Electronic Supplementary Information for Dalton Transactions

Electronic Supplementary information

Tetraalkylphosphonium polyoxometalates: Electroactive, "task-specific" ionic liquids

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Crystallographic Report

X-ray diffraction data for $[(n\text{-}C_4H_9)_4N]_2W_6O_{19}$ were collected at 100 K using a Bruker SMART APEX diffractometer at the University of Notre Dame (λ = 0.71073 Å). A sphere of data was collected using frame-widths of 0.3º in ω. Data were corrected for Lorentz and polarization using the Bruker program SAINT, absorption corrections were performed using the Bruker program XPREP (version 5.1, 1997), and the structure was solved by direct methods and refined on the basis of F^2 for all unique reflections using the Bruker SHELXTL system of programs (v. 6.10). Refinement of the structure was straightforward: 86,257 total reflections of which all 21,989 unique reflections were used in the refinement, 71.81º maximum 2-theta, $R1$ = 0.0272, $wR2$ = 0.0669, GOF = 1.132, μ = 14.57, cell weight = 3783.92, space group P-1, triclinic, a = 11.5863(3) Å, b = 12.5910(4) Å, c = 19.0145(6) Å, α = 78.832(2)º, β = 74.601(2)º, γ = 62.805(1)º, V = 2370.21(12) Å^3, Z = 2. The unit cell and parameters as well as the individual W-O_6 octahedra as well as the framework -W-O-W- connectivity are in agreement with previously reported structures.[1-4] The crystallographic data in CIF format are available on line. Details about the crystal data and structure refinement are presented in Table S1.

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In the molecular structure of $[(n\text{-}C_4H_9)_4N]_2W_6O_{19}$ there are two independent $[W_6O_{19}]^{2-}$ anions lying on inversion centers as well as two independent $n\text{-}Bu_4N^+$ cations in the asymmetric unit. These are shown in Figures S1 and S2, respectively, in which all atoms, except H, are labelled. In Figure S1, the W^{6+} ions are shown as yellow thermal ellipsoids and the O^{2-} ions are shown as red thermal ellipsoids. The oxygen atoms O1 and O11 are at the centers of each hexatungstate unit comprising atoms W1–W3, O1–O10, and W4–W6, O11–O20, respectively. The diameter of the essentially spherical Lindqvist hexatungstate cluster as measured by the 6 pairs of opposite, terminal O-O interatomic distances (O2–O2, O8–O8, O10–O10, O12–O12, O18–O18, O20–O20) is 8.08±0.02 Å. The interatomic distances to the neighboring atoms about the W1, W2, W3, W4, W5, and W6 sites within 0–5 Å are provided in Table S2.

In Figure S2, the two N atoms (N1 and N2) are shown as blue thermal ellipsoids and the C atoms (C1–C32) are shown as black thermal ellipsoids. The H atoms are indicated by the pink ends of the C–H stick bonds. To minimize congestion and overlap in the display, the H atom labels are not shown.

The packing diagram is shown in Figure S3, wherein all the atoms are rendered as described above, and where the unit cell is shown in blue.

Figure S1.

Figure S2.

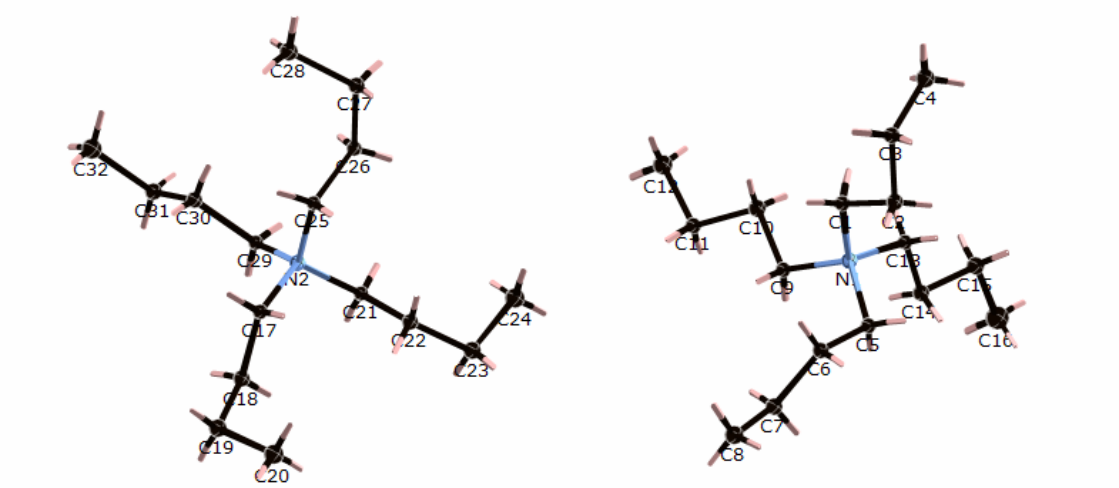

Figure S3.

