						
HETATM	854	S	0	6.442	18.055	-1.001
S						
HETATM	855	S	0	11.833	19.961	-3.913
S						
HETATM	856	N	0	9.845	16.052	-1.555
N						
HETATM	857	N	0	8.867	18.054	-0.223
N						
HETATM	858	N	0	8.294	19.116	0.425
N						
HETATM	859	N	0	11.230	18.450	-1.637
N						
HETATM	860	C	0	10.415	15.074	-2.247
C						
HETATM	861	H	0	11.345	14.916	-2.134
H						
HETATM	862	C	0	9.703	14.272	-3.129
C						
HETATM	863	H	0	10.144	13.567	-3.589
H						
HETATM	864	C	0	8.369	14.498	-3.340
C						
HETATM	865	H	0	7.873	13.953	-3.940
H						
HETATM	866	C	0	7.759	15.534	-2.659
C						
HETATM	867	H	0	6.837	15.726	-2.791
H						
HETATM	868	C	0	8.520	16.292	-1.776
C						
HETATM	869	C	0	8.035	17.414	-1.007
C						
HETATM	870	C	0	7.030	19.240	0.135
C						
HETATM	871	C	0	6.135	20.265	0.693
C						
HETATM	872	C	0	6.660	21.338	1.449
C						

HETATM	873	H	0	7.598	21.409	1.572
H						
HETATM	874	C	0	5.842	22.263	2.002
C						
HETATM	875	H	0	6.215	22.982	2.499
H						
HETATM	876	C	0	4.431	22.178	1.850
C						
HETATM	877	C	0	3.542	23.106	2.432
C						
HETATM	878	H	0	3.889	23.829	2.939
H						
HETATM	879	C	0	2.186	22.978	2.273
C						
HETATM	880	H	0	1.604	23.615	2.672
H						
HETATM	881	C	0	1.649	21.912	1.524
C						
HETATM	882	H	0	0.708	21.833	1.419
H						
HETATM	883	C	0	2.479	20.994	0.951
C						
HETATM	884	H	0	2.110	20.278	0.447
H						
HETATM	885	C	0	3.891	21.097	1.097
C						
HETATM	886	C	0	4.769	20.160	0.527
C						
HETATM	887	H	0	4.416	19.441	0.017
H						
HETATM	888	C	0	11.471	19.077	-2.565
C						
HETATM	889	S	0	14.969	16.479	0.627
S						
HETATM	890	S	0	9.579	14.574	3.539
S						
HETATM	891	N	0	11.567	18.482	1.181
N						
HETATM	892	N	0	12.546	16.480	-0.151
N						
HETATM	893	N	0	13.117	15.418	-0.799
N						
HETATM	894	N	0	10.181	16.084	1.263
N						
HETATM	895	C	0	10.997	19.460	1.872
C						
HETATM	896	H	0	10.067	19.618	1.760
H						
HETATM	897	C	0	11.708	20.262	2.755
C						
HETATM	898	H	0	11.269	20.968	3.215
H						
HETATM	899	C	0	13.042	20.036	2.965
C						
HETATM	900	H	0	13.538	20.581	3.565
H						

HETATM	901	C	0	13.654	19.000	2.285
C						
HETATM	902	H	0	14.574	18.808	2.417
H						
HETATM	903	C	0	12.893	18.242	1.401
C						
HETATM	904	C	0	13.377	17.120	0.632
C						
HETATM	905	C	0	14.381	15.293	-0.509
C						
HETATM	906	C	0	15.276	14.269	-1.067
C						
HETATM	907	C	0	14.753	13.196	-1.824
C						
HETATM	908	H	0	13.813	13.125	-1.947
H						
HETATM	909	C	0	15.569	12.271	-2.376
C						
HETATM	910	H	0	15.196	11.552	-2.873
H						
HETATM	911	C	0	16.981	12.357	-2.225
C						
HETATM	912	C	0	17.869	11.428	-2.806
C						
HETATM	913	H	0	17.523	10.705	-3.314
H						
HETATM	914	C	0	19.226	11.556	-2.648
C						
HETATM	915	H	0	19.808	10.919	-3.046
H						
HETATM	916	C	0	19.763	12.622	-1.898
C						
HETATM	917	H	0	20.704	12.701	-1.793
H						
HETATM	918	C	0	18.932	13.540	-1.325
C						
HETATM	919	H	0	19.302	14.255	-0.822
H						
HETATM	920	C	0	17.521	13.437	-1.471
C						
HETATM	921	C	0	16.642	14.374	-0.902
C						
HETATM	922	H	0	16.996	15.093	-0.392
H						
HETATM	923	C	0	9.940	15.457	2.191
C						
HETATM	924	Fe	0	14.546	5.522	0.284
Fe						
HETATM	925	S	0	10.283	6.310	-0.530
S						
HETATM	926	S	0	15.672	8.216	-3.441
S						
HETATM	927	N	0	13.685	4.306	-1.084
N						
HETATM	928	N	0	12.706	6.309	0.248
N						

HETATM	929	N	0	12.134	7.371	0.896
N						
HETATM	930	N	0	15.070	6.705	-1.165
N						
HETATM	931	C	0	14.255	3.329	-1.775
C						
HETATM	932	H	0	15.185	3.170	-1.663
H						
HETATM	933	C	0	13.543	2.526	-2.658
C						
HETATM	934	H	0	13.983	1.821	-3.117
H						
HETATM	935	C	0	12.209	2.752	-2.868
C						
HETATM	936	H	0	11.713	2.208	-3.468
H						
HETATM	937	C	0	11.598	3.789	-2.187
C						
HETATM	938	H	0	10.677	3.980	-2.320
H						
HETATM	939	C	0	12.359	4.547	-1.304
C						
HETATM	940	C	0	11.874	5.669	-0.535
C						
HETATM	941	C	0	10.870	7.495	0.606
C						
HETATM	942	C	0	9.976	8.520	1.164
C						
HETATM	943	C	0	10.499	9.592	1.922
C						
HETATM	944	H	0	11.438	9.665	2.044
H						
HETATM	945	C	0	9.682	10.518	2.473
C						
HETATM	946	H	0	10.055	11.236	2.970
H						
HETATM	947	C	0	8.271	10.432	2.322
C						
HETATM	948	C	0	7.383	11.360	2.903
C						
HETATM	949	H	0	7.729	12.084	3.412
H						
HETATM	950	C	0	6.027	11.233	2.745
C						
HETATM	951	H	0	5.444	11.870	3.143
H						
HETATM	952	C	0	5.488	10.167	1.996
C						
HETATM	953	H	0	4.548	10.088	1.890
H						
HETATM	954	C	0	6.319	9.249	1.422
C						
HETATM	955	H	0	5.950	8.534	0.920
H						
HETATM	956	C	0	7.731	9.352	1.569
C						

HETATM	957	C	0	8.610	8.415	0.999
C						
HETATM	958	H	0	8.256	7.695	0.489
H						
HETATM	959	C	0	15.311	7.332	-2.093
C						
HETATM	960	S	0	18.809	4.733	1.098
S						
HETATM	961	S	0	13.419	2.828	4.010
S						
HETATM	962	N	0	15.407	6.737	1.653
N						
HETATM	963	N	0	16.386	4.735	0.321
N						
HETATM	964	N	0	16.958	3.672	-0.327
N						
HETATM	965	N	0	14.022	4.339	1.734
N						
HETATM	966	C	0	14.837	7.714	2.344
C						
HETATM	967	H	0	13.907	7.873	2.231
H						
HETATM	968	C	0	15.549	8.517	3.226
C						
HETATM	969	H	0	15.108	9.222	3.686
H						
HETATM	970	C	0	16.883	8.291	3.438
C						
HETATM	971	H	0	17.378	8.836	4.038
H						
HETATM	972	C	0	17.493	7.255	2.756
C						
HETATM	973	H	0	18.414	7.063	2.889
H						
HETATM	974	C	0	16.733	6.497	1.873
C						
HETATM	975	C	0	17.217	5.375	1.104
C						
HETATM	976	C	0	18.221	3.549	-0.038
C						
HETATM	977	C	0	19.116	2.524	-0.596
C						
HETATM	978	C	0	18.592	1.451	-1.352
C						
HETATM	979	H	0	17.653	1.379	-1.475
H						
HETATM	980	C	0	19.410	0.526	-1.905
C						
HETATM	981	H	0	19.036	-0.193	-2.401
H						
HETATM	982	C	0	20.821	0.612	-1.752
C						
HETATM	983	C	0	21.709	-0.317	-2.335
C						
HETATM	984	H	0	21.363	-1.041	-2.842
H						

HETATM	985	C	0	23.065	-0.190	-2.176
C						
HETATM	986	H	0	23.648	-0.826	-2.574
H						
HETATM	987	C	0	23.603	0.877	-1.427
C						
HETATM	988	H	0	24.544	0.956	-1.321
H						
HETATM	989	C	0	22.772	1.794	-0.853
C						
HETATM	990	H	0	23.141	2.510	-0.350
H						
HETATM	991	C	0	21.361	1.691	-1.000
C						
HETATM	992	C	0	20.482	2.629	-0.429
C						
HETATM	993	H	0	20.835	3.349	0.081
H						
HETATM	994	C	0	13.780	3.711	2.662
C						
HETATM	995	Fe	0	18.386	-6.224	0.757
Fe						
HETATM	996	S	0	14.122	-5.435	-0.057
S						
HETATM	997	S	0	19.512	-3.530	-2.970
S						
HETATM	998	N	0	17.525	-7.439	-0.612
N						
HETATM	999	N	0	16.546	-5.437	0.719
N						
HETATM	1000	N	0	15.974	-4.375	1.368
N						
HETATM	1001	N	0	18.910	-5.041	-0.693
N						
HETATM	1002	C	0	18.094	-8.417	-1.303
C						
HETATM	1003	H	0	19.024	-8.576	-1.190
H						
HETATM	1004	C	0	17.382	-9.218	-2.185
C						
HETATM	1005	H	0	17.823	-9.923	-2.646
H						
HETATM	1006	C	0	16.048	-8.993	-2.397
C						
HETATM	1007	H	0	15.553	-9.537	-2.997
H						
HETATM	1008	C	0	15.438	-7.956	-1.715
C						
HETATM	1009	H	0	14.518	-7.765	-1.848
H						
HETATM	1010	C	0	16.199	-7.198	-0.832
C						
HETATM	1011	C	0	15.714	-6.077	-0.063
C						
HETATM	1012	C	0	14.710	-4.250	1.079
C						

HETATM 1013	C	0	13.815	-3.225	1.636
C					
HETATM 1014	C	0	14.339	-2.153	2.393
C					
HETATM 1015	H	0	15.278	-2.080	2.516
H					
HETATM 1016	C	0	13.521	-1.227	2.945
C					
HETATM 1017	H	0	13.896	-0.509	3.442
H					
HETATM 1018	C	0	12.111	-1.314	2.793
C					
HETATM 1019	C	0	11.222	-0.384	3.375
C					
HETATM 1020	H	0	11.569	0.339	3.883
H					
HETATM 1021	C	0	9.866	-0.513	3.217
C					
HETATM 1022	H	0	9.284	0.124	3.615
H					
HETATM 1023	C	0	9.328	-1.578	2.467
C					
HETATM 1024	H	0	8.388	-1.657	2.362
H					
HETATM 1025	C	0	10.159	-2.496	1.893
C					
HETATM 1026	H	0	9.790	-3.212	1.391
H					
HETATM 1027	C	0	11.570	-2.394	2.040
C					
HETATM 1028	C	0	12.449	-3.330	1.470
C					
HETATM 1029	H	0	12.096	-4.050	0.960
H					
HETATM 1030	C	0	19.152	-4.413	-1.622
C					
HETATM 1031	S	0	22.650	-7.012	1.570
S					
HETATM 1032	S	0	17.259	-8.917	4.482
S					
HETATM 1033	N	0	19.247	-5.009	2.125
N					
HETATM 1034	N	0	20.225	-7.010	0.793
N					
HETATM 1035	N	0	20.797	-8.072	0.144
N					
HETATM 1036	N	0	17.862	-7.407	2.205
N					
HETATM 1037	C	0	18.677	-4.030	2.816
C					
HETATM 1038	H	0	17.747	-3.872	2.703
H					
HETATM 1039	C	0	19.388	-3.229	3.698
C					
HETATM 1040	H	0	18.948	-2.524	4.158
H					

HETATM	1041	C	0	20.723	-3.454	3.909
C						
HETATM	1042	H	0	21.219	-2.909	4.509
H						
HETATM	1043	C	0	21.333	-4.491	3.227
C						
HETATM	1044	H	0	22.254	-4.682	3.360
H						
HETATM	1045	C	0	20.572	-5.249	2.345
C						
HETATM	1046	C	0	21.057	-6.370	1.575
C						
HETATM	1047	C	0	22.061	-8.197	0.434
C						
HETATM	1048	C	0	22.956	-9.221	-0.123
C						
HETATM	1049	C	0	22.432	-10.295	-0.881
C						
HETATM	1050	H	0	21.493	-10.366	-1.004
H						
HETATM	1051	C	0	23.250	-11.220	-1.433
C						
HETATM	1052	H	0	22.876	-11.938	-1.930
H						
HETATM	1053	C	0	24.660	-11.133	-1.281
C						
HETATM	1054	C	0	25.549	-12.063	-1.862
C						
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CONNECT	733	732		
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CONNECT	745	744		
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CONNECT	747	762	763	
CONNECT	748	781		

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CONECT	751	750	763	
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CONECT	754	753		
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CONECT	756	755		
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CONECT	758	757		
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CONECT	760	759		
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CONECT	768	767		
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CONECT	775	774		
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CONECT	777	776		
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CONECT	780	779		
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CONECT	782	788	823	
CONECT	783	798	799	
CONECT	784	817		
CONECT	785	789	797	
CONECT	786	787	798	
CONECT	787	786	799	
CONECT	788	782	817	
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CONECT	790	789		
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CONECT	794	793		
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CONECT	798	797	783	786
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CONECT	804	803		
CONECT	805	803	806	814

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CONNECT	815	814	800	816
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CONNECT	822	821	834	
CONNECT	823	782	852	
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CONNECT	825	824		
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CONNECT	862	860	863	864

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CONNECT	865	864		
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CONNECT	867	866		
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CONNECT	869	868	854	857
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CONNECT	875	874		
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CONNECT	877	876	878	879
CONNECT	878	877		
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CONNECT	880	879		
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CONNECT	886	885	871	887
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CONNECT	905	889	893	906
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CONNECT	915	914		
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CONNECT	919	918		

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CONNECT	930	924	959	
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CONNECT	938	937		
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CONNECT	940	925	928	939
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CONNECT	951	950		
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CONNECT	957	942	956	958
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CONNECT	973	972		
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CONNECT	975	963	960	974
CONNECT	976	960	964	977

CONNECT 977 976 978 992
CONNECT 978 977 979 980
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CONNECT 1000 999 1012
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CONNECT 1006 1004 1007 1008
CONNECT 1007 1006
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CONNECT 1025 1023 1026 1027
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CONNECT 1027 1025 1018 1028
CONNECT 1028 1013 1027 1029
CONNECT 1029 1028
CONNECT 1030 997 1001
CONNECT 1031 1046 1047
CONNECT 1032 1065
CONNECT 1033 1037 1045

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CONNECT 1034 1035 1046
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CONNECT 1036 995 1065
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CONNECT 1060 1058 1061 1062
CONNECT 1061 1060
CONNECT 1062 1053 1060 1063
CONNECT 1063 1048 1062 1064
CONNECT 1064 1063
CONNECT 1065 1032 1036

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Table 3. PDB file of the optimised structure of the 15-nuclear model of the LS centre in Zn matrix

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TITLE          CSD ENTRY jmk-126-09
REMARK        1 File created by GaussView 6.0.16
HETATM        1 Zn          0      19.114   5.736   0.752
Zn
HETATM        2 S           0      14.656   5.034  -0.111
S
HETATM        3 S           0      20.181   3.097  -3.176
S
HETATM        4 N           0      18.096   6.982  -0.749
N
HETATM        5 N           0      17.061   4.943   0.688
N
HETATM        6 N           0      16.435   3.925   1.358
N
HETATM        7 N           0      19.645   4.432  -0.793
N
HETATM        8 C           0      18.636   7.955  -1.467
C
HETATM        9 H           0      19.564   8.132  -1.367
H
HETATM       10 C           0      19.855   3.876  -1.789
C

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HETATM	11	C	0	17.909	8.725	-2.355
C						
HETATM	12	H	0	18.333	9.416	-2.850
H						
HETATM	13	C	0	16.574	8.485	-2.516
C						
HETATM	14	H	0	16.058	9.013	-3.115
H						
HETATM	15	C	0	15.983	7.461	-1.793
C						
HETATM	16	H	0	15.058	7.268	-1.891
H						
HETATM	17	C	0	16.775	6.721	-0.920
C						
HETATM	18	C	0	16.274	5.615	-0.116
C						
HETATM	19	C	0	15.156	3.852	1.050
C						
HETATM	20	C	0	14.221	2.885	1.642
C						
HETATM	21	C	0	14.698	1.833	2.446
C						
HETATM	22	H	0	15.631	1.736	2.592
H						
HETATM	23	C	0	13.833	0.958	3.012
C						
HETATM	24	H	0	14.173	0.235	3.525
H						
HETATM	25	C	0	12.414	1.102	2.853
C						
HETATM	26	C	0	11.501	0.235	3.454
C						
HETATM	27	H	0	11.818	-0.476	4.000
H						
HETATM	28	C	0	10.147	0.400	3.266
C						
HETATM	29	H	0	9.535	-0.209	3.665
H						
HETATM	30	C	0	9.671	1.450	2.496
C						
HETATM	31	H	0	8.736	1.565	2.385
H						
HETATM	32	C	0	10.539	2.328	1.890
C						
HETATM	33	H	0	10.204	3.044	1.363
H						
HETATM	34	C	0	11.949	2.159	2.054
C						
HETATM	35	C	0	12.862	3.033	1.449
C						
HETATM	36	H	0	12.542	3.738	0.896
H						
HETATM	37	S	0	23.571	6.438	1.614
S						
HETATM	38	S	0	18.047	8.375	4.680
S						

