

Table S1 xyz Cartesian coordinates of Huolinhe lignite model

element	x	y	z
C	13.5435	8.6571	-0.2071
C	14.905	9.0442	-0.3014
C	15.4806	9.3878	-1.5386
C	14.7053	9.354	-2.7105
C	13.3517	8.981	-2.639
C	12.7773	8.6416	-1.4003
O	15.2625	9.6817	-3.899
H	14.727	9.6609	-4.7199
C	12.9917	8.3091	1.0494
C	12.0205	7.1869	1.2706
C	10.661	7.7052	1.8583
O	13.3713	8.9616	2.0516
C	9.7103	8.3892	0.8434
O	9.3253	7.5378	-0.2512
C	5.8637	5.1827	-0.4927
C	6.8952	4.869	0.4128
C	8.0306	5.6809	0.4955
C	8.1792	6.8017	-0.3416
C	7.1724	7.1124	-1.2956
C	5.9789	6.3234	-1.3437
C	4.7142	4.3659	-0.5383
C	3.6507	4.6878	-1.3915
C	3.7067	5.8303	-2.2179
C	4.8718	6.6312	-2.1822
C	7.4002	8.193	-2.171
O	7.7814	9.4076	-1.7133
H	7.8926	9.5646	-0.7525
O	7.2753	8.0578	-3.4093
C	2.5401	6.167	-3.09
C	2.3591	5.1861	-4.3009
C	0.8869	5.0725	-4.8317
C	-0.8038	6.84	-3.9685
C	-1.3036	8.0285	-4.4932
N	-0.7726	8.2796	-5.6975
C	0.1495	7.2607	-6.0553
C	0.1021	6.3322	-4.9083
C	-1.2298	6.385	-2.6986
C	-2.1484	7.1726	-1.949
C	-2.6422	8.3788	-2.513
C	-2.2311	8.8087	-3.7886
O	-0.7526	5.2208	-2.1969
H	-1.0276	4.897	-1.3147
C	-2.5659	6.7645	-0.5761

C	-3.5744	5.5521	-0.4729
C	-4.9875	5.9282	-1.1307
C	-6.2799	5.3992	-0.4025
C	-10.0447	7.5262	-0.8765
C	-9.9026	6.1867	-1.3148
C	-8.682	5.5041	-1.19
C	-7.5528	6.1423	-0.6337
C	-7.6783	7.4916	-0.2344
C	-8.8997	8.1923	-0.3591
C	-11.4072	8.1694	-0.9102
C	-5.0143	5.5305	-2.6564
C	-5.9927	6.3068	-3.5743
O	-5.8037	7.7146	-3.4783
H	-6.4542	8.0993	-4.103
C	-11.1976	10.5977	-3.6766
N	-11.5952	11.4348	-2.7075
C	-11.7693	10.7483	-1.4751
C	-11.4128	9.3561	-1.8155
C	-11.0796	9.3168	-3.1669
C	-11.9619	8.4415	0.5321
C	-11.976	7.1886	1.4551
O	-9.0172	9.4966	0.0256
C	-8.0407	10.3762	0.5926
C	12.677	5.9864	2.083
C	12.0558	4.6179	1.629
C	12.3779	4.1511	0.1678
C	12.6149	6.1974	3.6446
C	13.5634	5.3733	4.5748
C	13.3265	3.8423	4.7834
C	11.8467	3.3536	5.0284
C	11.6835	1.8235	4.6855
C	10.3141	1.4268	4.0563
C	10.2857	-0.012	3.4687
C	11.3781	3.7368	6.4771
C	9.849	3.7333	6.7728
C	8.767	3.1227	-1.9488
C	9.5484	4.1759	-2.4186
C	10.7429	4.5378	-1.7648
C	11.1519	3.8127	-0.6113
C	10.3521	2.7271	-0.1654
C	9.1563	2.3853	-0.8204
C	7.6224	2.9364	-2.7081
C	7.5238	3.8382	-3.7758
S	8.8813	4.9407	-3.8226
O	11.4491	5.5782	-2.2704
H	12.287	5.8774	-1.8644