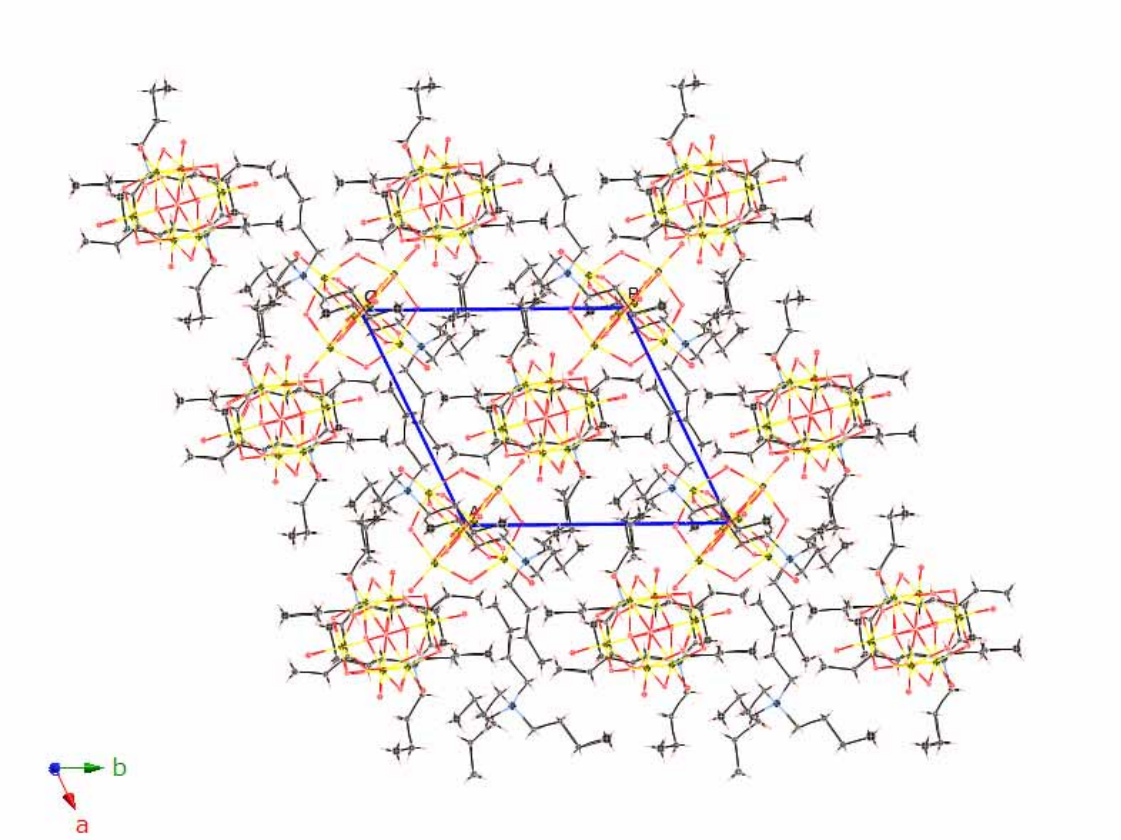

Table S1.

Crystal data and structure refinement

	data for $[(n\text{-}C_4H_9)_4N]_2W_6O_{19}$
Chemical formula	$[(n\text{-}C_4H_9)_4N]_2W_6O_{19}$
Formula weight	1891.96
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	triclinic, P-1
Unit cell dimensions	a = 11.5863(3)Å α = 78.832(2)° b = 12.5910(4)Å β = 74.601(2)° c = 19.0145(6)Å γ = 62.8050(10)°
Volume	2370.21(12) $Å^3$
Z, Calculated density	2, 2.651 Mg/m^3
Absorption coefficient, μ	14.570 mm^{-1}
F(000)	1748
Crystal size	0.140 x 0.110 x 0.080 mm
Theta range for data collection	1.11 to 35.90°
Limiting indices	-19<=h<=19, -20<=k<=20, -31<=l<=31
Reflections collected / unique	86257 / 21989 [R(int) = 0.0654]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	21989 / 72 / 751
Goodness-of-fit on F^2	1.132
Final R indices [I>2sigma(I)]	R1 = 0.0272, wR2 = 0.0641
R indices (all data)	R1 = 0.0320, wR2 = 0.0669

Table S2.

Bond search from target site: W1:
... Found 60 atoms within 0.00 - 5.00 Å of this site.