HETATM	39	N	0	20.131	4.491	2.253
N						
HETATM	40	N	0	21.167	6.528	0.815
N						
HETATM	41	N	0	21.793	7.546	0.145
N						
HETATM	42	N	0	18.582	7.040	2.296
N						
HETATM	43	C	0	19.592	3.517	2.970
C						
HETATM	44	H	0	18.664	3.340	2.871
H						
HETATM	45	C	0	18.373	7.595	3.292
C						
HETATM	46	C	0	20.319	2.747	3.859
C						
HETATM	47	H	0	19.894	2.057	4.353
H						
HETATM	48	C	0	21.654	2.986	4.019
C						
HETATM	49	H	0	22.169	2.459	4.618
H						
HETATM	50	C	0	22.245	4.010	3.296
C						
HETATM	51	H	0	23.170	4.204	3.395
H						
HETATM	52	C	0	21.453	4.750	2.424
C						
HETATM	53	C	0	21.954	5.857	1.619
C						
HETATM	54	C	0	23.071	7.620	0.453
C						
HETATM	55	C	0	24.007	8.587	-0.139
C						
HETATM	56	C	0	23.530	9.639	-0.943
C						
HETATM	57	H	0	22.596	9.736	-1.088
H						
HETATM	58	C	0	24.395	10.514	-1.509
C						
HETATM	59	H	0	24.054	11.237	-2.023
H						
HETATM	60	C	0	25.815	10.370	-1.350
C						
HETATM	61	C	0	26.727	11.237	-1.951
C						
HETATM	62	H	0	26.410	11.948	-2.496
H						
HETATM	63	C	0	28.081	11.073	-1.763
C						
HETATM	64	H	0	28.692	11.681	-2.162
H						
HETATM	65	C	0	28.556	10.022	-0.993
C						
HETATM	66	H	0	29.492	9.906	-0.883
H						

HETATM	67	C	0	27.688	9.145	-0.387
C						
HETATM	68	H	0	28.024	8.428	0.140
H						
HETATM	69	C	0	26.278	9.313	-0.551
C						
HETATM	70	C	0	25.366	8.438	0.054
C						
HETATM	71	H	0	25.686	7.734	0.607
H						
HETATM	72	Zn	0	14.899	-5.588	0.280
Zn						
HETATM	73	S	0	10.441	-6.290	-0.582
S						
HETATM	74	S	0	15.966	-8.227	-3.648
S						
HETATM	75	N	0	13.882	-4.342	-1.220
N						
HETATM	76	N	0	12.846	-6.380	0.217
N						
HETATM	77	N	0	12.219	-7.399	0.887
N						
HETATM	78	N	0	15.430	-6.892	-1.264
N						
HETATM	79	C	0	14.420	-3.369	-1.938
C						
HETATM	80	H	0	15.348	-3.192	-1.839
H						
HETATM	81	C	0	15.639	-7.447	-2.260
C						
HETATM	82	C	0	13.693	-2.599	-2.827
C						
HETATM	83	H	0	14.118	-1.908	-3.321
H						
HETATM	84	C	0	12.359	-2.838	-2.988
C						
HETATM	85	H	0	11.843	-2.311	-3.586
H						
HETATM	86	C	0	11.768	-3.862	-2.264
C						
HETATM	87	H	0	10.842	-4.056	-2.363
H						
HETATM	88	C	0	12.559	-4.602	-1.392
C						
HETATM	89	C	0	12.058	-5.709	-0.587
C						
HETATM	90	C	0	10.941	-7.473	0.579
C						
HETATM	91	C	0	10.006	-8.438	1.172
C						
HETATM	92	C	0	10.483	-9.491	1.975
C						
HETATM	93	H	0	11.417	-9.588	2.120
H						
HETATM	94	C	0	9.617	-10.366	2.540
C						

HETATM	95	H	0	9.958	-11.089	3.055
H						
HETATM	96	C	0	8.198	-10.222	2.382
C						
HETATM	97	C	0	7.286	-11.089	2.983
C						
HETATM	98	H	0	7.603	-11.800	3.528
H						
HETATM	99	C	0	5.932	-10.924	2.794
C						
HETATM	100	H	0	5.321	-11.533	3.194
H						
HETATM	101	C	0	5.457	-9.873	2.025
C						
HETATM	102	H	0	4.520	-9.758	1.914
H						
HETATM	103	C	0	6.325	-8.997	1.419
C						
HETATM	104	H	0	5.989	-8.281	0.893
H						
HETATM	105	C	0	7.735	-9.164	1.583
C						
HETATM	106	C	0	8.647	-8.290	0.977
C						
HETATM	107	H	0	8.326	-7.586	0.426
H						
HETATM	108	S	0	19.357	-4.886	1.143
S						
HETATM	109	S	0	13.831	-2.949	4.208
S						
HETATM	110	N	0	15.916	-6.833	1.781
N						
HETATM	111	N	0	16.951	-4.794	0.344
N						
HETATM	112	N	0	17.577	-3.777	-0.326
N						
HETATM	113	N	0	14.367	-4.284	1.826
N						
HETATM	114	C	0	15.376	-7.807	2.499
C						
HETATM	115	H	0	14.448	-7.984	2.399
H						
HETATM	116	C	0	14.158	-3.728	2.821
C						
HETATM	117	C	0	16.104	-8.577	3.388
C						
HETATM	118	H	0	15.679	-9.267	3.883
H						
HETATM	119	C	0	17.438	-8.337	3.548
C						
HETATM	120	H	0	17.954	-8.865	4.147
H						
HETATM	121	C	0	18.029	-7.313	2.826
C						
HETATM	122	H	0	18.954	-7.120	2.924
H						

HETATM	123	C	0	17.238	-6.572	1.953
C						
HETATM	124	C	0	17.738	-5.467	1.148
C						
HETATM	125	C	0	18.856	-3.704	-0.018
C						
HETATM	126	C	0	19.792	-2.737	-0.610
C						
HETATM	127	C	0	19.314	-1.685	-1.414
C						
HETATM	128	H	0	18.381	-1.588	-1.560
H						
HETATM	129	C	0	20.179	-0.810	-1.980
C						
HETATM	130	H	0	19.839	-0.087	-2.493
H						
HETATM	131	C	0	21.599	-0.953	-1.820
C						
HETATM	132	C	0	22.511	-0.087	-2.422
C						
HETATM	133	H	0	22.194	0.624	-2.968
H						
HETATM	134	C	0	23.865	-0.251	-2.233
C						
HETATM	135	H	0	24.477	0.357	-2.632
H						
HETATM	136	C	0	24.341	-1.302	-1.463
C						
HETATM	137	H	0	25.276	-1.417	-1.353
H						
HETATM	138	C	0	23.473	-2.180	-0.857
C						
HETATM	139	H	0	23.809	-2.896	-0.331
H						
HETATM	140	C	0	22.063	-2.011	-1.022
C						
HETATM	141	C	0	21.150	-2.885	-0.416
C						
HETATM	142	H	0	21.471	-3.589	0.136
H						
HETATM	143	Zn	0	10.683	-16.912	-0.190
Zn						
HETATM	144	S	0	6.226	-17.613	-1.053
S						
HETATM	145	S	0	11.750	-19.551	-4.119
S						
HETATM	146	N	0	9.666	-15.666	-1.691
N						
HETATM	147	N	0	8.631	-17.705	-0.255
N						
HETATM	148	N	0	8.005	-18.723	0.416
N						
HETATM	149	N	0	11.215	-18.215	-1.735
N						
HETATM	150	C	0	10.205	-14.692	-2.409
C						

HETATM	151	H	0	11.133	-14.516	-2.310
H						
HETATM	152	C	0	11.423	-18.771	-2.731
C						
HETATM	153	C	0	9.477	-13.923	-3.298
C						
HETATM	154	H	0	9.903	-13.232	-3.793
H						
HETATM	155	C	0	8.144	-14.163	-3.458
C						
HETATM	156	H	0	7.628	-13.634	-4.057
H						
HETATM	157	C	0	7.553	-15.186	-2.736
C						
HETATM	158	H	0	6.627	-15.379	-2.834
H						
HETATM	159	C	0	8.344	-15.927	-1.863
C						
HETATM	160	C	0	7.844	-17.032	-1.058
C						
HETATM	161	C	0	6.725	-18.796	0.108
C						
HETATM	162	C	0	5.790	-19.762	0.700
C						
HETATM	163	C	0	6.267	-20.814	1.505
C						
HETATM	164	H	0	7.201	-20.911	1.650
H						
HETATM	165	C	0	5.402	-21.689	2.070
C						
HETATM	166	H	0	5.742	-22.413	2.583
H						
HETATM	167	C	0	3.982	-21.545	1.910
C						
HETATM	168	C	0	3.071	-22.413	2.512
C						
HETATM	169	H	0	3.387	-23.124	3.057
H						
HETATM	170	C	0	1.716	-22.248	2.323
C						
HETATM	171	H	0	1.105	-22.857	2.722
H						
HETATM	172	C	0	1.241	-21.197	1.554
C						
HETATM	173	H	0	0.305	-21.081	1.443
H						
HETATM	174	C	0	2.109	-20.320	0.947
C						
HETATM	175	H	0	1.773	-19.604	0.421
H						
HETATM	176	C	0	3.519	-20.488	1.112
C						
HETATM	177	C	0	4.431	-19.614	0.506
C						
HETATM	178	H	0	4.111	-18.910	-0.046
H						

HETATM	179	S	0	15.141	-16.210	0.672
S						
HETATM	180	S	0	9.616	-14.273	3.738
S						
HETATM	181	N	0	11.700	-18.157	1.310
N						
HETATM	182	N	0	12.736	-16.118	-0.127
N						
HETATM	183	N	0	13.361	-15.101	-0.797
N						
HETATM	184	N	0	10.152	-15.608	1.354
N						
HETATM	185	C	0	11.161	-19.131	2.028
C						
HETATM	186	H	0	10.233	-19.308	1.929
H						
HETATM	187	C	0	9.943	-15.053	2.349
C						
HETATM	188	C	0	11.889	-19.901	2.917
C						
HETATM	189	H	0	11.464	-20.591	3.411
H						
HETATM	190	C	0	13.222	-19.661	3.078
C						
HETATM	191	H	0	13.738	-20.189	3.676
H						
HETATM	192	C	0	13.813	-18.636	2.354
C						
HETATM	193	H	0	14.739	-18.444	2.453
H						
HETATM	194	C	0	13.022	-17.896	1.482
C						
HETATM	195	C	0	13.522	-16.791	0.676
C						
HETATM	196	C	0	14.640	-15.027	-0.489
C						
HETATM	197	C	0	15.576	-14.061	-1.082
C						
HETATM	198	C	0	15.099	-13.009	-1.885
C						
HETATM	199	H	0	14.165	-12.912	-2.030
H						
HETATM	200	C	0	15.964	-12.134	-2.451
C						
HETATM	201	H	0	15.624	-11.410	-2.965
H						
HETATM	202	C	0	17.384	-12.277	-2.292
C						
HETATM	203	C	0	18.295	-11.410	-2.893
C						
HETATM	204	H	0	17.979	-10.699	-3.438
H						
HETATM	205	C	0	19.651	-11.575	-2.705
C						
HETATM	206	H	0	20.261	-10.967	-3.104
H						

HETATM	207	C	0	20.125	-12.626	-1.935
C						
HETATM	208	H	0	21.062	-12.742	-1.824
H						
HETATM	209	C	0	19.257	-13.503	-1.329
C						
HETATM	210	H	0	19.593	-14.219	-0.803
H						
HETATM	211	C	0	17.847	-13.335	-1.493
C						
HETATM	212	C	0	16.935	-14.210	-0.887
C						
HETATM	213	H	0	17.255	-14.913	-0.336
H						
HETATM	214	Zn	0	11.664	8.530	0.612
Zn						
HETATM	215	S	0	7.207	7.828	-0.251
S						
HETATM	216	S	0	12.731	5.891	-3.316
S						
HETATM	217	N	0	10.647	9.775	-0.889
N						
HETATM	218	N	0	9.612	7.737	0.547
N						
HETATM	219	N	0	8.986	6.719	1.218
N						
HETATM	220	N	0	12.196	7.226	-0.934
N						
HETATM	221	C	0	11.186	10.749	-1.607
C						
HETATM	222	H	0	12.115	10.926	-1.507
H						
HETATM	223	C	0	12.405	6.671	-1.929
C						
HETATM	224	C	0	10.460	11.518	-2.496
C						
HETATM	225	H	0	10.884	12.210	-2.991
H						
HETATM	226	C	0	9.125	11.279	-2.656
C						
HETATM	227	H	0	8.609	11.807	-3.255
H						
HETATM	228	C	0	8.534	10.255	-1.934
C						
HETATM	229	H	0	7.608	10.062	-2.032
H						
HETATM	230	C	0	9.326	9.515	-1.061
C						
HETATM	231	C	0	8.825	8.409	-0.256
C						
HETATM	232	C	0	7.707	6.646	0.910
C						
HETATM	233	C	0	6.771	5.679	1.502
C						
HETATM	234	C	0	7.248	4.627	2.306
C						

HETATM	235	H	0	8.182	4.530	2.452
H						
HETATM	236	C	0	6.384	3.752	2.872
C						
HETATM	237	H	0	6.724	3.029	3.385
H						
HETATM	238	C	0	4.965	3.896	2.712
C						
HETATM	239	C	0	4.052	3.029	3.314
C						
HETATM	240	H	0	4.368	2.318	3.860
H						
HETATM	241	C	0	2.697	3.194	3.126
C						
HETATM	242	H	0	2.086	2.585	3.524
H						
HETATM	243	C	0	2.222	4.244	2.355
C						
HETATM	244	H	0	1.286	4.359	2.245
H						
HETATM	245	C	0	3.090	5.121	1.749
C						
HETATM	246	H	0	2.755	5.837	1.223
H						
HETATM	247	C	0	4.500	4.953	1.914
C						
HETATM	248	C	0	5.413	5.827	1.308
C						
HETATM	249	H	0	5.093	6.532	0.756
H						
HETATM	250	S	0	16.122	9.232	1.474
S						
HETATM	251	S	0	10.598	11.168	4.540
S						
HETATM	252	N	0	12.682	7.285	2.112
N						
HETATM	253	N	0	13.717	9.323	0.675
N						
HETATM	254	N	0	14.343	10.341	0.005
N						
HETATM	255	N	0	11.133	9.834	2.156
N						
HETATM	256	C	0	12.143	6.311	2.830
C						
HETATM	257	H	0	11.214	6.134	2.731
H						
HETATM	258	C	0	10.924	10.389	3.151
C						
HETATM	259	C	0	12.870	5.541	3.719
C						
HETATM	260	H	0	12.445	4.851	4.213
H						
HETATM	261	C	0	14.205	5.780	3.879
C						
HETATM	262	H	0	14.720	5.253	4.478
H						

HETATM	263	C	0	14.795	6.805	3.156
C						
HETATM	264	H	0	15.721	6.998	3.255
H						
HETATM	265	C	0	14.003	7.545	2.284
C						
HETATM	266	C	0	14.504	8.651	1.479
C						
HETATM	267	C	0	15.622	10.414	0.313
C						
HETATM	268	C	0	16.557	11.381	-0.280
C						
HETATM	269	C	0	16.081	12.433	-1.083
C						
HETATM	270	H	0	15.146	12.530	-1.228
H						
HETATM	271	C	0	16.946	13.308	-1.649
C						
HETATM	272	H	0	16.605	14.031	-2.163
H						
HETATM	273	C	0	18.365	13.164	-1.490
C						
HETATM	274	C	0	19.277	14.031	-2.091
C						
HETATM	275	H	0	18.961	14.742	-2.636
H						
HETATM	276	C	0	20.632	13.867	-1.903
C						
HETATM	277	H	0	21.243	14.475	-2.302
H						
HETATM	278	C	0	21.107	12.816	-1.133
C						
HETATM	279	H	0	22.043	12.700	-1.023
H						
HETATM	280	C	0	20.239	11.938	-0.527
C						
HETATM	281	H	0	20.574	11.222	-0.001
H						
HETATM	282	C	0	18.829	12.107	-0.691
C						
HETATM	283	C	0	17.917	11.232	-0.086
C						
HETATM	284	H	0	18.236	10.528	0.466
H						
HETATM	285	Zn	0	7.449	-2.794	0.140
Zn						
HETATM	286	S	0	2.991	-3.496	-0.722
S						
HETATM	287	S	0	8.517	-5.433	-3.788
S						
HETATM	288	N	0	6.433	-1.549	-1.360
N						
HETATM	289	N	0	5.396	-3.587	0.077
N						
HETATM	290	N	0	4.770	-4.605	0.747
N						

HETATM	291	N	0	7.981	-4.098	-1.404
N						
HETATM	292	C	0	6.971	-0.575	-2.078
C						
HETATM	293	H	0	7.899	-0.398	-1.979
H						
HETATM	294	C	0	8.190	-4.653	-2.400
C						
HETATM	295	C	0	6.244	0.195	-2.967
C						
HETATM	296	H	0	6.669	0.886	-3.461
H						
HETATM	297	C	0	4.910	-0.045	-3.128
C						
HETATM	298	H	0	4.393	0.483	-3.726
H						
HETATM	299	C	0	4.319	-1.069	-2.404
C						
HETATM	300	H	0	3.394	-1.262	-2.504
H						
HETATM	301	C	0	5.110	-1.809	-1.532
C						
HETATM	302	C	0	4.609	-2.915	-0.727
C						
HETATM	303	C	0	3.492	-4.679	0.439
C						
HETATM	304	C	0	2.556	-5.644	1.032
C						
HETATM	305	C	0	3.033	-6.697	1.835
C						
HETATM	306	H	0	3.967	-6.794	1.980
H						
HETATM	307	C	0	2.168	-7.572	2.400
C						
HETATM	308	H	0	2.508	-8.295	2.915
H						
HETATM	309	C	0	0.749	-7.428	2.242
C						
HETATM	310	C	0	-0.163	-8.295	2.843
C						
HETATM	311	H	0	0.154	-9.006	3.388
H						
HETATM	312	C	0	-1.518	-8.130	2.654
C						
HETATM	313	H	0	-2.128	-8.739	3.054
H						
HETATM	314	C	0	-1.992	-7.079	1.885
C						
HETATM	315	H	0	-2.929	-6.965	1.774
H						
HETATM	316	C	0	-1.125	-6.202	1.279
C						
HETATM	317	H	0	-1.462	-5.486	0.753
H						
HETATM	318	C	0	0.286	-6.371	1.443
C						