C	6.4757	3.91	-4.7231
C	5.399	2.9936	-4.7829
C	3.4136	5.47	-5.4311
C	3.8041	4.262	-6.3393
C	4.2223	3.0389	-5.5754
C	3.2508	1.8928	-5.6236
C	3.3533	0.6853	-4.641
C	-3.5501	5.0576	1.0243
C	-4.002	3.5896	1.2853
C	-3.9492	3.2042	2.7932
C	-4.7841	1.9369	3.1537
O	-4.3005	0.8722	2.3095
C	-8.3511	-0.5896	-2.1459
C	-7.5719	-1.6603	-2.6787
C	-8.072	-2.4171	-3.7711
C	-9.3287	-2.1144	-4.3251
C	-10.0959	-1.0614	-3.8066
C	-9.6109	-0.3039	-2.7289
C	-7.868	0.1551	-1.0392
C	-6.6161	-0.1592	-0.4497
C	-5.8378	-1.2206	-0.9908
C	-6.3194	-1.9525	-2.0956
C	-4.5918	-1.5476	-0.4097
C	-4.1149	-0.8317	0.6993
C	-4.865	0.2224	1.2496
C	-6.1124	0.547	0.6705
O	-7.3923	-3.4509	-4.326
H	-6.5128	-3.7225	-3.9933
C	-4.6842	1.514	4.6648
C	-5.1841	2.6189	5.6717
C	-12.3465	7.4907	2.9321
O	-11.9399	6.4097	3.791
C	-9.2476	4.1076	4.9382
C	-9.0252	2.7992	5.4993
C	-7.696	2.3737	5.7519
C	-6.5694	3.1489	5.4501
C	-6.7996	4.4425	4.9563
C	-8.0981	4.9372	4.6661
C	-10.5335	4.6626	4.6293
C	-10.6814	5.9631	4.1037
C	-9.5412	6.7465	3.8772
C	-8.2482	6.2531	4.1253
C	-7.1898	7.1239	3.7847
O	-6.2261	6.7458	3.0825
O	-7.198	8.4231	4.1644
H	-7.9354	8.7785	4.7037

C	7.4957	-0.9886	0.9952
C	6.4282	-1.1293	1.9194
N	6.6384	-0.9002	3.2416
C	7.838	-0.5392	3.7512
C	8.9555	-0.3844	2.9044
C	8.7603	-0.6142	1.5212
C	7.2546	-1.2403	-0.3842
C	5.9564	-1.5999	-0.8681
C	4.9342	-1.7364	0.1127
C	5.1623	-1.5615	1.4906
O	8.2898	-1.114	-1.2545
H	9.1893	-0.8672	-0.9612
O	6.5527	4.836	-5.5628
C	5.6845	-1.8053	-2.2615
O	6.6382	-1.8133	-3.0759
C	4.4311	-0.3894	-4.9884
C	1.7132	-2.5638	-3.9653
C	2.1547	-3.4186	-2.7097
C	3.7132	-3.3988	-2.5024
C	4.3183	-2.0024	-2.8668
C	4.184	-1.8416	-4.4435
C	2.8597	-2.4809	-5.0245
C	0.3105	-2.8675	-4.5914
C	-1.2049	0.5216	-6.8434
C	-1.6687	1.6475	-7.5612
C	-2.1013	2.7988	-6.8788
C	-2.0783	2.838	-5.4733
C	-1.6123	1.7266	-4.7471
C	-1.1724	0.5634	-5.4207
C	-0.7737	-0.6447	-7.5125
C	-0.3014	-1.7521	-6.7855
C	-0.242	-1.72	-5.3743
C	-0.6981	-0.5585	-4.7054
O	-8.6305	1.1682	-0.5499
H	-8.3446	1.7112	0.2117
O	-2.5042	3.9419	-4.8175
H	-2.8306	4.7198	-5.3167
C	-10.0503	1.7632	5.8648
C	-10.9815	0.9325	3.6535
C	-11.1143	-0.044	2.6393
C	-10.4585	-1.2973	2.8043
C	-9.5831	-1.5031	3.905
C	-9.4707	-0.4928	4.8869
C	-10.1809	0.7238	4.7959
C	-5.3496	0.1289	4.9512
O	-4.705	-0.9531	4.2446