	Label	Elmt	Fractional Coordinates x	y	z	Orthogonal Coordinates xor[Å]	yor[Å]	zor[Å]	Bond Distance d[Å]	d/(rA+rB)
TARG.	W1	W	0.9781	0.0389	0.1187	-10.131	-7.085	0.072		
1.	O2	O	0.9582	0.0677	0.2063	-11.451	-6.383	-0.754	1.7071	0.66
2.	O6	O	1.1040	0.0971	0.0623	-10.935	-8.246	1.361	1.9123	0.74
3.	O4	O	1.1164	-0.1211	0.1116	-9.696	-8.629	-0.980	1.9191	0.74
4.	O5	O	0.8435	0.1823	0.0800	-9.809	-5.856	1.535	1.9379	0.75
5.	O3	O	0.8557	-0.0319	0.1286	-8.595	-6.231	-0.765	1.9465	0.75
6.	O1	O	1.0000	0.0000	0.0000	-8.304	-7.993	1.185	2.3253	0.89
7.	W3	W	1.1705	-0.1880	0.0186	-8.232	-9.728	-0.359	3.2837	1.93
8.	W3	W	0.8295	0.1880	-0.0186	-8.376	-6.258	2.730	3.2913	1.94
9.	W2	W	1.1544	0.0809	-0.0423	-9.749	-9.251	2.526	3.2955	1.94
10.	W2	W	0.8456	-0.0809	0.0423	-6.858	-6.735	-0.155	3.3001	1.94
11.	H3	H	0.9640	-0.2080	0.2240	-9.185	-7.027	-3.196	3.4027	17.01
12.	H44	H	1.0224	0.2550	0.1810	-13.372	-6.562	1.143	3.4527	17.26
13.	O7	O	1.2599	-0.0858	-0.0164	-9.437	-10.374	0.991	3.4848	1.34
14.	H50	H	0.6570	0.2250	0.2020	-10.351	-3.604	0.218	3.4904	17.45
15.	H62	H	1.3070	-0.0700	0.1390	-12.134	-9.878	-0.663	3.5144	17.57
16.	O9	O	0.9868	0.2159	-0.0483	-9.529	-7.604	3.495	3.5148	1.35
17.	O9	O	1.0132	-0.2160	0.0483	-7.079	-8.382	-1.124	3.5262	1.36
18.	H39	H	0.8760	0.3520	0.0920	-11.821	-5.625	2.810	3.5330	17.66
19.	O7	O	0.7401	0.0858	0.0164	-7.170	-5.612	1.380	3.5569	1.37
20.	H10	H	0.7720	-0.0380	0.2790	-9.933	-4.771	-2.693	3.6105	18.05
21.	H28	H	0.9780	-0.1080	0.3030	-11.327	-6.465	-3.301	3.6321	18.16
22.	H59	H	1.2310	-0.1910	0.2330	-11.685	-9.070	-2.848	3.8576	19.29
23.	H61	H	1.2700	-0.0180	0.2130	-13.337	-9.055	-1.160	3.9594	19.80
24.	C28	C	1.3340	-0.0876	0.1850	-12.833	-9.891	-1.318	4.1365	7.13
25.	H49	H	0.7350	0.3470	0.2260	-12.465	-3.793	1.018	4.1444	20.72
26.	H47	H	0.6700	0.3890	0.1140	-10.759	-3.768	2.606	4.2212	21.11
27.	C2	C	0.9165	-0.2585	0.2432	-8.588	-6.671	-3.890	4.2715	7.36
28.	C23	C	0.6084	0.2689	0.2454	-10.958	-2.873	0.004	4.2925	7.40
29.	H30	H	0.8600	0.0600	0.3540	-12.616	-4.827	-2.680	4.3406	21.70