HETATM	319	C	0	1.197	-5.497	0.837
C						
HETATM	320	H	0	0.877	-4.792	0.286
H						
HETATM	321	S	0	11.906	-2.092	1.003
S						
HETATM	322	S	0	6.382	-0.155	4.068
S						
HETATM	323	N	0	8.466	-4.039	1.641
N						
HETATM	324	N	0	9.502	-2.001	0.204
N						
HETATM	325	N	0	10.128	-0.984	-0.466
N						
HETATM	326	N	0	6.917	-1.490	1.685
N						
HETATM	327	C	0	7.927	-5.013	2.359
C						
HETATM	328	H	0	6.999	-5.190	2.259
H						
HETATM	329	C	0	6.708	-0.935	2.681
C						
HETATM	330	C	0	8.654	-5.783	3.248
C						
HETATM	331	H	0	8.229	-6.473	3.743
H						
HETATM	332	C	0	9.989	-5.544	3.408
C						
HETATM	333	H	0	10.504	-6.071	4.007
H						
HETATM	334	C	0	10.580	-4.519	2.686
C						
HETATM	335	H	0	11.505	-4.326	2.783
H						
HETATM	336	C	0	9.789	-3.779	1.813
C						
HETATM	337	C	0	10.289	-2.673	1.008
C						
HETATM	338	C	0	11.406	-0.910	-0.158
C						
HETATM	339	C	0	12.343	0.057	-0.750
C						
HETATM	340	C	0	11.865	1.109	-1.555
C						
HETATM	341	H	0	10.932	1.205	-1.700
H						
HETATM	342	C	0	12.730	1.984	-2.120
C						
HETATM	343	H	0	12.390	2.707	-2.633
H						
HETATM	344	C	0	14.150	1.840	-1.960
C						
HETATM	345	C	0	15.062	2.707	-2.562
C						
HETATM	346	H	0	14.745	3.418	-3.108
H						

HETATM	347	C	0	16.416	2.543	-2.374
C						
HETATM	348	H	0	17.027	3.151	-2.773
H						
HETATM	349	C	0	16.891	1.492	-1.604
C						
HETATM	350	H	0	17.827	1.376	-1.493
H						
HETATM	351	C	0	16.024	0.614	-0.998
C						
HETATM	352	H	0	16.360	-0.102	-0.471
H						
HETATM	353	C	0	14.613	0.783	-1.162
C						
HETATM	354	C	0	13.701	-0.092	-0.556
C						
HETATM	355	H	0	14.022	-0.795	-0.004
H						
HETATM	356	Zn	0	3.234	-14.118	-0.331
Zn						
HETATM	357	S	0	-1.224	-14.819	-1.194
S						
HETATM	358	S	0	4.301	-16.757	-4.259
S						
HETATM	359	N	0	2.217	-12.872	-1.831
N						
HETATM	360	N	0	1.182	-14.911	-0.395
N						
HETATM	361	N	0	0.555	-15.929	0.275
N						
HETATM	362	N	0	3.765	-15.421	-1.876
N						
HETATM	363	C	0	2.756	-11.898	-2.550
C						
HETATM	364	H	0	3.684	-11.722	-2.450
H						
HETATM	365	C	0	3.974	-15.977	-2.871
C						
HETATM	366	C	0	2.028	-11.129	-3.438
C						
HETATM	367	H	0	2.454	-10.438	-3.933
H						
HETATM	368	C	0	0.694	-11.368	-3.599
C						
HETATM	369	H	0	0.179	-10.840	-4.197
H						
HETATM	370	C	0	0.103	-12.392	-2.876
C						
HETATM	371	H	0	-0.822	-12.585	-2.974
H						
HETATM	372	C	0	0.895	-13.133	-2.003
C						
HETATM	373	C	0	0.394	-14.238	-1.198
C						
HETATM	374	C	0	-0.724	-16.002	-0.033
C						

HETATM	375	C	0	-1.659	-16.968	0.560
C						
HETATM	376	C	0	-1.182	-18.020	1.364
C						
HETATM	377	H	0	-0.248	-18.117	1.510
H						
HETATM	378	C	0	-2.047	-18.895	1.930
C						
HETATM	379	H	0	-1.707	-19.619	2.443
H						
HETATM	380	C	0	-3.467	-18.751	1.770
C						
HETATM	381	C	0	-4.379	-19.619	2.371
C						
HETATM	382	H	0	-4.062	-20.330	2.917
H						
HETATM	383	C	0	-5.733	-19.454	2.183
C						
HETATM	384	H	0	-6.344	-20.063	2.582
H						
HETATM	385	C	0	-6.208	-18.403	1.413
C						
HETATM	386	H	0	-7.144	-18.288	1.303
H						
HETATM	387	C	0	-5.340	-17.526	0.807
C						
HETATM	388	H	0	-5.676	-16.811	0.281
H						
HETATM	389	C	0	-3.930	-17.694	0.971
C						
HETATM	390	C	0	-3.018	-16.820	0.366
C						
HETATM	391	H	0	-3.338	-16.116	-0.186
H						
HETATM	392	S	0	7.692	-13.416	0.532
S						
HETATM	393	S	0	2.167	-11.479	3.598
S						
HETATM	394	N	0	4.251	-15.363	1.170
N						
HETATM	395	N	0	5.286	-13.324	-0.267
N						
HETATM	396	N	0	5.912	-12.307	-0.938
N						
HETATM	397	N	0	2.703	-12.814	1.214
N						
HETATM	398	C	0	3.711	-16.337	1.887
C						
HETATM	399	H	0	2.784	-16.514	1.789
H						
HETATM	400	C	0	2.493	-12.258	2.209
C						
HETATM	401	C	0	4.439	-17.107	2.777
C						
HETATM	402	H	0	4.015	-17.797	3.271
H						

HETATM	403	C	0	5.773	-16.867	2.937
C						
HETATM	404	H	0	6.289	-17.395	3.535
H						
HETATM	405	C	0	6.364	-15.842	2.214
C						
HETATM	406	H	0	7.290	-15.650	2.313
H						
HETATM	407	C	0	5.573	-15.102	1.342
C						
HETATM	408	C	0	6.073	-13.997	0.536
C						
HETATM	409	C	0	7.191	-12.234	-0.630
C						
HETATM	410	C	0	8.127	-11.267	-1.222
C						
HETATM	411	C	0	7.650	-10.215	-2.025
C						
HETATM	412	H	0	6.716	-10.118	-2.171
H						
HETATM	413	C	0	8.514	-9.340	-2.592
C						
HETATM	414	H	0	8.175	-8.616	-3.105
H						
HETATM	415	C	0	9.934	-9.483	-2.432
C						
HETATM	416	C	0	10.846	-8.616	-3.033
C						
HETATM	417	H	0	10.530	-7.905	-3.578
H						
HETATM	418	C	0	12.201	-8.781	-2.845
C						
HETATM	419	H	0	12.812	-8.173	-3.244
H						
HETATM	420	C	0	12.676	-9.832	-2.075
C						
HETATM	421	H	0	13.612	-9.948	-1.964
H						
HETATM	422	C	0	11.808	-10.710	-1.469
C						
HETATM	423	H	0	12.144	-11.425	-0.943
H						
HETATM	424	C	0	10.398	-10.541	-1.633
C						
HETATM	425	C	0	9.485	-11.415	-1.027
C						
HETATM	426	H	0	9.806	-12.119	-0.476
H						
HETATM	427	Zn	0	4.215	11.324	0.471
Zn						
HETATM	428	S	0	-0.242	10.622	-0.392
S						
HETATM	429	S	0	5.282	8.685	-3.457
S						
HETATM	430	N	0	3.198	12.569	-1.029
N						

HETATM	431	N	0	2.163	10.531	0.407
N						
HETATM	432	N	0	1.537	9.513	1.078
N						
HETATM	433	N	0	4.747	10.020	-1.074
N						
HETATM	434	C	0	3.737	13.543	-1.748
C						
HETATM	435	H	0	4.666	13.719	-1.648
H						
HETATM	436	C	0	4.956	9.464	-2.069
C						
HETATM	437	C	0	3.010	14.313	-2.636
C						
HETATM	438	H	0	3.435	15.004	-3.131
H						
HETATM	439	C	0	1.675	14.073	-2.797
C						
HETATM	440	H	0	1.160	14.600	-3.395
H						
HETATM	441	C	0	1.085	13.049	-2.074
C						
HETATM	442	H	0	0.159	12.856	-2.172
H						
HETATM	443	C	0	1.876	12.309	-1.201
C						
HETATM	444	C	0	1.376	11.203	-0.396
C						
HETATM	445	C	0	0.258	9.439	0.769
C						
HETATM	446	C	0	-0.678	8.473	1.362
C						
HETATM	447	C	0	-0.201	7.421	2.165
C						
HETATM	448	H	0	0.733	7.324	2.311
H						
HETATM	449	C	0	-1.066	6.546	2.731
C						
HETATM	450	H	0	-0.725	5.823	3.245
H						
HETATM	451	C	0	-2.485	6.690	2.572
C						
HETATM	452	C	0	-3.397	5.822	3.173
C						
HETATM	453	H	0	-3.081	5.112	3.719
H						
HETATM	454	C	0	-4.752	5.988	2.985
C						
HETATM	455	H	0	-5.363	5.379	3.384
H						
HETATM	456	C	0	-5.227	7.038	2.215
C						
HETATM	457	H	0	-6.163	7.153	2.105
H						
HETATM	458	C	0	-4.359	7.915	1.609
C						

HETATM	459	H	0	-4.695	8.631	1.083
H						
HETATM	460	C	0	-2.949	7.747	1.773
C						
HETATM	461	C	0	-2.037	8.621	1.168
C						
HETATM	462	H	0	-2.356	9.326	0.616
H						
HETATM	463	S	0	8.673	12.026	1.334
S						
HETATM	464	S	0	3.149	13.962	4.400
S						
HETATM	465	N	0	5.233	10.079	1.972
N						
HETATM	466	N	0	6.268	12.116	0.535
N						
HETATM	467	N	0	6.894	13.134	-0.136
N						
HETATM	468	N	0	3.684	12.628	2.016
N						
HETATM	469	C	0	4.694	9.105	2.690
C						
HETATM	470	H	0	3.765	8.928	2.591
H						
HETATM	471	C	0	3.475	13.183	3.011
C						
HETATM	472	C	0	5.420	8.335	3.579
C						
HETATM	473	H	0	4.996	7.645	4.073
H						
HETATM	474	C	0	6.755	8.574	3.739
C						
HETATM	475	H	0	7.271	8.047	4.337
H						
HETATM	476	C	0	7.346	9.598	3.016
C						
HETATM	477	H	0	8.272	9.791	3.115
H						
HETATM	478	C	0	6.554	10.338	2.144
C						
HETATM	479	C	0	7.055	11.445	1.338
C						
HETATM	480	C	0	8.173	13.208	0.173
C						
HETATM	481	C	0	9.108	14.175	-0.420
C						
HETATM	482	C	0	8.632	15.227	-1.223
C						
HETATM	483	H	0	7.697	15.323	-1.368
H						
HETATM	484	C	0	9.497	16.101	-1.789
C						
HETATM	485	H	0	9.156	16.825	-2.303
H						
HETATM	486	C	0	10.916	15.958	-1.630
C						

HETATM	487	C	0	11.827	16.825	-2.231
C						
HETATM	488	H	0	11.511	17.536	-2.776
H						
HETATM	489	C	0	13.183	16.660	-2.043
C						
HETATM	490	H	0	13.793	17.269	-2.442
H						
HETATM	491	C	0	13.658	15.609	-1.273
C						
HETATM	492	H	0	14.594	15.494	-1.163
H						
HETATM	493	C	0	12.790	14.732	-0.667
C						
HETATM	494	H	0	13.125	14.016	-0.141
H						
HETATM	495	C	0	11.380	14.901	-0.831
C						
HETATM	496	C	0	10.468	14.026	-0.226
C						
HETATM	497	H	0	10.787	13.322	0.326
H						
HETATM	498	Fe	0	0.001	0.000	-0.001
Fe						
HETATM	499	S	0	-4.355	-0.645	-0.945
S						
HETATM	500	S	0	1.025	-2.790	-3.821
S						
HETATM	501	N	0	-0.795	1.289	-1.344
N						
HETATM	502	N	0	-1.889	-0.752	-0.067
N						
HETATM	503	N	0	-2.543	-1.803	0.594
N						
HETATM	504	N	0	0.490	-1.165	-1.485
N						
HETATM	505	C	0	-0.157	2.306	-1.976
C						
HETATM	506	H	0	0.886	2.452	-1.705
H						
HETATM	507	C	0	0.693	-1.830	-2.448
C						
HETATM	508	C	0	-0.813	3.119	-2.931
C						
HETATM	509	H	0	-0.262	3.925	-3.414
H						
HETATM	510	C	0	-2.169	2.872	-3.245
C						
HETATM	511	H	0	-2.695	3.489	-3.974
H						
HETATM	512	C	0	-2.838	1.809	-2.595
C						
HETATM	513	H	0	-3.877	1.568	-2.826
H						
HETATM	514	C	0	-2.109	1.051	-1.653
C						

HETATM	515	C	0	-2.674	-0.072	-0.897
C						
HETATM	516	C	0	-3.826	-1.896	0.264
C						
HETATM	517	C	0	-4.793	-2.866	0.821
C						
HETATM	518	C	0	-4.331	-3.985	1.609
C						
HETATM	519	H	0	-3.261	-4.122	1.761
H						
HETATM	520	C	0	-5.253	-4.865	2.172
C						
HETATM	521	H	0	-4.918	-5.717	2.767
H						
HETATM	522	C	0	-6.674	-4.662	1.999
C						
HETATM	523	C	0	-7.652	-5.533	2.601
C						
HETATM	524	H	0	-7.302	-6.372	3.205
H						
HETATM	525	C	0	-9.018	-5.312	2.400
C						
HETATM	526	H	0	-9.761	-5.960	2.868
H						
HETATM	527	C	0	-9.470	-4.208	1.592
C						
HETATM	528	H	0	-10.543	-4.056	1.459
H						
HETATM	529	C	0	-8.547	-3.341	1.004
C						
HETATM	530	H	0	-8.877	-2.488	0.409
H						
HETATM	531	C	0	-7.132	-3.553	1.192
C						
HETATM	532	C	0	-6.164	-2.676	0.606
C						
HETATM	533	H	0	-6.529	-1.847	-0.004
H						
HETATM	534	S	0	4.357	0.647	0.944
S						
HETATM	535	S	0	-1.025	2.789	3.820
S						
HETATM	536	N	0	0.797	-1.288	1.342
N						
HETATM	537	N	0	1.892	0.753	0.065
N						
HETATM	538	N	0	2.545	1.804	-0.596
N						
HETATM	539	N	0	-0.487	1.166	1.483
N						
HETATM	540	C	0	0.160	-2.305	1.974
C						
HETATM	541	H	0	-0.884	-2.452	1.703
H						
HETATM	542	C	0	-0.691	1.830	2.446
C						

HETATM	543	C	0	0.816	-3.118	2.930
C						
HETATM	544	H	0	0.265	-3.924	3.413
H						
HETATM	545	C	0	2.171	-2.870	3.244
C						
HETATM	546	H	0	2.697	-3.487	3.973
H						
HETATM	547	C	0	2.840	-1.808	2.594
C						
HETATM	548	H	0	3.879	-1.566	2.825
H						
HETATM	549	C	0	2.112	-1.049	1.652
C						
HETATM	550	C	0	2.677	0.073	0.895
C						
HETATM	551	C	0	3.828	1.897	-0.266
C						
HETATM	552	C	0	4.795	2.867	-0.822
C						
HETATM	553	C	0	4.333	3.986	-1.611
C						
HETATM	554	H	0	3.263	4.123	-1.762
H						
HETATM	555	C	0	5.254	4.867	-2.173
C						
HETATM	556	H	0	4.919	5.719	-2.769
H						
HETATM	557	C	0	6.675	4.664	-2.001
C						
HETATM	558	C	0	7.652	5.536	-2.603
C						
HETATM	559	H	0	7.302	6.374	-3.207
H						
HETATM	560	C	0	9.019	5.315	-2.403
C						
HETATM	561	H	0	9.762	5.962	-2.871
H						
HETATM	562	C	0	9.471	4.210	-1.595
C						
HETATM	563	H	0	10.544	4.059	-1.463
H						
HETATM	564	C	0	8.549	3.344	-1.006
C						
HETATM	565	H	0	8.879	2.490	-0.412
H						
HETATM	566	C	0	7.134	3.555	-1.194
C						
HETATM	567	C	0	6.166	2.678	-0.607
C						
HETATM	568	H	0	6.531	1.849	0.002
H						
HETATM	569	Zn	0	-4.215	-11.324	-0.471
Zn						
HETATM	570	S	0	-8.673	-12.026	-1.334
S						

HETATM	571	S	0	-3.149	-13.962	-4.400
S						
HETATM	572	N	0	-5.233	-10.079	-1.972
N						
HETATM	573	N	0	-6.268	-12.116	-0.535
N						
HETATM	574	N	0	-6.894	-13.134	0.136
N						
HETATM	575	N	0	-3.684	-12.628	-2.016
N						
HETATM	576	C	0	-4.694	-9.105	-2.689
C						
HETATM	577	H	0	-3.765	-8.928	-2.591
H						
HETATM	578	C	0	-3.475	-13.183	-3.011
C						
HETATM	579	C	0	-5.420	-8.335	-3.579
C						
HETATM	580	H	0	-4.996	-7.645	-4.073
H						
HETATM	581	C	0	-6.755	-8.575	-3.738
C						
HETATM	582	H	0	-7.271	-8.047	-4.337
H						
HETATM	583	C	0	-7.346	-9.598	-3.016
C						
HETATM	584	H	0	-8.272	-9.791	-3.115
H						
HETATM	585	C	0	-6.554	-10.338	-2.144
C						
HETATM	586	C	0	-7.055	-11.445	-1.338
C						
HETATM	587	C	0	-8.173	-13.208	-0.172
C						
HETATM	588	C	0	-9.109	-14.175	0.420
C						
HETATM	589	C	0	-8.632	-15.227	1.223
C						
HETATM	590	H	0	-7.698	-15.323	1.369
H						
HETATM	591	C	0	-9.497	-16.102	1.790
C						
HETATM	592	H	0	-9.156	-16.825	2.303
H						
HETATM	593	C	0	-10.916	-15.958	1.630
C						
HETATM	594	C	0	-11.828	-16.825	2.232
C						
HETATM	595	H	0	-11.512	-17.536	2.776
H						
HETATM	596	C	0	-13.183	-16.661	2.043
C						
HETATM	597	H	0	-13.794	-17.269	2.442
H						
HETATM	598	C	0	-13.658	-15.609	1.273
C						