C	-4.8963	-2.2884	4.7625
C	-6.3661	-2.7734	4.9344
C	-7.2991	-2.6874	3.6757
C	-8.8156	-2.7746	4.1046
C	-6.9212	-3.7564	2.5863
C	-11.8349	0.3	1.4776
O	-11.4737	-0.0844	0.3422
O	-12.9276	1.0963	1.5363
H	-13.4083	1.3367	0.7164
C	7.9753	4.0836	5.1045
C	7.1823	4.9158	4.296
C	7.4009	6.3115	4.2602
C	8.4531	6.859	5.0516
C	9.2434	6.0085	5.8581
C	9.021	4.6126	5.8942
C	8.6914	8.252	5.0306
C	7.8924	9.0985	4.2446
C	6.8493	8.5636	3.4718
C	6.5996	7.1786	3.4731
O	5.5727	6.7357	2.7072
H	5.3398	5.7857	2.6683
O	4.199	-1.7746	2.4357
C	2.2281	-4.9466	2.2259
C	1.1811	-4.5955	3.1105
C	1.1357	-3.3233	3.7093
C	2.1538	-2.3897	3.4489
C	3.1931	-2.6924	2.5491
C	3.2052	-3.9617	1.9203
O	0.1284	-3.0023	4.554
H	-0.5815	-3.65	4.7478
C	1.6223	-4.8919	-2.5672
C	1.2877	-5.2294	-1.081
C	1.2585	-6.7348	-0.6831
C	0.1912	-7.5809	-1.4593
C	-4.009	-6.6512	-0.637
C	-3.4492	-7.8833	0.0006
C	-1.9884	-8.0978	-0.2306
C	-1.2459	-7.3027	-1.1411
C	-1.9043	-6.2431	-1.8024
C	-3.2401	-5.9087	-1.5505
C	-5.3262	-6.262	-0.3138
C	-6.0529	-6.8474	0.7555
C	-5.326	-7.6785	1.6489
C	-3.8664	-7.9157	1.5005
C	1.149	-6.9107	0.8711
C	2.3394	-6.3535	1.7225

C	-7.5109	-3.5073	1.1562
C	-8.736	-4.3854	0.6954
C	-8.3345	-5.7821	0.1051
C	-7.4395	-6.6031	0.9697
O	-8.0137	-7.1094	1.9652
C	-9.6486	-3.6061	-0.3331
C	-14.8755	-2.1621	2.8376
C	-15.7813	-2.5369	1.8382
C	-15.3321	-3.0844	0.6146
C	-13.9263	-3.264	0.4137
C	-12.9903	-2.7861	1.388
C	-13.4989	-2.296	2.6149
C	-11.586	-2.8708	1.1408
C	-11.1071	-3.5567	-0.0068
C	-12.0352	-4.1126	-0.9085
C	-13.4121	-3.9546	-0.7108
O	-10.6074	-2.3508	1.9467
C	-16.3209	-3.4036	-0.341
O	-17.4947	-3.9758	0.0162
H	-17.6751	-4.1997	0.9532
O	-16.1731	-3.136	-1.5549
O	-15.3334	-1.6694	4.0123
H	-14.7058	-1.4031	4.7167
O	-11.736	4.0492	4.7544
H	-11.8613	3.1101	4.9475
O	-1.4174	-9.1344	0.4328
H	-0.4703	-9.3543	0.3253
H	15.4981	9.072	0.5326
H	16.4652	9.6606	-1.5835
H	12.7809	8.9588	-3.4873
H	11.787	8.3942	-1.3869
H	11.7725	6.7884	0.2896
H	10.8522	8.4093	2.6726
H	10.1101	6.8768	2.2985
H	10.1977	9.2725	0.4278
H	8.8183	8.7359	1.3689
H	6.8287	4.0508	1.0251
H	8.7584	5.4298	1.1606
H	4.6348	3.5351	0.0552
H	2.8242	4.0841	-1.3965
H	4.8957	7.4602	-2.7775
H	2.6172	7.1895	-3.4708
H	1.6577	6.147	-2.4513
H	2.5754	4.1937	-3.9017
H	0.3505	4.3643	-4.2006
H	0.8834	4.6141	-5.8225