30.	H32	H	1.0800	0.0150	0.3280	-13.664	-6.837	-2.477	4.3627	21.81
31.	C20	C	1.0387	0.3244	0.1789	-14.123	-6.529	1.751	4.3655	7.53
32.	H51	H	0.6360	0.2260	0.2890	-11.394	-2.968	-0.828	4.3993	22.00
33.	C18	C	0.8900	0.4227	0.0840	-12.482	-5.602	3.496	4.4098	7.60
34.	H41	H	1.0990	0.3370	0.0680	-13.200	-7.574	3.236	4.4350	22.17
35.	H4	H	0.8360	-0.2380	0.2250	-7.857	-6.074	-3.603	4.4384	22.19
36.	C27	C	1.3206	-0.1984	0.2284	-12.296	-9.830	-2.747	4.4911	7.74
37.	C13	C	0.9450	-0.1193	0.3554	-11.676	-5.949	-4.052	4.5471	7.84
38.	C5	C	0.7260	-0.0571	0.3268	-10.038	-4.195	-3.468	4.5703	7.88
39.	O5	O	1.1565	-0.1823	-0.0800	-6.798	-10.130	0.836	4.5795	1.76
40.	O3	O	1.1443	0.0319	-0.1286	-8.012	-9.755	3.136	4.5843	1.76
41.	O6	O	0.8960	-0.0971	-0.0623	-5.672	-7.740	1.010	4.6037	1.77
42.	O4	O	0.8836	0.1211	-0.1116	-6.911	-7.357	3.351	4.6045	1.77
43.	C19	C	1.0238	0.3889	0.1021	-13.531	-6.660	3.166	4.6162	7.96
44.	H58	H	1.3700	-0.2960	0.1430	-10.614	-10.927	-2.472	4.6335	23.17
45.	O10	O	0.7041	0.3273	-0.0310	-8.456	-4.972	3.860	4.6498	1.79
46.	C22	C	0.6401	0.3784	0.2262	-11.971	-2.954	1.158	4.6498	8.02
47.	W1	W	1.0219	-0.0389	-0.1187	-6.476	-8.901	2.299	4.6505	2.74
48.	O8	O	0.7344	-0.1418	0.0742	-5.812	-5.829	-1.159	4.6637	1.79
49.	O10	O	1.2959	-0.3273	0.0310	-8.151	-11.014	-1.489	4.6687	1.80
50.	H7	H	1.1850	-0.3750	0.1750	-8.788	-9.475	-3.711	4.6724	23.36
51.	O8	O	1.2656	0.1418	-0.0742	-10.795	-10.157	3.530	4.6734	1.80
52.	H70	H	1.3310	0.1450	0.0890	-13.635	-9.798	1.703	4.7221	23.61
53.	H40	H	0.8980	0.4470	0.0327	-12.062	-5.880	4.309	4.8097	24.05
54.	H11	H	0.7000	0.0070	0.3550	-10.809	-3.675	-3.312	4.8507	24.25
55.	H43	H	0.9700	0.3750	0.2160	-14.537	-5.654	1.642	4.8911	24.46
56.	C21	C	0.6123	0.4392	0.1517	-11.270	-2.979	2.500	4.9042	8.46
57.	H45	H	1.1240	0.3090	0.1860	-14.786	-7.212	1.643	4.9147	24.57
58.	C14	C	0.9065	-0.0040	0.3881	-12.881	-5.176	-3.548	4.9300	8.50
59.	H5	H	0.9890	-0.3650	0.1617	-7.069	-7.955	-3.705	4.9397	24.70
60.	H63	H	1.4210	-0.0930	0.1780	-13.408	-10.638	-1.176	4.9921	24.96