HETATM	599	H	0	-14.594	-15.494	1.163
H						
HETATM	600	C	0	-12.790	-14.732	0.667
C						
HETATM	601	H	0	-13.125	-14.016	0.141
H						
HETATM	602	C	0	-11.380	-14.901	0.831
C						
HETATM	603	C	0	-10.468	-14.026	0.226
C						
HETATM	604	H	0	-10.787	-13.322	-0.326
H						
HETATM	605	S	0	0.242	-10.622	0.392
S						
HETATM	606	S	0	-5.282	-8.685	3.457
S						
HETATM	607	N	0	-3.198	-12.569	1.029
N						
HETATM	608	N	0	-2.163	-10.531	-0.407
N						
HETATM	609	N	0	-1.537	-9.513	-1.077
N						
HETATM	610	N	0	-4.747	-10.020	1.074
N						
HETATM	611	C	0	-3.737	-13.543	1.748
C						
HETATM	612	H	0	-4.666	-13.720	1.648
H						
HETATM	613	C	0	-4.956	-9.464	2.069
C						
HETATM	614	C	0	-3.010	-14.313	2.636
C						
HETATM	615	H	0	-3.435	-15.004	3.131
H						
HETATM	616	C	0	-1.675	-14.073	2.797
C						
HETATM	617	H	0	-1.160	-14.600	3.396
H						
HETATM	618	C	0	-1.085	-13.049	2.074
C						
HETATM	619	H	0	-0.159	-12.856	2.172
H						
HETATM	620	C	0	-1.877	-12.309	1.201
C						
HETATM	621	C	0	-1.376	-11.203	0.396
C						
HETATM	622	C	0	-0.258	-9.439	-0.769
C						
HETATM	623	C	0	0.677	-8.473	-1.362
C						
HETATM	624	C	0	0.201	-7.421	-2.165
C						
HETATM	625	H	0	-0.733	-7.324	-2.311
H						
HETATM	626	C	0	1.066	-6.546	-2.731
C						

HETATM	627	H	0	0.725	-5.823	-3.245
H						
HETATM	628	C	0	2.485	-6.690	-2.572
C						
HETATM	629	C	0	3.397	-5.823	-3.173
C						
HETATM	630	H	0	3.081	-5.112	-3.719
H						
HETATM	631	C	0	4.752	-5.988	-2.985
C						
HETATM	632	H	0	5.363	-5.379	-3.384
H						
HETATM	633	C	0	5.227	-7.038	-2.215
C						
HETATM	634	H	0	6.163	-7.153	-2.105
H						
HETATM	635	C	0	4.359	-7.915	-1.609
C						
HETATM	636	H	0	4.694	-8.631	-1.083
H						
HETATM	637	C	0	2.949	-7.747	-1.773
C						
HETATM	638	C	0	2.037	-8.621	-1.168
C						
HETATM	639	H	0	2.356	-9.326	-0.616
H						
HETATM	640	Zn	0	-3.234	14.118	0.331
Zn						
HETATM	641	S	0	-7.692	13.416	-0.531
S						
HETATM	642	S	0	-2.167	11.479	-3.597
S						
HETATM	643	N	0	-4.251	15.363	-1.170
N						
HETATM	644	N	0	-5.287	13.324	0.267
N						
HETATM	645	N	0	-5.912	12.307	0.938
N						
HETATM	646	N	0	-2.703	12.814	-1.214
N						
HETATM	647	C	0	-3.711	16.337	-1.887
C						
HETATM	648	H	0	-2.784	16.514	-1.788
H						
HETATM	649	C	0	-2.493	12.258	-2.209
C						
HETATM	650	C	0	-4.439	17.107	-2.777
C						
HETATM	651	H	0	-4.015	17.797	-3.271
H						
HETATM	652	C	0	-5.773	16.867	-2.937
C						
HETATM	653	H	0	-6.289	17.395	-3.535
H						
HETATM	654	C	0	-6.365	15.842	-2.214
C						

HETATM	655	H	0	-7.290	15.650	-2.313
H						
HETATM	656	C	0	-5.573	15.102	-1.342
C						
HETATM	657	C	0	-6.073	13.997	-0.536
C						
HETATM	658	C	0	-7.192	12.234	0.630
C						
HETATM	659	C	0	-8.127	11.267	1.222
C						
HETATM	660	C	0	-7.650	10.215	2.025
C						
HETATM	661	H	0	-6.716	10.118	2.171
H						
HETATM	662	C	0	-8.515	9.340	2.592
C						
HETATM	663	H	0	-8.175	8.616	3.105
H						
HETATM	664	C	0	-9.934	9.483	2.432
C						
HETATM	665	C	0	-10.846	8.616	3.033
C						
HETATM	666	H	0	-10.530	7.905	3.578
H						
HETATM	667	C	0	-12.202	8.781	2.845
C						
HETATM	668	H	0	-12.812	8.173	3.244
H						
HETATM	669	C	0	-12.676	9.832	2.075
C						
HETATM	670	H	0	-13.613	9.948	1.964
H						
HETATM	671	C	0	-11.808	10.709	1.469
C						
HETATM	672	H	0	-12.144	11.425	0.943
H						
HETATM	673	C	0	-10.398	10.541	1.634
C						
HETATM	674	C	0	-9.485	11.415	1.027
C						
HETATM	675	H	0	-9.806	12.119	0.476
H						
HETATM	676	S	0	1.223	14.819	1.194
S						
HETATM	677	S	0	-4.301	16.757	4.259
S						
HETATM	678	N	0	-2.217	12.872	1.831
N						
HETATM	679	N	0	-1.182	14.911	0.395
N						
HETATM	680	N	0	-0.556	15.929	-0.275
N						
HETATM	681	N	0	-3.766	15.421	1.876
N						
HETATM	682	C	0	-2.756	11.898	2.550
C						

HETATM	683	H	0	-3.684	11.722	2.450
H						
HETATM	684	C	0	-3.974	15.977	2.871
C						
HETATM	685	C	0	-2.028	11.129	3.438
C						
HETATM	686	H	0	-2.454	10.438	3.933
H						
HETATM	687	C	0	-0.694	11.368	3.599
C						
HETATM	688	H	0	-0.179	10.840	4.198
H						
HETATM	689	C	0	-0.103	12.392	2.876
C						
HETATM	690	H	0	0.822	12.585	2.974
H						
HETATM	691	C	0	-0.895	13.133	2.003
C						
HETATM	692	C	0	-0.394	14.238	1.198
C						
HETATM	693	C	0	0.723	16.002	0.033
C						
HETATM	694	C	0	1.659	16.968	-0.560
C						
HETATM	695	C	0	1.182	18.020	-1.364
C						
HETATM	696	H	0	0.248	18.117	-1.509
H						
HETATM	697	C	0	2.047	18.895	-1.929
C						
HETATM	698	H	0	1.707	19.619	-2.443
H						
HETATM	699	C	0	3.467	18.751	-1.770
C						
HETATM	700	C	0	4.379	19.619	-2.371
C						
HETATM	701	H	0	4.062	20.330	-2.917
H						
HETATM	702	C	0	5.733	19.454	-2.183
C						
HETATM	703	H	0	6.344	20.063	-2.582
H						
HETATM	704	C	0	6.208	18.403	-1.413
C						
HETATM	705	H	0	7.144	18.287	-1.303
H						
HETATM	706	C	0	5.340	17.526	-0.807
C						
HETATM	707	H	0	5.676	16.810	-0.281
H						
HETATM	708	C	0	3.930	17.694	-0.971
C						
HETATM	709	C	0	3.018	16.820	-0.366
C						
HETATM	710	H	0	3.338	16.116	0.186
H						

HETATM	711	Zn	0	-7.449	2.794	-0.140
Zn						
HETATM	712	S	0	-11.907	2.092	-1.003
S						
HETATM	713	S	0	-6.382	0.155	-4.068
S						
HETATM	714	N	0	-8.466	4.038	-1.641
N						
HETATM	715	N	0	-9.502	2.001	-0.203
N						
HETATM	716	N	0	-10.128	0.984	0.466
N						
HETATM	717	N	0	-6.918	1.490	-1.685
N						
HETATM	718	C	0	-7.927	5.013	-2.359
C						
HETATM	719	H	0	-6.999	5.190	-2.259
H						
HETATM	720	C	0	-6.709	0.935	-2.681
C						
HETATM	721	C	0	-8.655	5.783	-3.247
C						
HETATM	722	H	0	-8.229	6.473	-3.742
H						
HETATM	723	C	0	-9.989	5.543	-3.408
C						
HETATM	724	H	0	-10.504	6.071	-4.007
H						
HETATM	725	C	0	-10.580	4.519	-2.685
C						
HETATM	726	H	0	-11.505	4.326	-2.783
H						
HETATM	727	C	0	-9.789	3.778	-1.813
C						
HETATM	728	C	0	-10.289	2.673	-1.008
C						
HETATM	729	C	0	-11.406	0.910	0.158
C						
HETATM	730	C	0	-12.343	-0.057	0.751
C						
HETATM	731	C	0	-11.865	-1.109	1.555
C						
HETATM	732	H	0	-10.932	-1.206	1.700
H						
HETATM	733	C	0	-12.730	-1.984	2.120
C						
HETATM	734	H	0	-12.390	-2.707	2.634
H						
HETATM	735	C	0	-14.150	-1.840	1.961
C						
HETATM	736	C	0	-15.062	-2.707	2.562
C						
HETATM	737	H	0	-14.745	-3.418	3.108
H						
HETATM	738	C	0	-16.416	-2.543	2.374
C						

HETATM	739	H	0	-17.027	-3.151	2.773
H						
HETATM	740	C	0	-16.891	-1.492	1.604
C						
HETATM	741	H	0	-17.827	-1.377	1.494
H						
HETATM	742	C	0	-16.024	-0.614	0.998
C						
HETATM	743	H	0	-16.360	0.102	0.471
H						
HETATM	744	C	0	-14.613	-0.783	1.162
C						
HETATM	745	C	0	-13.701	0.091	0.557
C						
HETATM	746	H	0	-14.022	0.795	0.004
H						
HETATM	747	S	0	-2.991	3.496	0.722
S						
HETATM	748	S	0	-8.517	5.433	3.788
S						
HETATM	749	N	0	-6.433	1.549	1.361
N						
HETATM	750	N	0	-5.397	3.587	-0.077
N						
HETATM	751	N	0	-4.770	4.605	-0.747
N						
HETATM	752	N	0	-7.981	4.098	1.404
N						
HETATM	753	C	0	-6.971	0.575	2.078
C						
HETATM	754	H	0	-7.899	0.398	1.979
H						
HETATM	755	C	0	-8.190	4.653	2.401
C						
HETATM	756	C	0	-6.244	-0.195	2.967
C						
HETATM	757	H	0	-6.669	-0.886	3.461
H						
HETATM	758	C	0	-4.910	0.044	3.128
C						
HETATM	759	H	0	-4.393	-0.483	3.726
H						
HETATM	760	C	0	-4.319	1.069	2.404
C						
HETATM	761	H	0	-3.393	1.262	2.503
H						
HETATM	762	C	0	-5.110	1.809	1.532
C						
HETATM	763	C	0	-4.609	2.915	0.727
C						
HETATM	764	C	0	-3.492	4.679	-0.439
C						
HETATM	765	C	0	-2.556	5.644	-1.032
C						
HETATM	766	C	0	-3.034	6.697	-1.835
C						

HETATM	767	H	0	-3.967	6.794	-1.980
H						
HETATM	768	C	0	-2.168	7.572	-2.400
C						
HETATM	769	H	0	-2.508	8.295	-2.914
H						
HETATM	770	C	0	-0.749	7.428	-2.242
C						
HETATM	771	C	0	0.163	8.295	-2.843
C						
HETATM	772	H	0	-0.154	9.006	-3.388
H						
HETATM	773	C	0	1.517	8.130	-2.654
C						
HETATM	774	H	0	2.128	8.739	-3.054
H						
HETATM	775	C	0	1.992	7.079	-1.885
C						
HETATM	776	H	0	2.929	6.965	-1.773
H						
HETATM	777	C	0	1.125	6.202	-1.279
C						
HETATM	778	H	0	1.461	5.486	-0.752
H						
HETATM	779	C	0	-0.286	6.370	-1.443
C						
HETATM	780	C	0	-1.198	5.496	-0.837
C						
HETATM	781	H	0	-0.877	4.792	-0.285
H						
HETATM	782	Zn	0	-11.665	-8.530	-0.612
Zn						
HETATM	783	S	0	-16.122	-9.232	-1.474
S						
HETATM	784	S	0	-10.598	-11.169	-4.540
S						
HETATM	785	N	0	-12.682	-7.285	-2.112
N						
HETATM	786	N	0	-13.717	-9.323	-0.675
N						
HETATM	787	N	0	-14.343	-10.341	-0.005
N						
HETATM	788	N	0	-11.133	-9.834	-2.156
N						
HETATM	789	C	0	-12.143	-6.311	-2.830
C						
HETATM	790	H	0	-11.214	-6.134	-2.731
H						
HETATM	791	C	0	-10.924	-10.389	-3.151
C						
HETATM	792	C	0	-12.870	-5.541	-3.719
C						
HETATM	793	H	0	-12.445	-4.851	-4.213
H						
HETATM	794	C	0	-14.205	-5.780	-3.879
C						

HETATM	795	H	0	-14.720	-5.253	-4.478
H						
HETATM	796	C	0	-14.795	-6.805	-3.156
C						
HETATM	797	H	0	-15.721	-6.998	-3.255
H						
HETATM	798	C	0	-14.003	-7.545	-2.284
C						
HETATM	799	C	0	-14.504	-8.651	-1.478
C						
HETATM	800	C	0	-15.622	-10.414	-0.313
C						
HETATM	801	C	0	-16.558	-11.381	0.280
C						
HETATM	802	C	0	-16.081	-12.433	1.083
C						
HETATM	803	H	0	-15.147	-12.530	1.228
H						
HETATM	804	C	0	-16.946	-13.308	1.649
C						
HETATM	805	H	0	-16.605	-14.031	2.163
H						
HETATM	806	C	0	-18.366	-13.164	1.490
C						
HETATM	807	C	0	-19.277	-14.031	2.091
C						
HETATM	808	H	0	-18.961	-14.742	2.636
H						
HETATM	809	C	0	-20.632	-13.867	1.903
C						
HETATM	810	H	0	-21.243	-14.475	2.302
H						
HETATM	811	C	0	-21.107	-12.816	1.133
C						
HETATM	812	H	0	-22.043	-12.700	1.023
H						
HETATM	813	C	0	-20.239	-11.938	0.527
C						
HETATM	814	H	0	-20.575	-11.223	0.001
H						
HETATM	815	C	0	-18.829	-12.107	0.691
C						
HETATM	816	C	0	-17.917	-11.232	0.086
C						
HETATM	817	H	0	-18.236	-10.528	-0.466
H						
HETATM	818	S	0	-7.207	-7.828	0.252
S						
HETATM	819	S	0	-12.731	-5.891	3.317
S						
HETATM	820	N	0	-10.647	-9.775	0.889
N						
HETATM	821	N	0	-9.612	-7.737	-0.547
N						
HETATM	822	N	0	-8.986	-6.719	-1.218
N						

HETATM	823	N	0	-12.196	-7.226	0.934
N						
HETATM	824	C	0	-11.186	-10.749	1.607
C						
HETATM	825	H	0	-12.115	-10.926	1.508
H						
HETATM	826	C	0	-12.405	-6.671	1.929
C						
HETATM	827	C	0	-10.460	-11.518	2.496
C						
HETATM	828	H	0	-10.884	-12.210	2.991
H						
HETATM	829	C	0	-9.125	-11.279	2.656
C						
HETATM	830	H	0	-8.609	-11.807	3.255
H						
HETATM	831	C	0	-8.534	-10.255	1.934
C						
HETATM	832	H	0	-7.608	-10.062	2.032
H						
HETATM	833	C	0	-9.326	-9.515	1.061
C						
HETATM	834	C	0	-8.825	-8.409	0.256
C						
HETATM	835	C	0	-7.707	-6.646	-0.910
C						
HETATM	836	C	0	-6.772	-5.679	-1.502
C						
HETATM	837	C	0	-7.248	-4.627	-2.305
C						
HETATM	838	H	0	-8.182	-4.530	-2.452
H						
HETATM	839	C	0	-6.384	-3.752	-2.872
C						
HETATM	840	H	0	-6.724	-3.029	-3.385
H						
HETATM	841	C	0	-4.965	-3.896	-2.712
C						
HETATM	842	C	0	-4.052	-3.029	-3.314
C						
HETATM	843	H	0	-4.368	-2.318	-3.859
H						
HETATM	844	C	0	-2.697	-3.194	-3.125
C						
HETATM	845	H	0	-2.087	-2.585	-3.524
H						
HETATM	846	C	0	-2.222	-4.244	-2.355
C						
HETATM	847	H	0	-1.286	-4.360	-2.245
H						
HETATM	848	C	0	-3.091	-5.122	-1.749
C						
HETATM	849	H	0	-2.754	-5.837	-1.223
H						
HETATM	850	C	0	-4.500	-4.953	-1.913
C						

HETATM	851	C	0	-5.413	-5.827	-1.308
C						
HETATM	852	H	0	-5.093	-6.532	-0.756
H						
HETATM	853	Zn	0	-10.683	16.912	0.190
Zn						
HETATM	854	S	0	-15.141	16.210	-0.672
S						
HETATM	855	S	0	-9.616	14.273	-3.738
S						
HETATM	856	N	0	-11.701	18.157	-1.310
N						
HETATM	857	N	0	-12.736	16.118	0.127
N						
HETATM	858	N	0	-13.362	15.101	0.798
N						
HETATM	859	N	0	-10.152	15.608	-1.354
N						
HETATM	860	C	0	-11.161	19.131	-2.028
C						
HETATM	861	H	0	-10.233	19.308	-1.929
H						
HETATM	862	C	0	-9.943	15.052	-2.349
C						
HETATM	863	C	0	-11.889	19.901	-2.917
C						
HETATM	864	H	0	-11.464	20.591	-3.411
H						
HETATM	865	C	0	-13.222	19.661	-3.078
C						
HETATM	866	H	0	-13.739	20.188	-3.676
H						
HETATM	867	C	0	-13.814	18.636	-2.354
C						
HETATM	868	H	0	-14.739	18.444	-2.453
H						
HETATM	869	C	0	-13.022	17.896	-1.482
C						
HETATM	870	C	0	-13.523	16.791	-0.676
C						
HETATM	871	C	0	-14.641	15.027	0.489
C						
HETATM	872	C	0	-15.576	14.061	1.082
C						
HETATM	873	C	0	-15.099	13.009	1.885
C						
HETATM	874	H	0	-14.165	12.912	2.030
H						
HETATM	875	C	0	-15.965	12.134	2.451
C						
HETATM	876	H	0	-15.624	11.410	2.965
H						
HETATM	877	C	0	-17.384	12.277	2.292
C						
HETATM	878	C	0	-18.296	11.410	2.893
C						

