

Molecular mechanism of the cesium and rubidium selective binding to the calix[4]arene revealed by Born–Oppenheimer molecular dynamics simulation and electron density analysis

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XYZ coordinates of the model system utilized in simulations (929 atoms)

Me is a metal cation (Li⁺, Na⁺, K⁺, Rb⁺, Cs⁺)

Me	-0.479000	-0.284000	-3.421000
C1	0.562000	-3.904000	1.565000
H1	0.622000	-4.435000	2.509000
C24	1.723000	-3.421000	0.967000
H24	2.686000	-3.577000	1.444000
C23	1.675000	-2.750000	-0.258000
C22	2.940000	-2.174000	-0.883000
H95	2.852000	-2.176000	-1.973000
H96	3.780000	-2.827000	-0.635000
C2	-0.672000	-3.703000	0.952000
H77	-1.580000	-4.070000	1.424000
C3	-0.771000	-3.043000	-0.279000
C25	0.420000	-2.593000	-0.878000
O25	0.348000	-2.034000	-2.135000
H25	1.076081	-1.415252	-2.075204
C4	-2.134000	-2.824000	-0.931000
H41	-2.011000	-2.699000	-2.008000
H42	-2.725000	-3.727000	-0.763000
C5	-2.905000	-1.646000	-0.349000
C6	-3.829000	-1.821000	0.688000
H6	-4.031000	-2.827000	1.046000
C7	-4.497000	-0.738000	1.259000
H7	-5.220000	-0.891000	2.052000
C8	-4.222000	0.556000	0.808000
H89	-4.732000	1.404000	1.255000
C28	-2.677000	-0.339000	-0.822000
O28	-1.870000	-0.181000	-1.906000
C9	-3.303000	0.779000	-0.230000
C10	-2.948000	2.184000	-0.693000
H91	-2.872000	2.205000	-1.786000
H92	-3.762000	2.860000	-0.418000
C11	-1.652000	2.716000	-0.091000
C12	-1.685000	3.398000	1.125000
H12	-2.643000	3.538000	1.614000

C13	-0.523000	3.904000	1.716000
H13	-0.558000	4.434000	2.661000
C14	0.692000	3.755000	1.047000
H14	1.596000	4.179000	1.473000
C27	-0.402000	2.502000	-0.732000
O27	-0.314000	1.765000	-1.848000
H27	-1.482301	0.745768	-1.824376
C15	0.771000	3.071000	-0.169000
C16	2.120000	2.882000	-0.844000
H93	1.994000	2.830000	-1.930000
H94	2.738000	3.759000	-0.634000
C17	2.848000	1.650000	-0.333000
C18	3.749000	1.763000	0.733000
H18	3.932000	2.746000	1.155000
C26	2.591000	0.370000	-0.864000
O26	1.684000	0.214000	-1.883000
H26	1.062364	1.037112	-1.880225
C21	3.255000	-0.773000	-0.371000
C20	4.170000	-0.603000	0.676000
H20	4.692000	-1.472000	1.057000
C19	4.414000	0.649000	1.239000
H19	5.123000	0.754000	2.054000
O	-10.034211	-0.140906	-9.662771
H	-9.472496	-0.061987	-8.856083
H	-9.354822	-0.240495	-10.361240
O	9.270194	-2.326498	3.325087
H	9.891460	-2.941718	3.726438
H	8.982837	-1.866714	4.114111
O	-9.551727	8.800347	-10.534440
H	-9.120653	9.254366	-9.755607
H	-10.516321	8.851477	-10.270180
O	8.157738	0.857861	3.523884
H	7.957779	0.466945	2.697611
H	9.128474	0.967474	3.412980
O	8.075758	3.549808	3.454759
H	7.924800	2.610168	3.822036
H	8.703245	3.344686	2.749985
O	-7.232625	-0.190766	-10.768618
H	-6.781025	-0.992314	-10.532185
H	-6.429292	0.330675	-10.897017
O	-9.408944	-7.428502	-5.782711
H	-9.548106	-7.259915	-4.840372
H	-8.950786	-8.253119	-5.721966
O	-3.235553	8.405665	-14.404328
H	-3.611546	7.950549	-15.161313
H	-4.041369	8.356697	-13.858634
O	-5.275342	-1.628049	-2.513496
H	-6.003497	-1.681925	-1.888318
H	-4.573871	-1.772212	-1.929017
O	-7.369761	7.605957	-4.779942