H	1.1425	7.6929	-6.1817
H	-0.1692	6.767	-6.9756
H	-3.3084	8.9581	-1.9963
H	-2.5937	9.6764	-4.1893
H	-3.0046	7.6145	-0.044
H	-1.6375	6.5463	-0.041
H	-3.1441	4.7223	-1.0407
H	-5.0582	7.0165	-1.0872
H	-6.1536	5.4528	0.6752
H	-6.4112	4.3428	-0.6501
H	-10.6987	5.6817	-1.7122
H	-8.6284	4.5299	-1.4985
H	-6.8698	7.9649	0.1722
H	-12.1288	7.4798	-1.3614
H	-5.2284	4.4623	-2.7486
H	-4.0292	5.6756	-3.0967
H	-7.0261	6.0678	-3.3356
H	-5.8197	6.0126	-4.612
H	-11.0116	10.8676	-4.6435
H	-12.8077	10.824	-1.147
H	-11.1012	11.1605	-0.7172
H	-10.7947	8.4899	-3.6956
H	-12.9879	8.8132	0.4565
H	-11.3686	9.2222	1.0125
H	-10.9871	6.7316	1.4444
H	-12.6777	6.4513	1.056
H	-7.2024	10.5053	-0.0938
H	-7.6809	9.9802	1.5434
H	-8.5037	11.347	0.7689
H	13.7394	5.936	1.8206
H	10.979	4.6632	1.8024
H	12.4168	3.8203	2.2613
H	13.0074	3.2561	0.199
H	12.984	4.8994	-0.3417
H	11.5903	6.0839	3.9946
H	12.8737	7.239	3.8428
H	13.5242	5.8402	5.563
H	14.5878	5.5116	4.2175
H	13.9381	3.5198	5.6315
H	13.7656	3.341	3.9204
H	11.2112	3.8943	4.3319
H	11.8568	1.2197	5.5801
H	12.4451	1.5262	3.9609
H	10.0641	2.1277	3.2549
H	9.5468	1.4996	4.822
H	10.5453	-0.7298	4.2516

H	11.0584	-0.0848	2.6981
H	11.7397	4.7382	6.7181
H	11.8618	3.0635	7.1901
H	9.7059	4.0756	7.8017
H	9.4921	2.7032	6.7548
H	10.6322	2.1798	0.6524
H	8.5791	1.6173	-0.4755
H	6.9372	2.2135	-2.484
H	5.4804	2.1925	-4.1707
H	4.3285	5.8491	-4.9777
H	3.0487	6.2732	-6.0725
H	4.6003	4.5578	-7.0241
H	2.9498	4.0433	-6.9858
H	3.2473	1.5061	-6.646
H	2.2545	2.3126	-5.4544
H	2.3743	0.2152	-4.6805
H	3.4878	1.0398	-3.6163
H	-4.1248	5.7519	1.6391
H	-2.5261	5.0944	1.4077
H	-3.3525	2.9132	0.7227
H	-5.0142	3.4348	0.9281
H	-4.327	4.0469	3.3701
H	-2.9056	3.048	3.0804
H	-5.8323	2.1542	2.9457
H	-9.6905	-2.6616	-5.1101
H	-11.0089	-0.8461	-4.214
H	-10.1964	0.4565	-2.3753
H	-5.7474	-2.714	-2.4695
H	-4.0216	-2.3105	-0.7856
H	-3.2101	-1.0826	1.1059
H	-6.6547	1.3104	1.0669
H	-3.6202	1.3692	4.8809
H	-4.4653	3.4417	5.6487
H	-5.1261	2.2343	6.6938
H	-13.4296	7.6012	3.0123
H	-11.8923	8.422	3.277
H	-7.5314	1.4627	6.1856
H	-5.9807	5.0319	4.8169
H	-9.6615	7.6903	3.5011
H	7.9157	-0.3924	4.7593
H	9.5612	-0.5077	0.8972
H	3.974	-1.9408	-0.1534
H	5.4047	-0.0472	-4.6381
H	4.5091	-0.462	-6.077
H	1.612	-1.5514	-3.5677
H	1.7389	-2.8609	-1.8598