HETATM	879	H	0	-17.980	10.699	3.438
H						
HETATM	880	C	0	-19.651	11.575	2.705
C						
HETATM	881	H	0	-20.261	10.967	3.104
H						
HETATM	882	C	0	-20.125	12.626	1.935
C						
HETATM	883	H	0	-21.062	12.741	1.824
H						
HETATM	884	C	0	-19.257	13.503	1.329
C						
HETATM	885	H	0	-19.593	14.219	0.803
H						
HETATM	886	C	0	-17.847	13.335	1.493
C						
HETATM	887	C	0	-16.935	14.209	0.887
C						
HETATM	888	H	0	-17.255	14.913	0.336
H						
HETATM	889	S	0	-6.226	17.613	1.053
S						
HETATM	890	S	0	-11.750	19.551	4.119
S						
HETATM	891	N	0	-9.666	15.666	1.691
N						
HETATM	892	N	0	-8.631	17.704	0.255
N						
HETATM	893	N	0	-8.005	18.722	-0.416
N						
HETATM	894	N	0	-11.215	18.215	1.736
N						
HETATM	895	C	0	-10.205	14.692	2.409
C						
HETATM	896	H	0	-11.133	14.516	2.310
H						
HETATM	897	C	0	-11.423	18.771	2.731
C						
HETATM	898	C	0	-9.477	13.923	3.298
C						
HETATM	899	H	0	-9.903	13.232	3.793
H						
HETATM	900	C	0	-8.144	14.163	3.459
C						
HETATM	901	H	0	-7.628	13.634	4.057
H						
HETATM	902	C	0	-7.553	15.186	2.736
C						
HETATM	903	H	0	-6.627	15.379	2.834
H						
HETATM	904	C	0	-8.344	15.927	1.863
C						
HETATM	905	C	0	-7.844	17.032	1.058
C						
HETATM	906	C	0	-6.726	18.796	-0.108
C						

HETATM	907	C	0	-5.790	19.762	-0.700
C						
HETATM	908	C	0	-6.267	20.814	-1.504
C						
HETATM	909	H	0	-7.201	20.911	-1.650
H						
HETATM	910	C	0	-5.402	21.689	-2.070
C						
HETATM	911	H	0	-5.742	22.413	-2.583
H						
HETATM	912	C	0	-3.982	21.545	-1.910
C						
HETATM	913	C	0	-3.071	22.413	-2.511
C						
HETATM	914	H	0	-3.387	23.124	-3.057
H						
HETATM	915	C	0	-1.716	22.248	-2.323
C						
HETATM	916	H	0	-1.105	22.857	-2.722
H						
HETATM	917	C	0	-1.241	21.196	-1.553
C						
HETATM	918	H	0	-0.305	21.081	-1.443
H						
HETATM	919	C	0	-2.109	20.320	-0.947
C						
HETATM	920	H	0	-1.773	19.604	-0.421
H						
HETATM	921	C	0	-3.519	20.488	-1.112
C						
HETATM	922	C	0	-4.431	19.614	-0.506
C						
HETATM	923	H	0	-4.112	18.910	0.046
H						
HETATM	924	Zn	0	-14.899	5.588	-0.280
Zn						
HETATM	925	S	0	-19.357	4.886	-1.143
S						
HETATM	926	S	0	-13.831	2.949	-4.208
S						
HETATM	927	N	0	-15.916	6.833	-1.781
N						
HETATM	928	N	0	-16.951	4.794	-0.344
N						
HETATM	929	N	0	-17.577	3.777	0.326
N						
HETATM	930	N	0	-14.368	4.284	-1.825
N						
HETATM	931	C	0	-15.376	7.807	-2.499
C						
HETATM	932	H	0	-14.449	7.984	-2.399
H						
HETATM	933	C	0	-14.158	3.728	-2.821
C						
HETATM	934	C	0	-16.104	8.577	-3.388
C						

HETATM	935	H	0	-15.679	9.267	-3.883
H						
HETATM	936	C	0	-17.438	8.337	-3.548
C						
HETATM	937	H	0	-17.954	8.865	-4.147
H						
HETATM	938	C	0	-18.029	7.312	-2.826
C						
HETATM	939	H	0	-18.954	7.120	-2.924
H						
HETATM	940	C	0	-17.238	6.572	-1.953
C						
HETATM	941	C	0	-17.738	5.467	-1.148
C						
HETATM	942	C	0	-18.856	3.704	0.018
C						
HETATM	943	C	0	-19.792	2.737	0.610
C						
HETATM	944	C	0	-19.314	1.684	1.415
C						
HETATM	945	H	0	-18.381	1.588	1.560
H						
HETATM	946	C	0	-20.179	0.810	1.980
C						
HETATM	947	H	0	-19.840	0.087	2.493
H						
HETATM	948	C	0	-21.599	0.953	1.820
C						
HETATM	949	C	0	-22.511	0.087	2.422
C						
HETATM	950	H	0	-22.194	-0.624	2.968
H						
HETATM	951	C	0	-23.865	0.251	2.233
C						
HETATM	952	H	0	-24.477	-0.357	2.633
H						
HETATM	953	C	0	-24.341	1.302	1.464
C						
HETATM	954	H	0	-25.276	1.417	1.353
H						
HETATM	955	C	0	-23.473	2.180	0.857
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Table 4. PDB file of the optimised structure of the 15-nuclear model of the HS centre in LS matrix

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TITLE          CSD ENTRY jmk-126-09
REMARK        1 File created by GaussView 6.0.16
HETATM        1 Zn          0      -19.118   5.721  -0.752
Zn
HETATM        2 S           0      -14.660   5.023   0.111
S
HETATM        3 S           0      -20.184   3.082   3.177
S
HETATM        4 N           0      -18.102   6.968   0.749
N
HETATM        5 N           0      -17.065   4.930  -0.687
N
HETATM        6 N           0      -16.438   3.912  -1.358
N
HETATM        7 N           0      -19.648   4.417   0.794
N
HETATM        8 C           0      -18.642   7.940   1.467
C
HETATM        9 H           0      -19.570   8.117   1.367
H
HETATM       10 C           0      -19.858   3.861   1.789
C
HETATM       11 C           0      -17.915   8.711   2.355
C
HETATM       12 H           0      -18.341   9.402   2.850
H
HETATM       13 C           0      -16.581   8.473   2.516
C
HETATM       14 H           0      -16.065   9.001   3.115
H
HETATM       15 C           0      -15.989   7.449   1.793
C
HETATM       16 H           0      -15.064   7.256   1.891
H
HETATM       17 C           0      -16.780   6.708   0.920
C
HETATM       18 C           0      -16.279   5.602   0.116
C
HETATM       19 C           0      -15.159   3.840  -1.050
C
HETATM       20 C           0      -14.223   2.874  -1.642
C
HETATM       21 C           0      -14.700   1.821  -2.445
C
HETATM       22 H           0      -15.633   1.724  -2.591
H
HETATM       23 C           0      -13.834   0.947  -3.012
C

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HETATM	24	H	0	-14.173	0.224	-3.525
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HETATM	25	C	0	-12.415	1.092	-2.852
C						
HETATM	26	C	0	-11.502	0.226	-3.453
C						
HETATM	27	H	0	-11.818	-0.486	-3.999
H						
HETATM	28	C	0	-10.148	0.392	-3.265
C						
HETATM	29	H	0	-9.535	-0.217	-3.664
H						
HETATM	30	C	0	-9.673	1.443	-2.495
C						
HETATM	31	H	0	-8.737	1.558	-2.385
H						
HETATM	32	C	0	-10.541	2.319	-1.889
C						
HETATM	33	H	0	-10.206	3.035	-1.363
H						
HETATM	34	C	0	-11.951	2.149	-2.054
C						
HETATM	35	C	0	-12.865	3.023	-1.448
C						
HETATM	36	H	0	-12.545	3.728	-0.896
H						
HETATM	37	S	0	-23.576	6.419	-1.614
S						
HETATM	38	S	0	-18.053	8.360	-4.680
S						
HETATM	39	N	0	-20.135	4.475	-2.252
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HETATM	40	N	0	-21.172	6.512	-0.815
N						
HETATM	41	N	0	-21.799	7.529	-0.145
N						
HETATM	42	N	0	-18.588	7.026	-2.296
N						
HETATM	43	C	0	-19.595	3.502	-2.970
C						
HETATM	44	H	0	-18.667	3.325	-2.871
H						
HETATM	45	C	0	-18.379	7.581	-3.292
C						
HETATM	46	C	0	-20.322	2.731	-3.859
C						
HETATM	47	H	0	-19.896	2.041	-4.353
H						
HETATM	48	C	0	-21.656	2.969	-4.019
C						
HETATM	49	H	0	-22.171	2.442	-4.617
H						
HETATM	50	C	0	-22.248	3.993	-3.296
C						
HETATM	51	H	0	-23.173	4.185	-3.395
H						

HETATM	52	C	0	-21.457	4.733	-2.424
C						
HETATM	53	C	0	-21.959	5.839	-1.618
C						
HETATM	54	C	0	-23.077	7.602	-0.453
C						
HETATM	55	C	0	-24.014	8.568	0.140
C						
HETATM	56	C	0	-23.537	9.621	0.943
C						
HETATM	57	H	0	-22.603	9.718	1.088
H						
HETATM	58	C	0	-24.403	10.495	1.509
C						
HETATM	59	H	0	-24.063	11.218	2.022
H						
HETATM	60	C	0	-25.823	10.350	1.350
C						
HETATM	61	C	0	-26.735	11.216	1.951
C						
HETATM	62	H	0	-26.419	11.928	2.496
H						
HETATM	63	C	0	-28.090	11.051	1.763
C						
HETATM	64	H	0	-28.701	11.659	2.162
H						
HETATM	65	C	0	-28.564	10.000	0.993
C						
HETATM	66	H	0	-29.500	9.884	0.883
H						
HETATM	67	C	0	-27.695	9.123	0.387
C						
HETATM	68	H	0	-28.031	8.406	-0.139
H						
HETATM	69	C	0	-26.285	9.293	0.551
C						
HETATM	70	C	0	-25.372	8.419	-0.054
C						
HETATM	71	H	0	-25.692	7.714	-0.606
H						
HETATM	72	Zn	0	-14.894	-5.600	-0.279
Zn						
HETATM	73	S	0	-10.436	-6.298	0.583
S						
HETATM	74	S	0	-15.959	-8.239	3.649
S						
HETATM	75	N	0	-13.878	-4.353	1.221
N						
HETATM	76	N	0	-12.841	-6.390	-0.216
N						
HETATM	77	N	0	-12.214	-7.408	-0.886
N						
HETATM	78	N	0	-15.425	-6.904	1.265
N						
HETATM	79	C	0	-14.418	-3.380	1.939
C						

HETATM	80	H	0	-15.346	-3.204	1.840
H						
HETATM	81	C	0	-15.633	-7.459	2.262
C						
HETATM	82	C	0	-13.691	-2.610	2.828
C						
HETATM	83	H	0	-14.117	-1.919	3.322
H						
HETATM	84	C	0	-12.356	-2.848	2.989
C						
HETATM	85	H	0	-11.841	-2.320	3.586
H						
HETATM	86	C	0	-11.765	-3.871	2.265
C						
HETATM	87	H	0	-10.839	-4.064	2.364
H						
HETATM	88	C	0	-12.555	-4.612	1.393
C						
HETATM	89	C	0	-12.054	-5.718	0.587
C						
HETATM	90	C	0	-10.935	-7.481	-0.578
C						
HETATM	91	C	0	-10.000	-8.446	-1.171
C						
HETATM	92	C	0	-10.475	-9.500	-1.974
C						
HETATM	93	H	0	-11.409	-9.597	-2.119
H						
HETATM	94	C	0	-9.609	-10.373	-2.539
C						
HETATM	95	H	0	-9.949	-11.097	-3.053
H						
HETATM	96	C	0	-8.190	-10.228	-2.381
C						
HETATM	97	C	0	-7.277	-11.095	-2.982
C						
HETATM	98	H	0	-7.594	-11.806	-3.527
H						
HETATM	99	C	0	-5.923	-10.929	-2.793
C						
HETATM	100	H	0	-5.312	-11.537	-3.193
H						
HETATM	101	C	0	-5.449	-9.877	-2.024
C						
HETATM	102	H	0	-4.513	-9.762	-1.913
H						
HETATM	103	C	0	-6.318	-9.002	-1.418
C						
HETATM	104	H	0	-5.982	-8.285	-0.892
H						
HETATM	105	C	0	-7.728	-9.171	-1.582
C						
HETATM	106	C	0	-8.640	-8.297	-0.976
C						
HETATM	107	H	0	-8.320	-7.592	-0.425
H						

HETATM	108	S	0	-19.353	-4.901	-1.142
S						
HETATM	109	S	0	-13.829	-2.960	-4.208
S						
HETATM	110	N	0	-15.911	-6.845	-1.780
N						
HETATM	111	N	0	-16.948	-4.808	-0.343
N						
HETATM	112	N	0	-17.574	-3.791	0.327
N						
HETATM	113	N	0	-14.364	-4.295	-1.825
N						
HETATM	114	C	0	-15.370	-7.819	-2.498
C						
HETATM	115	H	0	-14.442	-7.995	-2.398
H						
HETATM	116	C	0	-14.155	-3.740	-2.820
C						
HETATM	117	C	0	-16.097	-8.589	-3.386
C						
HETATM	118	H	0	-15.672	-9.280	-3.881
H						
HETATM	119	C	0	-17.432	-8.351	-3.547
C						
HETATM	120	H	0	-17.947	-8.879	-4.146
H						
HETATM	121	C	0	-18.024	-7.327	-2.824
C						
HETATM	122	H	0	-18.949	-7.135	-2.922
H						
HETATM	123	C	0	-17.233	-6.586	-1.952
C						
HETATM	124	C	0	-17.734	-5.481	-1.147
C						
HETATM	125	C	0	-18.853	-3.718	0.019
C						
HETATM	126	C	0	-19.790	-2.753	0.611
C						
HETATM	127	C	0	-19.313	-1.699	1.415
C						
HETATM	128	H	0	-18.380	-1.602	1.560
H						
HETATM	129	C	0	-20.179	-0.826	1.981
C						
HETATM	130	H	0	-19.839	-0.102	2.494
H						
HETATM	131	C	0	-21.598	-0.970	1.821
C						
HETATM	132	C	0	-22.511	-0.104	2.422
C						
HETATM	133	H	0	-22.194	0.607	2.968
H						
HETATM	134	C	0	-23.865	-0.269	2.234
C						
HETATM	135	H	0	-24.477	0.338	2.633
H						

HETATM	136	C	0	-24.340	-1.321	1.464
C						
HETATM	137	H	0	-25.275	-1.437	1.354
H						
HETATM	138	C	0	-23.471	-2.198	0.858
C						
HETATM	139	H	0	-23.806	-2.914	0.332
H						
HETATM	140	C	0	-22.061	-2.028	1.023
C						
HETATM	141	C	0	-21.148	-2.902	0.417
C						
HETATM	142	H	0	-21.468	-3.606	-0.135
H						
HETATM	143	Zn	0	-10.670	-16.920	0.192
Zn						
HETATM	144	S	0	-6.212	-17.618	1.055
S						
HETATM	145	S	0	-11.734	-19.559	4.121
S						
HETATM	146	N	0	-9.654	-15.674	1.693
N						
HETATM	147	N	0	-8.617	-17.711	0.257
N						
HETATM	148	N	0	-7.990	-18.729	-0.414
N						
HETATM	149	N	0	-11.200	-18.224	1.738
N						
HETATM	150	C	0	-10.194	-14.700	2.411
C						
HETATM	151	H	0	-11.122	-14.525	2.311
H						
HETATM	152	C	0	-11.408	-18.780	2.733
C						
HETATM	153	C	0	-9.466	-13.930	3.299
C						
HETATM	154	H	0	-9.892	-13.239	3.794
H						
HETATM	155	C	0	-8.133	-14.169	3.460
C						
HETATM	156	H	0	-7.617	-13.640	4.059
H						
HETATM	157	C	0	-7.541	-15.192	2.737
C						
HETATM	158	H	0	-6.615	-15.384	2.835
H						
HETATM	159	C	0	-8.332	-15.933	1.865
C						
HETATM	160	C	0	-7.831	-17.038	1.060
C						
HETATM	161	C	0	-6.711	-18.801	-0.106
C						
HETATM	162	C	0	-5.775	-19.766	-0.698
C						
HETATM	163	C	0	-6.251	-20.819	-1.502
C						

HETATM	164	H	0	-7.185	-20.916	-1.648
H						
HETATM	165	C	0	-5.385	-21.693	-2.068
C						
HETATM	166	H	0	-5.725	-22.417	-2.581
H						
HETATM	167	C	0	-3.966	-21.549	-1.908
C						
HETATM	168	C	0	-3.054	-22.416	-2.509
C						
HETATM	169	H	0	-3.369	-23.127	-3.055
H						
HETATM	170	C	0	-1.699	-22.249	-2.321
C						
HETATM	171	H	0	-1.087	-22.858	-2.720
H						
HETATM	172	C	0	-1.225	-21.198	-1.552
C						
HETATM	173	H	0	-0.288	-21.082	-1.441
H						
HETATM	174	C	0	-2.093	-20.322	-0.945
C						
HETATM	175	H	0	-1.758	-19.606	-0.419
H						
HETATM	176	C	0	-3.503	-20.491	-1.110
C						
HETATM	177	C	0	-4.416	-19.618	-0.504
C						
HETATM	178	H	0	-4.097	-18.913	0.048
H						
HETATM	179	S	0	-15.128	-16.222	-0.670
S						
HETATM	180	S	0	-9.605	-14.281	-3.736
S						
HETATM	181	N	0	-11.686	-18.166	-1.308
N						
HETATM	182	N	0	-12.723	-16.128	0.129
N						
HETATM	183	N	0	-13.350	-15.111	0.799
N						
HETATM	184	N	0	-10.140	-15.616	-1.352
N						
HETATM	185	C	0	-11.147	-19.140	-2.026
C						
HETATM	186	H	0	-10.218	-19.316	-1.927
H						
HETATM	187	C	0	-9.931	-15.060	-2.347
C						
HETATM	188	C	0	-11.873	-19.910	-2.915
C						
HETATM	189	H	0	-11.448	-20.600	-3.409
H						
HETATM	190	C	0	-13.207	-19.672	-3.075
C						
HETATM	191	H	0	-13.723	-20.200	-3.673
H						

HETATM	192	C	0	-13.799	-18.647	-2.352
C						
HETATM	193	H	0	-14.725	-18.456	-2.451
H						
HETATM	194	C	0	-13.008	-17.906	-1.480
C						
HETATM	195	C	0	-13.509	-16.802	-0.674
C						
HETATM	196	C	0	-14.629	-15.039	0.491
C						
HETATM	197	C	0	-15.565	-14.073	1.084
C						
HETATM	198	C	0	-15.089	-13.020	1.887
C						
HETATM	199	H	0	-14.155	-12.923	2.032
H						
HETATM	200	C	0	-15.955	-12.146	2.453
C						
HETATM	201	H	0	-15.615	-11.422	2.966
H						
HETATM	202	C	0	-17.374	-12.291	2.294
C						
HETATM	203	C	0	-18.286	-11.424	2.895
C						
HETATM	204	H	0	-17.971	-10.713	3.440
H						
HETATM	205	C	0	-19.641	-11.590	2.707
C						
HETATM	206	H	0	-20.252	-10.982	3.106
H						
HETATM	207	C	0	-20.115	-12.642	1.937
C						
HETATM	208	H	0	-21.052	-12.758	1.826
H						
HETATM	209	C	0	-19.247	-13.518	1.331
C						
HETATM	210	H	0	-19.582	-14.234	0.805
H						
HETATM	211	C	0	-17.837	-13.348	1.495
C						
HETATM	212	C	0	-16.924	-14.223	0.889
C						
HETATM	213	H	0	-17.243	-14.926	0.338
H						
HETATM	214	Zn	0	-11.671	8.521	-0.612
Zn						
HETATM	215	S	0	-7.213	7.822	0.251
S						
HETATM	216	S	0	-12.736	5.882	3.316
S						
HETATM	217	N	0	-10.655	9.767	0.888
N						
HETATM	218	N	0	-9.618	7.730	-0.548
N						
HETATM	219	N	0	-8.991	6.712	-1.218
N						