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H	-6.655134	7.945050	-4.200649
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H	6.572078	1.953753	6.694698
O	2.632890	-5.194958	4.628741
H	3.305718	-5.436767	3.994706
H	2.771198	-4.208448	4.707848
O	4.734891	3.128703	-3.084414
H	3.878649	3.405268	-3.396416
H	4.794507	2.199353	-3.206439
O	8.655797	-4.854993	-5.230912
H	9.422537	-5.265806	-4.849807
H	8.884358	-3.911052	-5.169094
O	5.126931	-4.439696	6.876575
H	5.773675	-4.139895	7.564869
H	5.478636	-4.017417	6.119261
O	7.420575	-9.220451	1.231399
H	6.752762	-9.743525	1.657892
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H	-0.911819	7.903040	4.985658
O	3.323126	5.758821	-12.140916
H	3.525996	5.471817	-13.028060
H	3.268385	4.928688	-11.628737
O	-2.314135	-3.532303	-9.319463
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H	-2.982492	-3.984702	-9.847217
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H	-5.541194	-1.716450	-8.620682
O	7.972997	-0.360064	-11.896620
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H	7.672474	-0.726176	-11.083078
O	-9.027852	-0.750154	-12.610947
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O	-8.851463	2.570571	-3.665221
H	-8.485717	2.722666	-2.761282
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O	2.463866	-8.815895	-2.519597
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O	-1.736445	-8.501058	-5.464925
H	-1.667177	-8.173848	-4.494845
H	-0.859226	-8.643729	-5.762598
O	5.481587	-1.301866	-13.670355
H	5.359495	-2.231356	-13.425705
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O	8.878627	3.475572	-0.705801
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O	6.059299	7.020645	-12.067986
H	6.578347	6.223637	-11.918731
H	5.227232	6.674294	-11.681710
O	-9.938421	-2.068918	0.930221
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O	-0.110689	-5.908287	-1.537410
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O	4.497750	5.760605	-6.197657
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H	9.428092	-2.716677	-1.945880
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O	-2.109853	1.469714	3.740654
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O	0.384531	-6.005980	-7.585979
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H	-0.418860	-6.153087	-8.130493
O	4.553206	-7.967264	2.864302
H	4.755856	-6.995472	2.692571
H	4.206664	-8.291905	2.055382
O	-3.688457	3.664192	4.135738
H	-3.229052	2.865828	3.804516
H	-3.375448	3.841192	5.027346
O	4.682426	-5.208310	2.565665
H	5.107474	-4.370012	2.769292
H	4.615020	-5.178513	1.592744
O	0.862438	-7.368777	-13.819512
H	1.727958	-7.610102	-13.458045
H	0.540556	-6.576368	-13.350698
O	-9.709896	-2.299180	-2.374078
H	-9.436063	-2.571884	-3.238681
H	-9.932705	-1.376150	-2.518884
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O	1.917012	8.135679	4.353974
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O	-0.606204	3.346425	-6.765284
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O	6.389977	4.279678	0.241187

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O	8.269246	-5.151665	5.056417
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H	7.350482	-5.435856	5.305711
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O	-3.056319	-5.994481	2.338828
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H	-7.678924	4.424529	-7.794353
O	7.255737	-1.491409	6.275186
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H	6.766579	-2.242652	5.849773
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H	4.981410	0.182631	-2.520880
H	3.584032	0.214001	-2.982258
O	-7.264575	-6.624690	-12.846528
H	-6.921816	-5.994582	-13.427182
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H	4.154861	-9.035404	-6.961375
H	2.615072	-8.813752	-7.074629
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H	4.731009	-9.669166	-0.608343
O	-5.444865	1.196252	-2.852853
H	-6.051255	1.065299	-3.568458
H	-5.139217	0.276829	-2.673679
O	2.968542	-6.720713	-8.880807
H	3.667315	-6.998036	-9.477475
H	3.481216	-6.814788	-8.074253
O	-4.111528	-9.877312	-5.191415
H	-4.698422	-9.090580	-4.908887
H	-3.232645	-9.546472	-5.158310
O	9.509457	4.761463	-8.386518
H	8.555319	4.641833	-8.187506
H	9.737128	4.974910	-7.486855