Bond search from target site: W2:
... Found 53 atoms within 0.00 - 5.00 Å of this site.

	Label	Elmt	Fractional Coordinates x	y	z	Orthogonal Coordinates xor[Å]	yor[Å]	zor[Å]	Bond Distance d[Å]	d/(rA+rB)
TARG.	W2	W	0.8456	0.9191	0.0423	-16.144	-4.225	7.969		
1.	O8	O	0.7344	0.8582	0.0742	-15.098	-3.318	6.965	1.7099	0.66
2.	O3	O	0.8557	0.9681	0.1286	-17.882	-3.720	7.359	1.9096	0.73
3.	O9	O	1.0132	0.7840	0.0483	-16.365	-5.871	7.000	1.9237	0.74
4.	O7	O	0.7401	1.0858	0.0164	-16.456	-3.102	9.504	1.9273	0.74
5.	O6	O	0.8960	0.9029	-0.0623	-14.958	-5.229	9.134	1.9419	0.75
6.	O1	O	1.0000	1.0000	0.0000	-17.590	-5.482	9.309	2.3385	0.90
7.	W3	W	0.8295	1.1880	-0.0186	-17.662	-3.747	10.854	3.2943	1.94
8.	W1	W	1.0219	0.9611	-0.1187	-15.762	-6.391	10.423	3.2955	1.94
9.	W3	W	1.1705	0.8120	0.0186	-17.518	-7.217	7.765	3.2994	1.94
10.	W1	W	0.9781	1.0389	0.1187	-19.418	-4.574	8.196	3.3001	1.94
11.	O4	O	1.1164	0.8789	0.1116	-18.982	-6.119	7.144	3.5109	1.35
12.	O5	O	0.8435	1.1823	0.0800	-19.095	-3.345	9.659	3.5125	1.35
13.	O5	O	1.1565	0.8177	-0.0800	-16.084	-7.620	8.960	3.5373	1.36
14.	O4	O	0.8836	1.1211	-0.1116	-16.197	-4.846	11.475	3.5611	1.37
15.	H72	H	0.4880	1.0900	0.0800	-15.285	-0.735	8.487	3.6305	18.15
16.	H4	H	0.8360	0.7620	0.2250	-17.143	-3.563	4.521	3.6511	18.26
17.	H5	H	0.9890	0.6350	0.1617	-16.355	-5.444	4.419	3.7602	18.80
18.	H3	H	0.9640	0.7920	0.2240	-18.471	-4.517	4.928	3.8408	19.20
19.	H67	H	0.6830	0.7210	0.0220	-12.672	-3.531	6.407	3.8696	19.35
20.	H41	H	0.9010	0.6630	-0.0680	-12.694	-5.901	7.259	3.9015	19.51
21.	H70	H	0.6690	0.8550	-0.0890	-12.258	-3.678	8.792	4.0090	20.05
22.	H62	H	0.6930	1.0700	-0.1390	-13.760	-3.598	11.158	4.0306	20.15
23.	C2	C	0.9165	0.7415	0.2432	-17.874	-4.161	4.234	4.1170	7.10
24.	H39	H	1.1240	0.6480	-0.0920	-14.073	-7.850	7.685	4.1852	20.93
25.	H38	H	0.7880	0.6000	0.1110	-13.657	-4.197	4.496	4.2722	21.36
26.	H10	H	0.7720	0.9620	0.2790	-19.219	-2.260	5.431	4.4453	22.23
27.	H40	H	1.1020	0.5530	-0.0327	-13.832	-7.595	6.186	4.4597	22.30
28.	C3	C	1.0021	0.6188	0.2118	-17.010	-5.321	3.710	4.4825	7.73
29.	C32	C	0.4074	1.1523	0.1003	-15.477	0.174	8.658	4.5020	7.76
30.	H68	H	0.4810	1.2770	0.0690	-16.811	-0.269	10.128	4.5557	22.78
31.	O6	O	1.1040	1.0971	0.0623	-20.221	-5.736	9.485	4.6047	1.77
32.	O7	O	1.2599	0.9142	-0.0164	-18.724	-7.863	9.115	4.6048	1.77
33.	O9	O	0.9868	1.2160	-0.0483	-18.815	-5.093	11.619	4.6054	1.77
34.	O3	O	1.1443	1.0319	-0.1286	-17.298	-7.245	11.260	4.6132	1.77
35.	C19	C	0.9762	0.6111	-0.1021	-12.362	-6.816	7.329	4.6284	7.98
36.	O2	O	0.9582	1.0677	0.2063	-20.737	-3.873	7.370	4.6455	1.79
37.	H12	H	0.5860	0.9520	0.2770	-17.554	-0.810	5.153	4.6460	23.23
38.	H71	H	0.4060	1.1420	0.1490	-16.046	0.420	7.997	4.6460	23.23
39.	C18	C	1.1100	0.5773	-0.0840	-13.411	-7.873	6.999	4.6605	8.04
40.	O10	O	1.2959	0.6727	0.0310	-17.438	-8.503	6.635	4.6649	1.79
41.	O10	O	0.7041	1.3273	-0.0310	-17.742	-2.461	11.984	4.6667	1.79
42.	O2	O	1.0418	0.9323	-0.2063	-14.442	-7.092	11.249	4.6767	1.80
43.	W2	W	1.1544	1.0809	-0.0423	-19.036	-6.740	10.650	4.6769	2.75
44.	H50	H	0.6570	1.2250	0.2020	-19.637	-1.093	8.342	4.7058	23.53
45.	H44	H	0.9776	0.7450	-0.1810	-12.521	-6.913	9.352	4.7184	23.59
46.	H66	H	0.4740	1.2350	-0.0420	-14.821	-0.913	11.092	4.7398	23.70
47.	C30	C	0.6078	0.7097	0.0156	-11.854	-2.993	6.301	4.7646	8.21
48.	H56	H	0.5770	0.7120	0.1540	-13.542	-1.999	4.647	4.7706	23.85
49.	H7	H	1.1850	0.6250	0.1750	-18.075	-6.965	4.413	4.8875	24.44
50.	H66	H	0.5260	0.7650	0.0420	-12.055	-2.059	6.342	4.9050	24.53
51.	C32	C	0.5926	0.8477	-0.1003	-11.399	-3.146	8.775	4.9320	8.50
52.	H63	H	0.4210	0.9070	0.1780	-14.391	-0.134	5.762	4.9674	24.84
53.	C28	C	0.6660	1.0876	-0.1850	-13.060	-3.584	11.813	4.9695	8.57