HETATM	220	N	0	-12.201	7.216	0.933
N						
HETATM	221	C	0	-11.195	10.740	1.607
C						
HETATM	222	H	0	-12.123	10.916	1.507
H						
HETATM	223	C	0	-12.410	6.661	1.929
C						
HETATM	224	C	0	-10.469	11.510	2.495
C						
HETATM	225	H	0	-10.894	12.202	2.990
H						
HETATM	226	C	0	-9.134	11.272	2.656
C						
HETATM	227	H	0	-8.618	11.800	3.255
H						
HETATM	228	C	0	-8.542	10.249	1.933
C						
HETATM	229	H	0	-7.616	10.056	2.031
H						
HETATM	230	C	0	-9.333	9.508	1.060
C						
HETATM	231	C	0	-8.832	8.402	0.256
C						
HETATM	232	C	0	-7.712	6.639	-0.910
C						
HETATM	233	C	0	-6.776	5.674	-1.502
C						
HETATM	234	C	0	-7.252	4.621	-2.306
C						
HETATM	235	H	0	-8.186	4.523	-2.452
H						
HETATM	236	C	0	-6.387	3.747	-2.872
C						
HETATM	237	H	0	-6.726	3.023	-3.385
H						
HETATM	238	C	0	-4.968	3.892	-2.712
C						
HETATM	239	C	0	-4.055	3.025	-3.314
C						
HETATM	240	H	0	-4.370	2.314	-3.860
H						
HETATM	241	C	0	-2.700	3.192	-3.126
C						
HETATM	242	H	0	-2.089	2.583	-3.525
H						
HETATM	243	C	0	-2.226	4.242	-2.356
C						
HETATM	244	H	0	-1.289	4.358	-2.246
H						
HETATM	245	C	0	-3.094	5.119	-1.750
C						
HETATM	246	H	0	-2.759	5.835	-1.223
H						
HETATM	247	C	0	-4.504	4.949	-1.914
C						

HETATM	248	C	0	-5.418	5.823	-1.309
C						
HETATM	249	H	0	-5.098	6.528	-0.757
H						
HETATM	250	S	0	-16.130	9.219	-1.474
S						
HETATM	251	S	0	-10.607	11.160	-4.540
S						
HETATM	252	N	0	-12.688	7.275	-2.113
N						
HETATM	253	N	0	-13.724	9.312	-0.675
N						
HETATM	254	N	0	-14.351	10.329	-0.005
N						
HETATM	255	N	0	-11.141	9.825	-2.156
N						
HETATM	256	C	0	-12.148	6.301	-2.830
C						
HETATM	257	H	0	-11.219	6.125	-2.731
H						
HETATM	258	C	0	-10.933	10.380	-3.152
C						
HETATM	259	C	0	-12.875	5.531	-3.719
C						
HETATM	260	H	0	-12.449	4.841	-4.213
H						
HETATM	261	C	0	-14.209	5.769	-3.879
C						
HETATM	262	H	0	-14.724	5.241	-4.478
H						
HETATM	263	C	0	-14.800	6.793	-3.156
C						
HETATM	264	H	0	-15.726	6.985	-3.255
H						
HETATM	265	C	0	-14.009	7.533	-2.284
C						
HETATM	266	C	0	-14.511	8.639	-1.479
C						
HETATM	267	C	0	-15.630	10.402	-0.313
C						
HETATM	268	C	0	-16.566	11.368	0.279
C						
HETATM	269	C	0	-16.090	12.421	1.083
C						
HETATM	270	H	0	-15.156	12.518	1.228
H						
HETATM	271	C	0	-16.956	13.295	1.649
C						
HETATM	272	H	0	-16.616	14.018	2.162
H						
HETATM	273	C	0	-18.376	13.150	1.489
C						
HETATM	274	C	0	-19.288	14.016	2.091
C						
HETATM	275	H	0	-18.972	14.727	2.635
H						

HETATM	276	C	0	-20.643	13.851	1.902
C						
HETATM	277	H	0	-21.254	14.458	2.301
H						
HETATM	278	C	0	-21.117	12.799	1.133
C						
HETATM	279	H	0	-22.053	12.683	1.022
H						
HETATM	280	C	0	-20.248	11.923	0.527
C						
HETATM	281	H	0	-20.583	11.206	0.000
H						
HETATM	282	C	0	-18.838	12.092	0.691
C						
HETATM	283	C	0	-17.926	11.218	0.085
C						
HETATM	284	H	0	-18.244	10.514	-0.467
H						
HETATM	285	Zn	0	-7.447	-2.800	-0.140
Zn						
HETATM	286	S	0	-2.988	-3.498	0.723
S						
HETATM	287	S	0	-8.512	-5.439	3.789
S						
HETATM	288	N	0	-6.431	-1.553	1.361
N						
HETATM	289	N	0	-5.394	-3.591	-0.076
N						
HETATM	290	N	0	-4.767	-4.608	-0.746
N						
HETATM	291	N	0	-7.978	-4.105	1.405
N						
HETATM	292	C	0	-6.971	-0.581	2.078
C						
HETATM	293	H	0	-7.899	-0.404	1.979
H						
HETATM	294	C	0	-8.186	-4.660	2.401
C						
HETATM	295	C	0	-6.244	0.190	2.968
C						
HETATM	296	H	0	-6.670	0.881	3.461
H						
HETATM	297	C	0	-4.909	-0.048	3.128
C						
HETATM	298	H	0	-4.394	0.480	3.726
H						
HETATM	299	C	0	-4.318	-1.072	2.404
C						
HETATM	300	H	0	-3.392	-1.264	2.504
H						
HETATM	301	C	0	-5.108	-1.812	1.533
C						
HETATM	302	C	0	-4.607	-2.918	0.727
C						
HETATM	303	C	0	-3.489	-4.681	-0.438
C						

HETATM	304	C	0	-2.552	-5.646	-1.031
C						
HETATM	305	C	0	-3.028	-6.700	-1.834
C						
HETATM	306	H	0	-3.961	-6.797	-1.979
H						
HETATM	307	C	0	-2.162	-7.574	-2.399
C						
HETATM	308	H	0	-2.502	-8.297	-2.914
H						
HETATM	309	C	0	-0.743	-7.428	-2.241
C						
HETATM	310	C	0	0.170	-8.295	-2.842
C						
HETATM	311	H	0	-0.147	-9.007	-3.387
H						
HETATM	312	C	0	1.524	-8.129	-2.653
C						
HETATM	313	H	0	2.135	-8.738	-3.053
H						
HETATM	314	C	0	1.998	-7.078	-1.884
C						
HETATM	315	H	0	2.934	-6.962	-1.773
H						
HETATM	316	C	0	1.130	-6.202	-1.278
C						
HETATM	317	H	0	1.466	-5.485	-0.752
H						
HETATM	318	C	0	-0.281	-6.371	-1.442
C						
HETATM	319	C	0	-1.193	-5.498	-0.836
C						
HETATM	320	H	0	-0.873	-4.793	-0.285
H						
HETATM	321	S	0	-11.905	-2.101	-1.003
S						
HETATM	322	S	0	-6.382	-0.161	-4.068
S						
HETATM	323	N	0	-8.463	-4.045	-1.640
N						
HETATM	324	N	0	-9.501	-2.008	-0.203
N						
HETATM	325	N	0	-10.127	-0.991	0.466
N						
HETATM	326	N	0	-6.916	-1.495	-1.685
N						
HETATM	327	C	0	-7.923	-5.019	-2.358
C						
HETATM	328	H	0	-6.995	-5.196	-2.258
H						
HETATM	329	C	0	-6.708	-0.940	-2.680
C						
HETATM	330	C	0	-8.650	-5.790	-3.247
C						
HETATM	331	H	0	-8.224	-6.480	-3.742
H						

HETATM	332	C	0	-9.985	-5.552	-3.407
C						
HETATM	333	H	0	-10.500	-6.079	-4.006
H						
HETATM	334	C	0	-10.577	-4.527	-2.685
C						
HETATM	335	H	0	-11.502	-4.335	-2.783
H						
HETATM	336	C	0	-9.786	-3.786	-1.812
C						
HETATM	337	C	0	-10.287	-2.681	-1.007
C						
HETATM	338	C	0	-11.406	-0.918	0.158
C						
HETATM	339	C	0	-12.343	0.047	0.751
C						
HETATM	340	C	0	-11.866	1.100	1.555
C						
HETATM	341	H	0	-10.933	1.197	1.700
H						
HETATM	342	C	0	-12.732	1.974	2.120
C						
HETATM	343	H	0	-12.392	2.697	2.634
H						
HETATM	344	C	0	-14.151	1.830	1.961
C						
HETATM	345	C	0	-15.064	2.695	2.562
C						
HETATM	346	H	0	-14.747	3.407	3.108
H						
HETATM	347	C	0	-16.418	2.530	2.374
C						
HETATM	348	H	0	-17.029	3.138	2.773
H						
HETATM	349	C	0	-16.892	1.479	1.604
C						
HETATM	350	H	0	-17.828	1.363	1.494
H						
HETATM	351	C	0	-16.024	0.602	0.998
C						
HETATM	352	H	0	-16.360	-0.114	0.472
H						
HETATM	353	C	0	-14.614	0.772	1.162
C						
HETATM	354	C	0	-13.701	-0.102	0.557
C						
HETATM	355	H	0	-14.021	-0.806	0.005
H						
HETATM	356	Zn	0	-3.223	-14.121	0.332
Zn						
HETATM	357	S	0	1.235	-14.818	1.195
S						
HETATM	358	S	0	-4.288	-16.760	4.260
S						
HETATM	359	N	0	-2.207	-12.874	1.832
N						

HETATM	360	N	0	-1.170	-14.912	0.396
N						
HETATM	361	N	0	-0.543	-15.929	-0.274
N						
HETATM	362	N	0	-3.753	-15.424	1.877
N						
HETATM	363	C	0	-2.747	-11.900	2.551
C						
HETATM	364	H	0	-3.675	-11.725	2.451
H						
HETATM	365	C	0	-3.962	-15.980	2.873
C						
HETATM	366	C	0	-2.019	-11.130	3.439
C						
HETATM	367	H	0	-2.445	-10.440	3.934
H						
HETATM	368	C	0	-0.685	-11.369	3.600
C						
HETATM	369	H	0	-0.170	-10.840	4.198
H						
HETATM	370	C	0	-0.093	-12.392	2.877
C						
HETATM	371	H	0	0.832	-12.584	2.975
H						
HETATM	372	C	0	-0.885	-13.133	2.004
C						
HETATM	373	C	0	-0.383	-14.238	1.200
C						
HETATM	374	C	0	0.736	-16.002	0.034
C						
HETATM	375	C	0	1.672	-16.967	-0.559
C						
HETATM	376	C	0	1.196	-18.019	-1.363
C						
HETATM	377	H	0	0.262	-18.117	-1.508
H						
HETATM	378	C	0	2.062	-18.893	-1.928
C						
HETATM	379	H	0	1.722	-19.618	-2.441
H						
HETATM	380	C	0	3.481	-18.749	-1.768
C						
HETATM	381	C	0	4.394	-19.616	-2.370
C						
HETATM	382	H	0	4.078	-20.327	-2.915
H						
HETATM	383	C	0	5.748	-19.450	-2.182
C						
HETATM	384	H	0	6.360	-20.058	-2.581
H						
HETATM	385	C	0	6.222	-18.398	-1.412
C						
HETATM	386	H	0	7.159	-18.282	-1.302
H						
HETATM	387	C	0	5.354	-17.522	-0.806
C						

HETATM	388	H	0	5.689	-16.806	-0.279
H						
HETATM	389	C	0	3.944	-17.691	-0.970
C						
HETATM	390	C	0	3.031	-16.818	-0.364
C						
HETATM	391	H	0	3.350	-16.113	0.188
H						
HETATM	392	S	0	-7.681	-13.422	-0.530
S						
HETATM	393	S	0	-2.158	-11.481	-3.596
S						
HETATM	394	N	0	-4.239	-15.366	-1.169
N						
HETATM	395	N	0	-5.276	-13.328	0.269
N						
HETATM	396	N	0	-5.903	-12.312	0.939
N						
HETATM	397	N	0	-2.693	-12.816	-1.212
N						
HETATM	398	C	0	-3.699	-16.340	-1.886
C						
HETATM	399	H	0	-2.771	-16.516	-1.787
H						
HETATM	400	C	0	-2.483	-12.260	-2.208
C						
HETATM	401	C	0	-4.425	-17.110	-2.775
C						
HETATM	402	H	0	-4.001	-17.800	-3.269
H						
HETATM	403	C	0	-5.760	-16.872	-2.936
C						
HETATM	404	H	0	-6.276	-17.400	-3.534
H						
HETATM	405	C	0	-6.352	-15.848	-2.212
C						
HETATM	406	H	0	-7.278	-15.656	-2.311
H						
HETATM	407	C	0	-5.561	-15.107	-1.340
C						
HETATM	408	C	0	-6.062	-14.002	-0.535
C						
HETATM	409	C	0	-7.182	-12.239	0.631
C						
HETATM	410	C	0	-8.118	-11.273	1.223
C						
HETATM	411	C	0	-7.642	-10.221	2.027
C						
HETATM	412	H	0	-6.708	-10.123	2.172
H						
HETATM	413	C	0	-8.507	-9.346	2.593
C						
HETATM	414	H	0	-8.168	-8.622	3.106
H						
HETATM	415	C	0	-9.927	-9.491	2.433
C						

HETATM	416	C	0	-10.840	-8.624	3.035
C						
HETATM	417	H	0	-10.524	-7.913	3.579
H						
HETATM	418	C	0	-12.195	-8.790	2.846
C						
HETATM	419	H	0	-12.806	-8.183	3.246
H						
HETATM	420	C	0	-12.668	-9.842	2.077
C						
HETATM	421	H	0	-13.605	-9.958	1.966
H						
HETATM	422	C	0	-11.800	-10.719	1.471
C						
HETATM	423	H	0	-12.135	-11.435	0.944
H						
HETATM	424	C	0	-10.390	-10.549	1.635
C						
HETATM	425	C	0	-9.476	-11.423	1.029
C						
HETATM	426	H	0	-9.796	-12.127	0.477
H						
HETATM	427	Zn	0	-4.224	11.320	-0.472
Zn						
HETATM	428	S	0	0.234	10.622	0.391
S						
HETATM	429	S	0	-5.289	8.681	3.456
S						
HETATM	430	N	0	-3.208	12.567	1.028
N						
HETATM	431	N	0	-2.172	10.529	-0.408
N						
HETATM	432	N	0	-1.544	9.512	-1.078
N						
HETATM	433	N	0	-4.754	10.016	1.073
N						
HETATM	434	C	0	-3.748	13.540	1.747
C						
HETATM	435	H	0	-4.676	13.716	1.647
H						
HETATM	436	C	0	-4.963	9.461	2.068
C						
HETATM	437	C	0	-3.021	14.310	2.635
C						
HETATM	438	H	0	-3.447	15.001	3.130
H						
HETATM	439	C	0	-1.686	14.072	2.795
C						
HETATM	440	H	0	-1.171	14.600	3.394
H						
HETATM	441	C	0	-1.095	13.048	2.073
C						
HETATM	442	H	0	-0.169	12.856	2.171
H						
HETATM	443	C	0	-1.886	12.308	1.200
C						

HETATM	444	C	0	-1.385	11.202	0.395
C						
HETATM	445	C	0	-0.265	9.439	-0.770
C						
HETATM	446	C	0	0.671	8.473	-1.363
C						
HETATM	447	C	0	0.195	7.421	-2.166
C						
HETATM	448	H	0	-0.739	7.323	-2.312
H						
HETATM	449	C	0	1.061	6.547	-2.732
C						
HETATM	450	H	0	0.721	5.823	-3.245
H						
HETATM	451	C	0	2.480	6.692	-2.573
C						
HETATM	452	C	0	3.392	5.825	-3.174
C						
HETATM	453	H	0	3.077	5.114	-3.720
H						
HETATM	454	C	0	4.747	5.991	-2.986
C						
HETATM	455	H	0	5.358	5.383	-3.385
H						
HETATM	456	C	0	5.221	7.042	-2.216
C						
HETATM	457	H	0	6.157	7.158	-2.106
H						
HETATM	458	C	0	4.352	7.919	-1.610
C						
HETATM	459	H	0	4.688	8.635	-1.084
H						
HETATM	460	C	0	2.943	7.749	-1.774
C						
HETATM	461	C	0	2.030	8.623	-1.169
C						
HETATM	462	H	0	2.349	9.328	-0.617
H						
HETATM	463	S	0	-8.683	12.019	-1.334
S						
HETATM	464	S	0	-3.160	13.960	-4.401
S						
HETATM	465	N	0	-5.241	10.075	-1.973
N						
HETATM	466	N	0	-6.277	12.111	-0.536
N						
HETATM	467	N	0	-6.904	13.129	0.135
N						
HETATM	468	N	0	-3.694	12.625	-2.017
N						
HETATM	469	C	0	-4.701	9.101	-2.690
C						
HETATM	470	H	0	-3.772	8.925	-2.591
H						
HETATM	471	C	0	-3.486	13.180	-3.012
C						