O	9.077934	-5.510850	-0.000257
H	9.920837	-5.412614	-0.389291
H	8.560946	-4.821078	-0.397595
O	4.437537	-5.460530	-0.151712
H	3.564648	-5.731747	-0.366046
H	4.693581	-4.993213	-0.959508
O	10.207692	-5.853177	-10.082823
H	11.088032	-6.076192	-9.651323
H	9.581758	-5.962619	-9.404694
O	-2.364230	5.793490	-0.918856
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H	-2.960004	5.446619	-1.630159
O	8.258448	7.330656	1.948796
H	8.074232	7.040689	2.834353
H	7.375571	7.436978	1.632141
O	6.464370	-6.650225	-5.548887
H	6.650785	-7.308268	-4.769847
H	7.268366	-6.004236	-5.472032
O	-3.463568	-2.112547	-12.289867
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H	-2.721099	-2.439288	-12.854926
O	7.499576	-6.096631	-11.802511
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H	-5.755475	-4.633255	-3.987879
H	-7.290298	-4.314381	-3.982073
O	10.331944	4.973909	-5.549968
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O	-1.192003	9.526627	6.566590
H	-1.695722	9.182982	7.288038
H	-0.341626	9.792747	6.819190
O	-4.998819	6.438883	1.981355
H	-4.848017	5.610042	1.509295
H	-5.656940	6.183035	2.686204
O	-3.265246	-6.361031	-6.479864
H	-2.875056	-5.963387	-5.666659
H	-2.804742	-7.260819	-6.451107
O	5.263028	-0.601534	-10.506694
H	4.876877	0.260842	-10.250115
H	4.479232	-1.111884	-10.669018
O	-5.750793	4.031588	0.400818
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H	-6.302570	4.688584	-0.050649
O	5.277824	2.915684	-11.195990
H	6.126850	2.965681	-10.801483
H	4.809184	3.502419	-10.561783
O	-10.332232	2.873102	2.335501
H	-10.181375	2.256072	1.614373

H	-9.464890	3.270041	2.607884
O	-2.025548	0.594872	7.198607
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H	-2.273860	0.019271	6.509814
O	8.872547	8.352531	-9.342647
H	8.273956	9.092111	-8.985704
H	9.004625	7.862980	-8.520475
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H	-6.116445	-2.811563	-11.041140
O	-4.615643	7.605975	-2.437302
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H	-4.511051	7.901899	-1.528188
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H	5.306265	-4.638669	-10.469231
H	6.691984	-5.090060	-10.538303
O	-5.946078	2.308189	3.520721
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H	-5.200225	2.867936	3.847532
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H	8.148642	3.838649	-2.421039
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H	-1.377434	-5.979705	-3.294931
O	6.384220	-3.935075	-7.213877
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H	6.656431	-4.722227	-6.719561
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H	6.189678	3.750184	3.372696
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H	3.117340	-8.538452	-13.807492
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O	8.566336	5.194839	-11.363532
H	8.420140	5.615977	-10.549008
H	9.512157	5.204975	-11.388213
O	-8.119061	-3.745084	-8.085958

H	-8.487568	-4.645143	-8.070572
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H	8.608557	8.323774	-6.075172
H	8.816408	6.856595	-6.454587
O	0.100701	8.691881	-5.638109
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O	-3.924911	-3.852942	-4.259929
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H	-3.685855	-2.882671	-4.106374
O	2.662987	6.837432	-0.241213
H	1.729049	6.782841	-0.431237
H	3.059368	6.822713	-1.160805
O	-7.779892	-8.856913	4.554451
H	-8.539952	-9.084943	4.008367
H	-7.088577	-9.252226	4.081947
O	1.674288	6.334837	-5.429171
H	1.562892	7.264046	-5.049494
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O	2.895349	8.374333	-11.304557
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O	2.464594	-1.881918	-10.907506
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O	1.320073	0.208914	-8.051329
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O	-1.841804	-3.639165	-14.160954
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O	5.392323	-2.727259	4.658883
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O	-6.633865	-4.695189	7.451486
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H	-4.712618	4.075974	-2.145518
O	0.584491	-6.341950	5.933704
H	0.554535	-6.481278	6.897316
H	1.390231	-5.799813	5.732591
O	0.364452	1.538286	5.193764
H	0.712067	1.520446	6.094818
H	0.486895	2.447266	4.864592
O	7.377058	-1.911913	-9.428053
H	7.288438	-2.868272	-9.677809
H	6.487318	-1.619992	-9.747848
O	-2.951913	6.774399	-7.432117
H	-3.232897	5.870625	-7.602487
H	-3.807688	7.166967	-7.240646
O	-2.087794	0.750280	-4.948068
H	-1.620130	0.698571	-5.864154
H	-3.011800	0.651066	-5.156003
O	7.440936	1.883652	-9.786296
H	7.613472	1.179356	-10.446400
H	6.802960	1.423784	-9.214032
O	2.540053	8.956829	-4.620590
H	1.654897	8.858547	-5.006184
H	2.928367	9.626461	-5.205487
O	5.461454	7.901153	1.761215
H	5.232166	6.984906	1.477700
H	5.020607	7.824559	2.625267
O	-0.016187	7.837777	-12.963169
H	-0.189428	7.847676	-12.033167
H	-0.838915	7.559715	-13.319942
O	9.857656	-1.250490	6.187258
H	9.826383	-2.223052	6.238239