Bond search from target site: W3:
... Found 57 atoms within 0.00 - 5.00 Å of this site.

	Label	Elmt	Fractional Coordinates x	y	z	Orthogonal Coordinates xor[Å]	yor[Å]	zor[Å]	Bond Distance d[Å]	d/(rA+rB)
TARG.	W3	W	0.8295	0.1880	0.9814	-22.267	-0.900	-9.097		
1.	O10	O	0.7041	0.3273	0.9690	-22.347	0.386	-7.967	1.7137	0.66
2.	O5	O	0.8435	0.1823	1.0800	-23.700	-0.497	-10.292	1.9091	0.73
3.	O7	O	0.7401	0.0858	1.0164	-21.061	-0.254	-10.446	1.9215	0.74
4.	O9	O	0.9868	0.2159	0.9517	-23.420	-2.246	-8.331	1.9306	0.74
5.	O4	O	0.8836	0.1211	0.8884	-20.802	-1.998	-8.475	1.9335	0.74
6.	O1	O	1.0000	0.0000	1.0000	-22.195	-2.635	-10.641	2.3240	0.89
7.	W1	W	1.0219	-0.0389	0.8813	-20.367	-3.543	-9.527	3.2837	1.93
8.	W1	W	0.9781	0.0389	1.1187	-24.023	-1.726	-11.755	3.2913	1.94
9.	W2	W	0.8456	-0.0809	1.0423	-20.749	-1.377	-11.981	3.2943	1.94
10.	W2	W	1.1544	0.0809	0.9577	-23.641	-3.893	-9.301	3.2994	1.94
11.	H58	H	0.6300	0.2960	0.8570	-19.885	0.300	-6.984	3.4024	17.01
12.	H7	H	0.8150	0.3750	0.8250	-21.710	-1.152	-5.744	3.4077	17.04
13.	H47	H	0.6700	0.3890	1.1140	-24.651	1.590	-9.220	3.4494	17.25
14.	O3	O	0.8557	-0.0319	1.1286	-22.487	-0.872	-12.592	3.5021	1.35
15.	H39	H	0.8760	0.3520	1.0920	-25.712	-0.267	-9.017	3.5036	17.52
16.	O6	O	1.1040	0.0971	1.0623	-24.826	-2.888	-10.466	3.5184	1.35
17.	O6	O	0.8960	-0.0971	0.9377	-19.564	-2.381	-10.816	3.5299	1.36
18.	O3	O	1.1443	0.0319	0.8714	-21.903	-4.397	-8.691	3.5395	1.36
19.	H68	H	0.4810	0.2770	1.0690	-21.416	2.579	-9.822	3.6538	18.27
20.	H64	H	0.6740	0.5230	1.0210	-24.636	1.397	-7.027	3.8948	19.47
21.	H62	H	0.6930	0.0700	0.8610	-18.365	-0.750	-8.793	3.9168	19.58
22.	H65	H	0.4710	0.4160	0.9490	-20.957	2.365	-7.286	3.9563	19.78
23.	H5	H	1.0110	0.3650	0.8383	-23.430	-2.673	-5.751	3.9613	19.81
24.	H66	H	0.4740	0.2350	0.9580	-19.426	1.935	-8.859	4.0199	20.10
25.	H40	H	0.8980	0.4470	1.0327	-25.953	-0.522	-7.517	4.0280	20.14
26.	H3	H	1.0360	0.2080	0.7760	-21.314	-3.601	-6.260	4.0315	20.16
27.	H50	H	0.6570	0.2250	1.2020	-24.242	1.754	-11.609	4.1540	20.77
28.	C18	C	0.8900	0.4227	1.0840	-26.374	-0.244	-8.331	4.2286	7.29
29.	C4	C	0.8509	0.4253	0.7908	-22.000	-1.496	-4.889	4.2585	7.34
30.	H59	H	0.7690	0.1910	0.7670	-18.814	-1.557	-6.608	4.3072	21.54
31.	C26	C	0.5982	0.3133	0.8118	-19.154	0.355	-6.347	4.3395	7.48
32.	C21	C	0.6123	0.4392	1.1517	-25.162	2.380	-9.327	4.3801	7.55
33.	C31	C	0.4023	0.2732	1.0643	-20.662	3.173	-9.890	4.4490	7.67
34.	C3	C	0.9979	0.3812	0.7882	-22.775	-2.796	-5.042	4.5050	7.77
35.	H72	H	0.4880	0.0900	1.0800	-19.891	2.112	-11.463	4.5077	22.54
36.	H8	H	0.7950	0.5010	0.8080	-22.478	-0.767	-4.543	4.5601	22.80
37.	O9	O	1.0132	-0.2160	1.0483	-20.970	-3.024	-12.951	4.5879	1.76
38.	O5	O	1.1565	-0.1823	0.9200	-20.690	-4.772	-10.991	4.5903	1.77
39.	O7	O	1.2599	-0.0858	0.9836	-23.329	-5.015	-10.836	4.5925	1.77
40.	H57	H	0.6260	0.3750	0.7860	-19.599	0.149	-5.507	4.5939	22.97
41.	O4	O	1.1164	-0.1211	1.1116	-23.588	-3.271	-12.807	4.5972	1.77
42.	C30	C	0.3922	0.2903	0.9844	-19.627	2.869	-8.819	4.6094	7.95
43.	W3	W	1.1705	-0.1880	1.0186	-22.123	-4.370	-12.186	4.6480	2.73
44.	O2	O	0.9582	0.0677	1.2063	-25.342	-1.025	-12.581	4.6488	1.79
45.	O8	O	1.2656	0.1418	0.9258	-24.687	-4.799	-8.297	4.6584	1.79
46.	O2	O	1.0418	-0.0677	0.7937	-19.048	-4.244	-8.702	4.6590	1.79
47.	O8	O	0.7344	-0.1418	1.0742	-19.703	-0.470	-12.985	4.6774	1.80
48.	C2	C	1.0835	0.2585	0.7568	-21.910	-3.956	-5.566	4.6836	8.08
49.	C28	C	0.6660	0.0876	0.8150	-17.665	-0.736	-8.138	4.7036	8.11
50.	C29	C	0.3885	0.4120	0.9507	-20.259	3.023	-7.437	4.7095	8.12
51.	H46	H	0.5200	0.4650	1.1510	-24.625	3.178	-9.218	4.7123	23.56
52.	C27	C	0.6794	0.1984	0.7716	-18.202	-0.798	-6.708	4.7155	8.13
53.	C29	C	0.6115	0.5880	1.0493	-25.113	2.211	-6.907	4.7508	8.19
54.	H65	H	0.5290	0.5840	1.0510	-24.416	2.869	-7.058	4.7935	23.97
55.	H9	H	0.8430	0.4180	0.7450	-21.231	-1.697	-4.416	4.8602	24.30
56.	H4	H	1.1640	0.2380	0.7750	-22.641	-4.554	-5.852	4.9008	24.50
57.	C32	C	0.4074	0.1523	1.1003	-20.082	3.022	-11.293	4.9974	8.62

Bond search from target site: W4:
... Found 58 atoms within 0.00 - 5.00 Å of this site.