H	4.1888	-4.1519	-3.139
H	3.9455	-3.7039	-1.4841
H	3.6941	-1.2238	-2.42
H	4.9914	-2.4393	-4.8827
H	3.0657	-3.4998	-5.3675
H	2.5264	-1.9294	-5.9065
H	-0.4071	-3.0925	-3.7977
H	0.389	-3.7615	-5.2161
H	-1.6963	1.6389	-8.5843
H	-2.4349	3.6076	-7.4082
H	-1.5967	1.7726	-3.7245
H	-0.7962	-0.697	-8.5346
H	0.0115	-2.5808	-7.2972
H	-0.677	-0.5294	-3.6817
H	-11.0087	2.1756	6.1483
H	-9.7537	1.2785	6.8015
H	-11.4609	1.8248	3.5458
H	-8.863	-0.6516	5.6946
H	-6.391	0.157	4.6327
H	-5.3154	-0.0586	6.0292
H	-4.3913	-2.3593	5.7299
H	-4.3689	-2.9668	4.0918
H	-6.7954	-2.1754	5.7419
H	-6.347	-3.8076	5.2897
H	-7.1166	-1.7064	3.2275
H	-8.9091	-3.065	5.1555
H	-9.3129	-3.5937	3.5927
H	-7.1995	-4.7431	2.9563
H	-5.8353	-3.7671	2.4737
H	7.7705	3.0827	5.1176
H	6.4388	4.4853	3.7423
H	9.9873	6.4117	6.4342
H	9.4458	8.6627	5.5874
H	8.0703	10.1054	4.235
H	6.2717	9.1888	2.9045
H	0.4542	-5.2758	3.345
H	2.1367	-1.4813	3.9191
H	3.9706	-4.1927	1.2842
H	2.3595	-5.6015	-2.9512
H	0.7255	-5.0477	-3.1572
H	0.3422	-4.7548	-0.8068
H	2.0582	-4.7608	-0.4763
H	2.2306	-7.1493	-0.9722
H	0.4092	-8.6369	-1.2855
H	0.3458	-7.4537	-2.5339
H	-3.9439	-8.7322	-0.4838

H	-1.4053	-5.6811	-2.4918
H	-3.6439	-5.1016	-2.0347
H	-5.7393	-5.5123	-0.8675
H	-5.791	-8.1109	2.4518
H	-3.6236	-8.891	1.9311
H	-3.3264	-7.1486	2.0623
H	1.1011	-7.9849	1.0715
H	0.2059	-6.4849	1.2205
H	3.2666	-6.4896	1.1597
H	2.4389	-6.9841	2.6111
H	-6.7163	-3.6423	0.4205
H	-7.7701	-2.4492	1.1094
H	-9.3325	-4.6069	1.5805
H	-7.9064	-5.6474	-0.8864
H	-9.25	-6.3588	-0.0624
H	-9.4928	-3.9974	-1.3424
H	-9.3498	-2.5619	-0.4115
H	-16.7806	-2.3997	2.0182
H	-12.8792	-2.0451	3.3826
H	-11.7162	-4.6233	-1.7363
H	-14.0302	-4.3757	-1.4053