H	8.935661	-1.029295	6.447001
O	-4.819030	1.141391	-6.557108
H	-5.660440	1.374681	-6.238773
H	-5.068302	0.363612	-7.074124
O	4.306151	-4.752106	-5.103303
H	4.658206	-4.657434	-4.199526
H	5.003770	-5.302324	-5.503283
O	-9.440809	9.091132	2.850257
H	-9.327874	8.172176	2.603225
H	-10.279449	8.983624	3.302641
O	-9.342034	4.996394	5.200055
H	-9.067892	5.224697	6.086709
H	-9.607586	4.025582	5.291335
O	-6.877571	7.770701	6.343319
H	-6.804749	8.353459	7.058916
H	-7.839538	7.826245	6.151604
O	-7.353254	-6.047533	4.898859
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H	-6.618237	-6.563416	4.448901
O	1.578735	-0.007702	-5.129223
H	1.438481	0.407491	-5.959585
H	2.317134	-0.599417	-5.311999
O	6.537663	8.733496	-1.338893
H	7.460898	8.810887	-1.415157
H	6.499118	7.767526	-1.262718
O	-5.983121	4.410849	6.409270
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H	5.130712	-7.952023	-11.141686
H	5.918136	-7.351101	-9.915377
O	5.866402	10.002412	-12.062726
H	6.795193	9.853854	-11.955113
H	5.577757	9.077827	-11.858732
O	7.021786	-7.926558	-3.176236
H	6.448343	-8.654915	-2.837352
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O	3.398512	6.784535	-3.023539
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O	-6.125083	5.115304	-13.006557
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O	7.189053	3.436819	-7.463778
H	7.435658	2.994281	-8.317897
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O	6.670547	1.333082	-0.820601

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H	5.934500	1.881010	-0.587361
O	-1.559352	1.674493	-10.993275
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H	-2.343912	1.882618	-11.548013
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H	8.232227	-7.666524	2.495795
O	-9.781852	7.982877	6.080983
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H	-6.960589	-6.264125	-2.422186
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H	9.307137	-4.386588	6.518836
O	7.197206	-0.563923	-5.110697
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H	7.156084	0.341308	-4.815606
O	6.780619	-3.707919	-13.545993
H	7.644302	-3.243016	-13.399975
H	6.793880	-4.483279	-12.951214
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H	8.968175	2.597319	-4.467642
O	-2.049107	5.314009	-13.282851
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O	-1.166896	3.209593	-3.839291
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H	-0.857304	2.804248	-2.986093
O	6.213799	-6.678682	5.966519
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H	5.798659	-7.518012	6.214207
O	-0.938627	-8.553759	-12.002984
H	-1.355067	-8.630558	-12.911662
H	-0.046555	-8.332855	-12.234666
O	0.866687	-3.756540	-13.644814
H	0.967231	-2.900870	-13.990630
H	1.800280	-4.005374	-13.768816
O	-2.699003	-2.892045	-6.612094
H	-3.630943	-2.927989	-6.525732
H	-2.508344	-3.314874	-7.425756
O	-6.314644	7.832721	-9.771412
H	-7.296340	7.933229	-9.598401
H	-6.017086	8.066951	-8.901548

O	-0.564246	0.586359	1.752484
H	-0.097196	1.267840	1.308959
H	-1.144006	0.205237	1.110050
O	2.565882	-6.081341	-1.906374
H	2.545875	-7.045510	-2.029247
H	1.589084	-5.887381	-1.901904
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H	-4.176753	-6.260195	-10.745258
H	-4.641348	-6.343047	-12.229403
O	-4.013790	-4.386836	6.282898
H	-3.270284	-4.361648	6.978861
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O	8.655830	4.186049	-14.001045
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O	-7.321482	2.604315	-1.454317
H	-6.676859	2.081987	-1.940932
H	-7.576169	2.048883	-0.752087
O	-7.339650	-1.731514	-0.712819
H	-7.078075	-2.427823	-0.082480
H	-8.254851	-2.028588	-0.935379
O	9.899068	2.517905	-10.766676
H	9.008677	2.912264	-10.748295
H	9.860543	1.849876	-10.078583
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H	-3.721783	3.783974	-8.025018
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H	-8.955971	-6.682361	-7.441785
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O	-9.289178	6.121691	-10.657396
H	-9.451288	7.035903	-10.721032
H	-8.826843	6.143845	-9.813834
O	-3.406298	-0.938057	5.009847
H	-3.534143	-0.094014	4.519030
H	-4.353282	-1.281508	5.131033
O	-2.922351	-7.583321	5.892743
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O	3.356703	-4.495226	-11.020082
H	2.803380	-4.737251	-10.218676
H	2.961252	-4.795475	-11.833376