	Label	Elmt	Fractional Coordinates x	y	z	Orthogonal Coordinates xor[Å]	yor[Å]	zor[Å]	Bond Distance d[Å]	d/(rA+rB)
TARG.	W4	W	0.4454	0.6917	0.5280	-17.455	1.006	-0.097		
1.	O12	O	0.4079	0.8319	0.5490	-18.739	1.770	0.748	1.7166	0.66
2.	O15	O	0.3232	0.7182	0.4679	-15.853	1.727	0.683	1.9223	0.74
3.	O16	O	0.5785	0.6701	0.4393	-17.129	-0.587	0.934	1.9253	0.74
4.	O13	O	0.3350	0.6373	0.6064	-17.123	2.172	-1.597	1.9287	0.74
5.	O14	O	0.5892	0.5882	0.5775	-18.377	-0.138	-1.352	1.9325	0.74
6.	O11	O	0.5000	0.5000	0.5000	-15.741	-0.062	-1.259	2.3305	0.90
7.	W5	W	0.3494	0.4796	0.6041	-15.746	1.649	-2.834	3.2902	1.94
8.	W5	W	0.6506	0.5204	0.3959	-15.735	-1.773	0.316	3.2939	1.94
9.	W6	W	0.3331	0.5803	0.4324	-14.162	1.112	-0.005	3.2962	1.94
10.	W6	W	0.6669	0.4197	0.5676	-17.319	-1.236	-2.512	3.2985	1.94
11.	H18	H	0.3930	0.8760	0.3730	-16.579	1.057	3.171	3.3835	16.92
12.	O19	O	0.4875	0.5825	0.3621	-14.487	-0.494	1.028	3.5108	1.35
13.	O17	O	0.2457	0.5480	0.5291	-14.479	2.247	-1.514	3.5229	1.35
14.	O17	O	0.7543	0.4520	0.4709	-17.003	-2.371	-1.003	3.5255	1.36
15.	O19	O	0.5125	0.4175	0.6379	-16.994	0.370	-3.545	3.5365	1.36
16.	H51	H	0.3640	0.7740	0.7110	-20.087	2.844	-1.689	3.5830	17.92
17.	H23	H	0.7240	0.7030	0.5710	-20.472	-0.962	-0.184	3.6029	18.01
18.	H15	H	0.5080	0.9420	0.4300	-18.939	0.609	3.170	3.6093	18.05
19.	H20	H	0.7030	0.8030	0.4460	-19.490	-1.213	2.082	3.7162	18.58
20.	H34	H	0.0600	0.8550	0.5482	-16.053	4.604	0.534	3.9133	19.57
21.	H30	H	0.1400	0.9400	0.6460	-18.865	4.702	0.162	3.9649	19.82
22.	H17	H	0.2870	1.0000	0.4070	-17.323	2.397	3.651	3.9996	20.00
23.	C8	C	0.3679	0.9633	0.3715	-17.161	1.468	3.868	4.0027	6.90
24.	H48	H	0.4020	0.5650	0.7390	-18.850	2.165	-3.673	4.0104	20.05
25.	H52	H	0.5890	0.6420	0.7080	-20.688	0.698	-2.459	4.0157	20.08
26.	H35	H	0.0590	0.7990	0.6320	-16.689	4.921	-0.913	4.0721	20.36
27.	H31	H	0.1240	1.0130	0.5608	-18.227	4.557	1.744	4.0737	20.37
28.	H11	H	0.3000	0.9930	0.6450	-20.672	3.551	0.795	4.1978	20.99
29.	C7	C	0.4850	0.9776	0.3825	-18.419	0.627	3.993	4.2188	7.27
30.	C23	C	0.3916	0.7311	0.7546	-20.523	2.749	-2.521	4.2809	7.38
31.	C14	C	0.0935	1.0040	0.6119	-18.600	5.052	1.031	4.3534	7.51
32.	H13	H	0.6360	0.8370	0.3300	-17.638	-1.214	3.651	4.3594	21.80
33.	C16	C	0.0086	0.8610	0.5962	-16.349	5.288	-0.046	4.4227	7.63
34.	H14	H	0.5320	0.9390	0.6250	-21.819	1.454	0.867	4.4916	22.46
35.	C22	C	0.3599	0.6216	0.7738	-19.510	2.830	-3.675	4.5123	7.78
36.	C24	C	0.5380	0.7003	0.7437	-21.301	1.443	-2.469	4.5397	7.83
37.	C11	C	0.8044	0.7132	0.5670	-21.179	-1.601	0.042	4.5474	7.84
38.	O14	O	0.4108	0.4118	0.4225	-13.104	0.014	-1.165	4.5887	1.76
39.	O15	O	0.6768	0.2818	0.5321	-15.628	-1.851	-3.201	4.5975	1.77
40.	O13	O	0.6650	0.3627	0.3936	-14.358	-2.296	-0.920	4.6015	1.77
41.	O16	O	0.4215	0.3299	0.5607	-14.352	0.463	-3.451	4.6022	1.77
42.	C9	C	0.7766	0.8200	0.4434	-20.223	-1.773	2.338	4.6159	7.96
43.	H49	H	0.2650	0.6530	0.7740	-19.016	3.669	-3.535	4.6204	23.10
44.	O18	O	0.7876	0.3624	0.6180	-18.490	-2.074	-3.431	4.6554	1.79
45.	W4	W	0.5546	0.3083	0.4720	-14.026	-1.130	-2.421	4.6609	2.74
46.	O20	O	0.2405	0.4632	0.6820	-15.772	2.895	-4.018	4.6666	1.79
47.	H19	H	0.2640	1.1070	0.5320	-19.862	3.520	3.014	4.6680	23.34
48.	O20	O	0.7595	0.5368	0.3180	-15.709	-3.019	1.501	4.6692	1.80
49.	O18	O	0.2124	0.6376	0.3820	-12.991	1.950	0.914	4.6733	1.80
50.	H53	H	0.5550	0.7700	0.7320	-21.927	1.419	-1.744	4.7836	23.92
51.	H33	H	0.0850	0.9570	0.4090	-15.274	3.915	3.038	4.8008	24.00
52.	C6	C	0.6094	0.9182	0.3246	-18.096	-0.826	4.343	4.8452	8.35
53.	H19	H	0.7360	0.8930	0.4680	-20.905	-1.133	2.592	4.8689	24.34
54.	H16	H	0.3550	0.9970	0.3219	-16.678	1.390	4.713	4.8877	24.44
55.	H21	H	0.9050	0.6450	0.4680	-20.006	-3.107	0.778	4.9173	24.59
56.	H1	H	0.8440	0.6810	0.3450	-18.125	-3.188	2.453	4.9531	24.77
57.	H24	H	0.7770	0.7870	0.5880	-21.928	-1.084	0.361	4.9581	24.79
58.	C10	C	0.8733	0.7209	0.4873	-20.715	-2.559	1.129	4.9837	8.59