HETATM	472	C	0	-5.427	8.331	-3.579
C						
HETATM	473	H	0	-5.002	7.640	-4.073
H						
HETATM	474	C	0	-6.761	8.569	-3.739
C						
HETATM	475	H	0	-7.277	8.041	-4.338
H						
HETATM	476	C	0	-7.353	9.592	-3.016
C						
HETATM	477	H	0	-8.280	9.785	-3.115
H						
HETATM	478	C	0	-6.562	10.333	-2.145
C						
HETATM	479	C	0	-7.064	11.439	-1.339
C						
HETATM	480	C	0	-8.183	13.202	-0.173
C						
HETATM	481	C	0	-9.120	14.168	0.419
C						
HETATM	482	C	0	-8.643	15.220	1.222
C						
HETATM	483	H	0	-7.709	15.318	1.367
H						
HETATM	484	C	0	-9.509	16.094	1.788
C						
HETATM	485	H	0	-9.169	16.818	2.302
H						
HETATM	486	C	0	-10.929	15.950	1.629
C						
HETATM	487	C	0	-11.841	16.816	2.230
C						
HETATM	488	H	0	-11.525	17.527	2.775
H						
HETATM	489	C	0	-13.196	16.650	2.042
C						
HETATM	490	H	0	-13.807	17.258	2.441
H						
HETATM	491	C	0	-13.670	15.599	1.272
C						
HETATM	492	H	0	-14.606	15.483	1.162
H						
HETATM	493	C	0	-12.801	14.722	0.666
C						
HETATM	494	H	0	-13.136	14.006	0.140
H						
HETATM	495	C	0	-11.391	14.892	0.830
C						
HETATM	496	C	0	-10.479	14.018	0.225
C						
HETATM	497	H	0	-10.797	13.313	-0.327
H						
HETATM	498	Fe	0	0.000	0.000	-0.000
Fe						
HETATM	499	S	0	4.518	-0.716	0.897
S						

HETATM	500	S	0	-1.027	-2.848	3.934
S						
HETATM	501	N	0	1.006	1.320	1.416
N						
HETATM	502	N	0	2.035	-0.843	0.087
N						
HETATM	503	N	0	2.671	-1.899	-0.581
N						
HETATM	504	N	0	-0.539	-1.213	1.600
N						
HETATM	505	C	0	0.426	2.355	2.067
C						
HETATM	506	H	0	-0.621	2.542	1.820
H						
HETATM	507	C	0	-0.725	-1.885	2.567
C						
HETATM	508	C	0	1.142	3.138	3.006
C						
HETATM	509	H	0	0.650	3.969	3.509
H						
HETATM	510	C	0	2.493	2.817	3.273
C						
HETATM	511	H	0	3.072	3.398	3.992
H						
HETATM	512	C	0	3.098	1.729	2.597
C						
HETATM	513	H	0	4.128	1.446	2.809
H						
HETATM	514	C	0	2.313	1.009	1.669
C						
HETATM	515	C	0	2.829	-0.142	0.890
C						
HETATM	516	C	0	3.964	-1.983	-0.282
C						
HETATM	517	C	0	4.916	-2.955	-0.856
C						
HETATM	518	C	0	4.428	-4.064	-1.642
C						
HETATM	519	H	0	3.354	-4.185	-1.777
H						
HETATM	520	C	0	5.330	-4.951	-2.226
C						
HETATM	521	H	0	4.976	-5.795	-2.821
H						
HETATM	522	C	0	6.755	-4.764	-2.074
C						
HETATM	523	C	0	7.712	-5.645	-2.695
C						
HETATM	524	H	0	7.342	-6.474	-3.300
H						
HETATM	525	C	0	9.083	-5.447	-2.509
C						
HETATM	526	H	0	9.810	-6.102	-2.991
H						
HETATM	527	C	0	9.563	-4.356	-1.698
C						

HETATM	528	H	0	10.639	-4.224	-1.578
H						
HETATM	529	C	0	8.660	-3.480	-1.093
C						
HETATM	530	H	0	9.010	-2.635	-0.497
H						
HETATM	531	C	0	7.240	-3.668	-1.265
C						
HETATM	532	C	0	6.292	-2.782	-0.660
C						
HETATM	533	H	0	6.674	-1.961	-0.051
H						
HETATM	534	S	0	-4.518	0.716	-0.897
S						
HETATM	535	S	0	1.027	2.848	-3.935
S						
HETATM	536	N	0	-1.006	-1.320	-1.416
N						
HETATM	537	N	0	-2.035	0.843	-0.088
N						
HETATM	538	N	0	-2.670	1.899	0.581
N						
HETATM	539	N	0	0.539	1.213	-1.600
N						
HETATM	540	C	0	-0.426	-2.355	-2.067
C						
HETATM	541	H	0	0.621	-2.542	-1.820
H						
HETATM	542	C	0	0.725	1.885	-2.567
C						
HETATM	543	C	0	-1.142	-3.138	-3.006
C						
HETATM	544	H	0	-0.650	-3.969	-3.509
H						
HETATM	545	C	0	-2.493	-2.817	-3.273
C						
HETATM	546	H	0	-3.071	-3.398	-3.992
H						
HETATM	547	C	0	-3.098	-1.729	-2.597
C						
HETATM	548	H	0	-4.128	-1.446	-2.810
H						
HETATM	549	C	0	-2.313	-1.009	-1.669
C						
HETATM	550	C	0	-2.829	0.142	-0.890
C						
HETATM	551	C	0	-3.964	1.983	0.282
C						
HETATM	552	C	0	-4.916	2.955	0.856
C						
HETATM	553	C	0	-4.428	4.064	1.642
C						
HETATM	554	H	0	-3.354	4.185	1.777
H						
HETATM	555	C	0	-5.330	4.951	2.225
C						

HETATM	556	H	0	-4.977	5.795	2.820
H						
HETATM	557	C	0	-6.755	4.764	2.074
C						
HETATM	558	C	0	-7.712	5.645	2.695
C						
HETATM	559	H	0	-7.342	6.474	3.299
H						
HETATM	560	C	0	-9.083	5.446	2.509
C						
HETATM	561	H	0	-9.810	6.102	2.991
H						
HETATM	562	C	0	-9.563	4.356	1.698
C						
HETATM	563	H	0	-10.639	4.224	1.578
H						
HETATM	564	C	0	-8.660	3.480	1.093
C						
HETATM	565	H	0	-9.010	2.634	0.498
H						
HETATM	566	C	0	-7.240	3.668	1.265
C						
HETATM	567	C	0	-6.292	2.781	0.660
C						
HETATM	568	H	0	-6.674	1.960	0.051
H						
HETATM	569	Zn	0	4.224	-11.320	0.472
Zn						
HETATM	570	S	0	8.683	-12.019	1.334
S						
HETATM	571	S	0	3.160	-13.959	4.401
S						
HETATM	572	N	0	5.241	-10.075	1.973
N						
HETATM	573	N	0	6.277	-12.111	0.536
N						
HETATM	574	N	0	6.904	-13.129	-0.135
N						
HETATM	575	N	0	3.694	-12.625	2.017
N						
HETATM	576	C	0	4.701	-9.101	2.690
C						
HETATM	577	H	0	3.772	-8.925	2.591
H						
HETATM	578	C	0	3.486	-13.180	3.012
C						
HETATM	579	C	0	5.427	-8.331	3.579
C						
HETATM	580	H	0	5.002	-7.640	4.073
H						
HETATM	581	C	0	6.761	-8.569	3.739
C						
HETATM	582	H	0	7.277	-8.041	4.338
H						
HETATM	583	C	0	7.353	-9.592	3.016
C						

HETATM	584	H	0	8.280	-9.785	3.115
H						
HETATM	585	C	0	6.562	-10.333	2.145
C						
HETATM	586	C	0	7.064	-11.439	1.339
C						
HETATM	587	C	0	8.183	-13.202	0.173
C						
HETATM	588	C	0	9.120	-14.168	-0.419
C						
HETATM	589	C	0	8.643	-15.220	-1.222
C						
HETATM	590	H	0	7.709	-15.318	-1.367
H						
HETATM	591	C	0	9.509	-16.094	-1.788
C						
HETATM	592	H	0	9.169	-16.818	-2.302
H						
HETATM	593	C	0	10.929	-15.950	-1.629
C						
HETATM	594	C	0	11.841	-16.816	-2.230
C						
HETATM	595	H	0	11.525	-17.527	-2.775
H						
HETATM	596	C	0	13.196	-16.650	-2.042
C						
HETATM	597	H	0	13.807	-17.258	-2.441
H						
HETATM	598	C	0	13.670	-15.599	-1.272
C						
HETATM	599	H	0	14.606	-15.483	-1.162
H						
HETATM	600	C	0	12.801	-14.722	-0.666
C						
HETATM	601	H	0	13.136	-14.006	-0.140
H						
HETATM	602	C	0	11.391	-14.892	-0.830
C						
HETATM	603	C	0	10.479	-14.018	-0.225
C						
HETATM	604	H	0	10.797	-13.313	0.327
H						
HETATM	605	S	0	-0.234	-10.622	-0.391
S						
HETATM	606	S	0	5.289	-8.681	-3.456
S						
HETATM	607	N	0	3.208	-12.567	-1.028
N						
HETATM	608	N	0	2.172	-10.529	0.408
N						
HETATM	609	N	0	1.544	-9.512	1.078
N						
HETATM	610	N	0	4.754	-10.016	-1.073
N						
HETATM	611	C	0	3.748	-13.540	-1.747
C						

HETATM	612	H	0	4.676	-13.716	-1.647
H						
HETATM	613	C	0	4.963	-9.461	-2.068
C						
HETATM	614	C	0	3.021	-14.310	-2.635
C						
HETATM	615	H	0	3.447	-15.001	-3.130
H						
HETATM	616	C	0	1.686	-14.072	-2.795
C						
HETATM	617	H	0	1.171	-14.600	-3.394
H						
HETATM	618	C	0	1.095	-13.048	-2.073
C						
HETATM	619	H	0	0.169	-12.856	-2.171
H						
HETATM	620	C	0	1.886	-12.308	-1.200
C						
HETATM	621	C	0	1.385	-11.202	-0.395
C						
HETATM	622	C	0	0.265	-9.439	0.770
C						
HETATM	623	C	0	-0.671	-8.473	1.363
C						
HETATM	624	C	0	-0.195	-7.421	2.166
C						
HETATM	625	H	0	0.739	-7.323	2.312
H						
HETATM	626	C	0	-1.061	-6.547	2.732
C						
HETATM	627	H	0	-0.721	-5.823	3.245
H						
HETATM	628	C	0	-2.480	-6.692	2.573
C						
HETATM	629	C	0	-3.392	-5.825	3.174
C						
HETATM	630	H	0	-3.077	-5.114	3.720
H						
HETATM	631	C	0	-4.747	-5.991	2.986
C						
HETATM	632	H	0	-5.358	-5.383	3.385
H						
HETATM	633	C	0	-5.221	-7.042	2.216
C						
HETATM	634	H	0	-6.157	-7.158	2.106
H						
HETATM	635	C	0	-4.352	-7.919	1.610
C						
HETATM	636	H	0	-4.688	-8.635	1.084
H						
HETATM	637	C	0	-2.943	-7.749	1.774
C						
HETATM	638	C	0	-2.030	-8.623	1.169
C						
HETATM	639	H	0	-2.349	-9.328	0.617
H						

HETATM	640	Zn	0	3.223	14.121	-0.332
Zn						
HETATM	641	S	0	7.681	13.422	0.530
S						
HETATM	642	S	0	2.158	11.481	3.596
S						
HETATM	643	N	0	4.239	15.366	1.169
N						
HETATM	644	N	0	5.276	13.329	-0.269
N						
HETATM	645	N	0	5.903	12.312	-0.939
N						
HETATM	646	N	0	2.693	12.816	1.212
N						
HETATM	647	C	0	3.699	16.340	1.886
C						
HETATM	648	H	0	2.771	16.516	1.787
H						
HETATM	649	C	0	2.483	12.260	2.208
C						
HETATM	650	C	0	4.425	17.110	2.775
C						
HETATM	651	H	0	4.001	17.800	3.269
H						
HETATM	652	C	0	5.760	16.872	2.936
C						
HETATM	653	H	0	6.276	17.400	3.534
H						
HETATM	654	C	0	6.352	15.848	2.212
C						
HETATM	655	H	0	7.278	15.656	2.311
H						
HETATM	656	C	0	5.561	15.107	1.340
C						
HETATM	657	C	0	6.062	14.002	0.535
C						
HETATM	658	C	0	7.182	12.239	-0.631
C						
HETATM	659	C	0	8.118	11.273	-1.223
C						
HETATM	660	C	0	7.642	10.221	-2.027
C						
HETATM	661	H	0	6.708	10.123	-2.172
H						
HETATM	662	C	0	8.507	9.346	-2.593
C						
HETATM	663	H	0	8.168	8.622	-3.106
H						
HETATM	664	C	0	9.927	9.491	-2.433
C						
HETATM	665	C	0	10.840	8.624	-3.035
C						
HETATM	666	H	0	10.524	7.913	-3.579
H						
HETATM	667	C	0	12.195	8.790	-2.846
C						

HETATM	668	H	0	12.806	8.183	-3.246
H						
HETATM	669	C	0	12.668	9.842	-2.077
C						
HETATM	670	H	0	13.605	9.958	-1.966
H						
HETATM	671	C	0	11.800	10.719	-1.471
C						
HETATM	672	H	0	12.135	11.435	-0.944
H						
HETATM	673	C	0	10.390	10.549	-1.635
C						
HETATM	674	C	0	9.476	11.423	-1.029
C						
HETATM	675	H	0	9.796	12.127	-0.477
H						
HETATM	676	S	0	-1.235	14.818	-1.195
S						
HETATM	677	S	0	4.288	16.760	-4.260
S						
HETATM	678	N	0	2.207	12.874	-1.832
N						
HETATM	679	N	0	1.170	14.912	-0.396
N						
HETATM	680	N	0	0.543	15.929	0.274
N						
HETATM	681	N	0	3.753	15.424	-1.877
N						
HETATM	682	C	0	2.747	11.900	-2.551
C						
HETATM	683	H	0	3.675	11.725	-2.451
H						
HETATM	684	C	0	3.962	15.980	-2.873
C						
HETATM	685	C	0	2.019	11.130	-3.439
C						
HETATM	686	H	0	2.445	10.440	-3.934
H						
HETATM	687	C	0	0.685	11.369	-3.600
C						
HETATM	688	H	0	0.170	10.840	-4.198
H						
HETATM	689	C	0	0.093	12.392	-2.877
C						
HETATM	690	H	0	-0.832	12.584	-2.975
H						
HETATM	691	C	0	0.885	13.133	-2.004
C						
HETATM	692	C	0	0.383	14.238	-1.200
C						
HETATM	693	C	0	-0.736	16.002	-0.034
C						
HETATM	694	C	0	-1.672	16.967	0.559
C						
HETATM	695	C	0	-1.196	18.019	1.363
C						

HETATM	696	H	0	-0.262	18.117	1.508
H						
HETATM	697	C	0	-2.062	18.893	1.928
C						
HETATM	698	H	0	-1.722	19.618	2.441
H						
HETATM	699	C	0	-3.481	18.749	1.768
C						
HETATM	700	C	0	-4.394	19.616	2.370
C						
HETATM	701	H	0	-4.078	20.327	2.915
H						
HETATM	702	C	0	-5.748	19.450	2.182
C						
HETATM	703	H	0	-6.360	20.058	2.581
H						
HETATM	704	C	0	-6.222	18.398	1.412
C						
HETATM	705	H	0	-7.159	18.282	1.302
H						
HETATM	706	C	0	-5.354	17.522	0.806
C						
HETATM	707	H	0	-5.689	16.806	0.279
H						
HETATM	708	C	0	-3.944	17.691	0.970
C						
HETATM	709	C	0	-3.031	16.818	0.364
C						
HETATM	710	H	0	-3.350	16.113	-0.188
H						
HETATM	711	Zn	0	7.447	2.800	0.140
Zn						
HETATM	712	S	0	11.905	2.101	1.003
S						
HETATM	713	S	0	6.382	0.161	4.068
S						
HETATM	714	N	0	8.463	4.045	1.640
N						
HETATM	715	N	0	9.501	2.008	0.203
N						
HETATM	716	N	0	10.127	0.991	-0.466
N						
HETATM	717	N	0	6.916	1.495	1.685
N						
HETATM	718	C	0	7.923	5.019	2.358
C						
HETATM	719	H	0	6.995	5.196	2.258
H						
HETATM	720	C	0	6.708	0.940	2.680
C						
HETATM	721	C	0	8.650	5.790	3.247
C						
HETATM	722	H	0	8.224	6.480	3.742
H						
HETATM	723	C	0	9.985	5.552	3.407
C						

HETATM	724	H	0	10.500	6.079	4.006
H						
HETATM	725	C	0	10.577	4.527	2.685
C						
HETATM	726	H	0	11.502	4.335	2.783
H						
HETATM	727	C	0	9.786	3.786	1.812
C						
HETATM	728	C	0	10.287	2.682	1.007
C						
HETATM	729	C	0	11.406	0.918	-0.158
C						
HETATM	730	C	0	12.343	-0.047	-0.751
C						
HETATM	731	C	0	11.866	-1.100	-1.555
C						
HETATM	732	H	0	10.933	-1.197	-1.700
H						
HETATM	733	C	0	12.732	-1.974	-2.120
C						
HETATM	734	H	0	12.392	-2.697	-2.634
H						
HETATM	735	C	0	14.151	-1.830	-1.961
C						
HETATM	736	C	0	15.064	-2.695	-2.562
C						
HETATM	737	H	0	14.747	-3.407	-3.108
H						
HETATM	738	C	0	16.418	-2.530	-2.374
C						
HETATM	739	H	0	17.029	-3.138	-2.773
H						
HETATM	740	C	0	16.892	-1.479	-1.604
C						
HETATM	741	H	0	17.828	-1.363	-1.494
H						
HETATM	742	C	0	16.024	-0.602	-0.998
C						
HETATM	743	H	0	16.360	0.114	-0.472
H						
HETATM	744	C	0	14.614	-0.772	-1.162
C						
HETATM	745	C	0	13.701	0.102	-0.557
C						
HETATM	746	H	0	14.021	0.806	-0.005
H						
HETATM	747	S	0	2.988	3.498	-0.723
S						
HETATM	748	S	0	8.512	5.439	-3.789
S						
HETATM	749	N	0	6.431	1.554	-1.361
N						
HETATM	750	N	0	5.394	3.591	0.076
N						
HETATM	751	N	0	4.767	4.608	0.746
N						

HETATM	752	N	0	7.978	4.105	-1.405
N						
HETATM	753	C	0	6.971	0.581	-2.078
C						
HETATM	754	H	0	7.899	0.404	-1.979
H						
HETATM	755	C	0	8.186	4.660	-2.401
C						
HETATM	756	C	0	6.244	-0.190	-2.968
C						
HETATM	757	H	0	6.670	-0.881	-3.461
H						
HETATM	758	C	0	4.909	0.048	-3.128
C						
HETATM	759	H	0	4.394	-0.480	-3.726
H						
HETATM	760	C	0	4.318	1.072	-2.405
C						
HETATM	761	H	0	3.392	1.264	-2.504
H						
HETATM	762	C	0	5.108	1.812	-1.533
C						
HETATM	763	C	0	4.607	2.918	-0.727
C						
HETATM	764	C	0	3.489	4.681	0.438
C						
HETATM	765	C	0	2.552	5.646	1.031
C						
HETATM	766	C	0	3.028	6.700	1.834
C						
HETATM	767	H	0	3.961	6.797	1.979
H						
HETATM	768	C	0	2.162	7.574	2.399
C						
HETATM	769	H	0	2.502	8.297	2.914
H						
HETATM	770	C	0	0.743	7.429	2.241
C						
HETATM	771	C	0	-0.170	8.295	2.842
C						
HETATM	772	H	0	0.147	9.007	3.387
H						
HETATM	773	C	0	-1.524	8.129	2.653
C						
HETATM	774	H	0	-2.135	8.738	3.053
H						
HETATM	775	C	0	-1.998	7.078	1.884
C						
HETATM	776	H	0	-2.934	6.962	1.773
H						
HETATM	777	C	0	-1.130	6.202	1.278
C						
HETATM	778	H	0	-1.465	5.485	0.752
H						
HETATM	779	C	0	0.281	6.371	1.442
C						

HETATM	780	C	0	1.193	5.498	0.836
C						
HETATM	781	H	0	0.873	4.793	0.285
H						
HETATM	782	Zn	0	11.671	-8.521	0.612
Zn						
HETATM	783	S	0	16.130	-9.219	1.474
S						
HETATM	784	S	0	10.607	-11.160	4.540
S						
HETATM	785	N	0	12.688	-7.275	2.113
N						
HETATM	786	N	0	13.724	-9.312	0.675
N						
HETATM	787	N	0	14.351	-10.329	0.005
N						
HETATM	788	N	0	11.141	-9.825	2.156
N						
HETATM	789	C	0	12.148	-6.301	2.830
C						
HETATM	790	H	0	11.219	-6.125	2.731
H						
HETATM	791	C	0	10.933	-10.380	3.152
C						
HETATM	792	C	0	12.875	-5.531	3.719
C						
HETATM	793	H	0	12.449	-4.841	4.213
H						
HETATM	794	C	0	14.209	-5.769	3.879
C						
HETATM	795	H	0	14.724	-5.241	4.478
H						
HETATM	796	C	0	14.800	-6.793	3.156
C						
HETATM	797	H	0	15.726	-6.985	3.255
H						
HETATM	798	C	0	14.009	-7.533	2.284
C						
HETATM	799	C	0	14.511	-8.639	1.479
C						
HETATM	800	C	0	15.630	-10.402	0.313
C						
HETATM	801	C	0	16.566	-11.368	-0.279
C						
HETATM	802	C	0	16.090	-12.421	-1.083
C						
HETATM	803	H	0	15.156	-12.518	-1.228
H						
HETATM	804	C	0	16.956	-13.295	-1.649
C						
HETATM	805	H	0	16.616	-14.018	-2.162
H						
HETATM	806	C	0	18.376	-13.150	-1.489
C						
HETATM	807	C	0	19.288	-14.016	-2.091
C						

HETATM	808	H	0	18.972	-14.727	-2.635
H						
HETATM	809	C	0	20.643	-13.851	-1.902
C						
HETATM	810	H	0	21.254	-14.458	-2.301
H						
HETATM	811	C	0	21.117	-12.799	-1.133
C						
HETATM	812	H	0	22.053	-12.683	-1.022
H						
HETATM	813	C	0	20.248	-11.923	-0.527
C						
HETATM	814	H	0	20.583	-11.206	-0.000
H						
HETATM	815	C	0	18.838	-12.092	-0.691
C						
HETATM	816	C	0	17.926	-11.218	-0.085
C						
HETATM	817	H	0	18.244	-10.514	0.467
H						
HETATM	818	S	0	7.213	-7.822	-0.251
S						
HETATM	819	S	0	12.736	-5.882	-3.316
S						
HETATM	820	N	0	10.655	-9.767	-0.888
N						
HETATM	821	N	0	9.618	-7.730	0.548
N						
HETATM	822	N	0	8.991	-6.712	1.218
N						
HETATM	823	N	0	12.201	-7.216	-0.933
N						
HETATM	824	C	0	11.195	-10.740	-1.607
C						
HETATM	825	H	0	12.123	-10.916	-1.507
H						
HETATM	826	C	0	12.410	-6.661	-1.929
C						
HETATM	827	C	0	10.469	-11.510	-2.495
C						
HETATM	828	H	0	10.894	-12.202	-2.990
H						
HETATM	829	C	0	9.134	-11.272	-2.656
C						
HETATM	830	H	0	8.618	-11.800	-3.255
H						
HETATM	831	C	0	8.542	-10.249	-1.933
C						
HETATM	832	H	0	7.616	-10.056	-2.031
H						
HETATM	833	C	0	9.333	-9.508	-1.060
C						
HETATM	834	C	0	8.832	-8.402	-0.256
C						
HETATM	835	C	0	7.712	-6.639	0.910
C						

HETATM	836	C	0	6.776	-5.674	1.502
C						
HETATM	837	C	0	7.252	-4.621	2.306
C						
HETATM	838	H	0	8.186	-4.523	2.452
H						
HETATM	839	C	0	6.387	-3.747	2.872
C						
HETATM	840	H	0	6.726	-3.023	3.385
H						
HETATM	841	C	0	4.968	-3.892	2.712
C						
HETATM	842	C	0	4.055	-3.025	3.314
C						
HETATM	843	H	0	4.370	-2.314	3.860
H						
HETATM	844	C	0	2.700	-3.192	3.126
C						
HETATM	845	H	0	2.089	-2.583	3.525
H						
HETATM	846	C	0	2.226	-4.242	2.356
C						
HETATM	847	H	0	1.289	-4.358	2.246
H						
HETATM	848	C	0	3.094	-5.119	1.750
C						
HETATM	849	H	0	2.759	-5.835	1.223
H						
HETATM	850	C	0	4.504	-4.949	1.914
C						
HETATM	851	C	0	5.418	-5.823	1.309
C						
HETATM	852	H	0	5.098	-6.528	0.757
H						
HETATM	853	Zn	0	10.670	16.920	-0.192
Zn						
HETATM	854	S	0	15.128	16.222	0.670
S						
HETATM	855	S	0	9.605	14.281	3.736
S						
HETATM	856	N	0	11.686	18.166	1.308
N						
HETATM	857	N	0	12.723	16.128	-0.129
N						
HETATM	858	N	0	13.350	15.111	-0.799
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HETATM	859	N	0	10.140	15.616	1.352
N						
HETATM	860	C	0	11.147	19.140	2.026
C						
HETATM	861	H	0	10.218	19.316	1.927
H						
HETATM	862	C	0	9.931	15.060	2.347
C						
HETATM	863	C	0	11.873	19.910	2.915
C						

HETATM	864	H	0	11.448	20.600	3.409
H						
HETATM	865	C	0	13.207	19.672	3.075
C						
HETATM	866	H	0	13.723	20.200	3.673
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HETATM	867	C	0	13.799	18.647	2.352
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HETATM	868	H	0	14.725	18.456	2.451
H						
HETATM	869	C	0	13.008	17.906	1.480
C						
HETATM	870	C	0	13.509	16.802	0.674
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HETATM	871	C	0	14.629	15.039	-0.491
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HETATM	872	C	0	15.565	14.073	-1.084
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HETATM	873	C	0	15.089	13.020	-1.887
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HETATM	874	H	0	14.155	12.923	-2.032
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HETATM	875	C	0	15.955	12.146	-2.453
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HETATM	876	H	0	15.615	11.422	-2.966
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HETATM	877	C	0	17.374	12.291	-2.294
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HETATM	878	C	0	18.286	11.424	-2.895
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HETATM	879	H	0	17.971	10.713	-3.440
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HETATM	880	C	0	19.641	11.590	-2.707
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HETATM	881	H	0	20.252	10.982	-3.106
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HETATM	882	C	0	20.115	12.642	-1.937
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HETATM	883	H	0	21.052	12.758	-1.826
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HETATM	884	C	0	19.247	13.518	-1.331
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HETATM	885	H	0	19.582	14.235	-0.805
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HETATM	886	C	0	17.837	13.348	-1.495
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HETATM	887	C	0	16.924	14.223	-0.889
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HETATM	888	H	0	17.243	14.926	-0.338
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HETATM	889	S	0	6.212	17.618	-1.055
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HETATM	890	S	0	11.734	19.559	-4.121
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HETATM	891	N	0	9.654	15.674	-1.693
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HETATM	893	N	0	7.990	18.729	0.414
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HETATM	894	N	0	11.200	18.224	-1.738
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HETATM	895	C	0	10.194	14.700	-2.411
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HETATM	896	H	0	11.122	14.525	-2.311
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HETATM	897	C	0	11.408	18.780	-2.733
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HETATM	898	C	0	9.466	13.930	-3.299
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HETATM	899	H	0	9.892	13.239	-3.794
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HETATM	901	H	0	7.617	13.640	-4.059
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HETATM	902	C	0	7.541	15.192	-2.737
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HETATM	903	H	0	6.615	15.384	-2.835
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HETATM	904	C	0	8.332	15.933	-1.865
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HETATM	905	C	0	7.831	17.038	-1.060
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HETATM	908	C	0	6.251	20.819	1.502
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HETATM	909	H	0	7.185	20.916	1.648
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HETATM	910	C	0	5.385	21.693	2.068
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HETATM	911	H	0	5.725	22.417	2.581
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HETATM	912	C	0	3.966	21.549	1.908
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HETATM	913	C	0	3.054	22.416	2.509
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HETATM	914	H	0	3.369	23.127	3.055
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HETATM	915	C	0	1.699	22.249	2.321
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HETATM	916	H	0	1.087	22.858	2.720
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HETATM	917	C	0	1.225	21.198	1.552
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HETATM	918	H	0	0.288	21.082	1.441
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HETATM	919	C	0	2.093	20.322	0.945
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HETATM	920	H	0	1.758	19.606	0.419
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HETATM	921	C	0	3.503	20.491	1.110
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HETATM	922	C	0	4.416	19.618	0.504
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HETATM	923	H	0	4.097	18.913	-0.048
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HETATM	926	S	0	13.829	2.960	4.208
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HETATM	927	N	0	15.911	6.845	1.780
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HETATM	928	N	0	16.948	4.808	0.343
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HETATM	929	N	0	17.574	3.791	-0.327
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HETATM	930	N	0	14.364	4.295	1.825
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HETATM	932	H	0	14.442	7.995	2.398
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HETATM	933	C	0	14.155	3.740	2.820
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HETATM	934	C	0	16.097	8.589	3.386
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HETATM	935	H	0	15.672	9.280	3.881
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HETATM	936	C	0	17.432	8.351	3.547
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HETATM	937	H	0	17.947	8.879	4.146
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HETATM	938	C	0	18.024	7.327	2.824
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HETATM	939	H	0	18.949	7.135	2.922
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HETATM	940	C	0	17.233	6.586	1.952
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HETATM	941	C	0	17.734	5.481	1.147
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HETATM	942	C	0	18.853	3.718	-0.019
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HETATM	943	C	0	19.790	2.753	-0.611
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HETATM	944	C	0	19.313	1.699	-1.415
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HETATM	945	H	0	18.380	1.603	-1.560
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HETATM	946	C	0	20.179	0.826	-1.981
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HETATM	947	H	0	19.839	0.102	-2.494
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HETATM	950	H	0	22.194	-0.607	-2.968
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HETATM	951	C	0	23.865	0.269	-2.234
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HETATM	952	H	0	24.477	-0.338	-2.633
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HETATM	953	C	0	24.340	1.321	-1.464
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HETATM	954	H	0	25.275	1.437	-1.354
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HETATM	955	C	0	23.471	2.198	-0.858
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HETATM	956	H	0	23.806	2.914	-0.332
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HETATM	957	C	0	22.061	2.028	-1.023
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HETATM	958	C	0	21.148	2.902	-0.417
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HETATM	959	H	0	21.468	3.606	0.135
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HETATM	960	S	0	10.436	6.298	-0.583
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HETATM	961	S	0	15.959	8.239	-3.649
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HETATM	962	N	0	13.878	4.353	-1.221
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HETATM	963	N	0	12.841	6.390	0.216
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HETATM	964	N	0	12.214	7.408	0.886
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HETATM	965	N	0	15.425	6.904	-1.265
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HETATM	966	C	0	14.418	3.380	-1.939
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HETATM	967	H	0	15.346	3.204	-1.840
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HETATM	968	C	0	15.633	7.459	-2.262
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HETATM	969	C	0	13.691	2.610	-2.828
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HETATM	970	H	0	14.117	1.919	-3.322
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HETATM	971	C	0	12.356	2.848	-2.989
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HETATM	972	H	0	11.841	2.320	-3.586
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HETATM	973	C	0	11.765	3.871	-2.265
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HETATM	974	H	0	10.839	4.064	-2.364
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HETATM	975	C	0	12.555	4.612	-1.393
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HETATM	976	C	0	12.054	5.718	-0.587
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HETATM	977	C	0	10.935	7.481	0.578
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HETATM	978	C	0	10.000	8.446	1.171
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HETATM	979	C	0	10.475	9.500	1.974
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HETATM	980	H	0	11.409	9.597	2.119
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HETATM	981	C	0	9.609	10.373	2.539
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HETATM	982	H	0	9.949	11.097	3.053
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HETATM	983	C	0	8.190	10.228	2.381
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HETATM	984	C	0	7.277	11.095	2.982
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HETATM	985	H	0	7.594	11.806	3.527
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HETATM	986	C	0	5.923	10.929	2.793
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HETATM	987	H	0	5.312	11.537	3.193
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HETATM	988	C	0	5.449	9.877	2.024
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HETATM	989	H	0	4.513	9.762	1.913
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HETATM	990	C	0	6.318	9.002	1.418
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HETATM	991	H	0	5.982	8.285	0.892
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HETATM	992	C	0	7.728	9.171	1.582
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HETATM	993	C	0	8.640	8.297	0.976
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HETATM	994	H	0	8.320	7.592	0.425
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HETATM	995	Zn	0	19.118	-5.721	0.752
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HETATM	996	S	0	23.576	-6.419	1.614
S						
HETATM	997	S	0	18.053	-8.360	4.680
S						
HETATM	998	N	0	20.135	-4.475	2.252
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HETATM	999	N	0	21.172	-6.512	0.815
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HETATM	1000	N	0	21.799	-7.529	0.145
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HETATM	1001	N	0	18.588	-7.025	2.296
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HETATM	1002	C	0	19.595	-3.502	2.970
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HETATM	1003	H	0	18.667	-3.325	2.871
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HETATM 1004	C	0	18.379	-7.581	3.292
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HETATM 1005	C	0	20.322	-2.731	3.859
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HETATM 1006	H	0	19.896	-2.041	4.353
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HETATM 1007	C	0	21.656	-2.969	4.019
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HETATM 1008	H	0	22.171	-2.442	4.617
H					
HETATM 1009	C	0	22.248	-3.993	3.296
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HETATM 1010	H	0	23.173	-4.185	3.395
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HETATM 1011	C	0	21.457	-4.733	2.424
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HETATM 1012	C	0	21.959	-5.839	1.618
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HETATM 1013	C	0	23.077	-7.602	0.453
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HETATM 1014	C	0	24.014	-8.568	-0.140
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HETATM 1015	C	0	23.537	-9.621	-0.943
C					
HETATM 1016	H	0	22.603	-9.718	-1.088
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HETATM 1017	C	0	24.403	-10.495	-1.509
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HETATM 1018	H	0	24.063	-11.218	-2.022
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HETATM 1019	C	0	25.823	-10.350	-1.350
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HETATM 1020	C	0	26.735	-11.216	-1.951
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HETATM 1021	H	0	26.419	-11.928	-2.496
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HETATM 1022	C	0	28.090	-11.051	-1.763
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HETATM 1023	H	0	28.701	-11.659	-2.162
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HETATM 1024	C	0	28.564	-10.000	-0.993
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HETATM 1025	H	0	29.500	-9.884	-0.883
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HETATM 1026	C	0	27.695	-9.123	-0.387
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HETATM 1027	H	0	28.031	-8.406	0.139
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HETATM 1028	C	0	26.285	-9.293	-0.551
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HETATM 1029	C	0	25.372	-8.419	0.054
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HETATM 1030	H	0	25.692	-7.714	0.606
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HETATM 1031	S	0	14.660	-5.023	-0.111
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HETATM 1032	S	0	20.184	-3.082	-3.177
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HETATM 1033	N	0	18.102	-6.968	-0.749
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HETATM 1034	N	0	17.065	-4.930	0.687
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HETATM 1035	N	0	16.438	-3.912	1.358
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HETATM 1036	N	0	19.648	-4.417	-0.794
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HETATM 1037	C	0	18.642	-7.940	-1.467
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HETATM 1038	H	0	19.570	-8.117	-1.367
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HETATM 1039	C	0	19.858	-3.861	-1.789
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HETATM 1040	C	0	17.915	-8.711	-2.355
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HETATM 1041	H	0	18.341	-9.402	-2.850
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HETATM 1042	C	0	16.581	-8.473	-2.516
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HETATM 1043	H	0	16.065	-9.001	-3.115
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HETATM 1044	C	0	15.989	-7.449	-1.793
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HETATM 1045	H	0	15.064	-7.256	-1.891
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HETATM 1046	C	0	16.780	-6.708	-0.920
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HETATM 1047	C	0	16.279	-5.602	-0.116
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HETATM 1048	C	0	15.159	-3.840	1.050
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HETATM 1049	C	0	14.223	-2.874	1.642
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HETATM 1050	C	0	14.700	-1.821	2.445
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HETATM 1051	H	0	15.633	-1.724	2.591
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HETATM 1052	C	0	13.834	-0.947	3.012
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HETATM 1053	H	0	14.173	-0.224	3.525
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HETATM 1054	C	0	12.415	-1.092	2.852
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HETATM 1055	C	0	11.502	-0.226	3.453
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HETATM 1056	H	0	11.818	0.486	3.999
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HETATM 1058	H	0	9.535	0.217	3.664
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HETATM 1059	C	0	9.673	-1.443	2.495
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HETATM	1060	H	0	8.737	-1.558	2.385
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HETATM	1061	C	0	10.541	-2.319	1.889
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HETATM	1062	H	0	10.206	-3.035	1.363
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HETATM	1063	C	0	11.951	-2.149	2.054
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HETATM	1064	C	0	12.865	-3.023	1.448
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HETATM	1065	H	0	12.545	-3.728	0.896
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END

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The description of the movies illustrating the first 10 vibrational modes for model systems.

40 movies are attached separately as gif-files. They illustrate the first 10 vibrational modes of the central Fe molecule in the corresponding matrix. The names are coded in the following way: the name HS_in_HS_mode1_25 means that the shown vibration is the first mode of the HS molecule in the model HS matrix (Zn matrix) that occur with energy of 25 cm⁻¹. Similarly, LS_in_LS_mode2_36 shows the second mode (at 36 cm⁻¹) of the LS molecule in the LS matrix.