Bond search from target site: W5:
... Found 56 atoms within 0.00 - 5.00 Å of this site.

	Label	Elmt	Fractional Coordinates x	y	z	Orthogonal Coordinates xor[Å]	yor[Å]	zor[Å]	Bond Distance d[Å]	d/(rA+rB)
TARG.	W5	W	0.6506	0.5204	0.3959	-15.735	-1.773	0.316		
1.	O20	O	0.7595	0.5368	0.3180	-15.709	-3.019	1.501	1.7195	0.66
2.	O19	O	0.4875	0.5825	0.3621	-14.487	-0.494	1.028	1.9232	0.74
3.	O13	O	0.6650	0.3627	0.3936	-14.358	-2.296	-0.920	1.9235	0.74
4.	O17	O	0.7543	0.4520	0.4709	-17.003	-2.371	-1.003	1.9251	0.74
5.	O16	O	0.5785	0.6701	0.4393	-17.129	-0.587	0.934	1.9314	0.74
6.	O11	O	0.5000	0.5000	0.5000	-15.741	-0.062	-1.259	2.3252	0.89
7.	H48	H	0.5980	0.4350	0.2610	-12.631	-2.289	1.156	3.2571	16.29
8.	W6	W	0.6669	0.4197	0.5676	-17.319	-1.236	-2.512	3.2861	1.93
9.	W4	W	0.5546	0.3083	0.4720	-14.026	-1.130	-2.421	3.2902	1.94
10.	W4	W	0.4454	0.6917	0.5280	-17.455	1.006	-0.097	3.2939	1.94
11.	W6	W	0.3331	0.5803	0.4324	-14.162	1.112	-0.005	3.3012	1.94
12.	H55	H	0.5760	0.6260	0.2250	-13.722	-1.827	3.107	3.4420	17.21
13.	H1	H	0.8440	0.6810	0.3450	-18.125	-3.188	2.453	3.5039	17.52
14.	O14	O	0.4108	0.4118	0.4225	-13.104	0.014	-1.165	3.5083	1.35
15.	O15	O	0.6768	0.2818	0.5321	-15.628	-1.851	-3.201	3.5193	1.35
16.	O15	O	0.3232	0.7182	0.4679	-15.853	1.727	0.683	3.5210	1.35
17.	O14	O	0.5892	0.5882	0.5775	-18.377	-0.138	-1.352	3.5262	1.36
18.	H27	H	1.0260	0.3840	0.3880	-17.475	-5.158	-0.253	3.8485	19.24
19.	H13	H	0.6360	0.8370	0.3300	-17.638	-1.214	3.651	3.8798	19.40
20.	H49	H	0.7350	0.3470	0.2260	-12.465	-3.793	1.018	3.9072	19.54
21.	H35	H	0.9410	0.2010	0.3680	-14.792	-5.045	-1.604	3.9094	19.55
22.	H37	H	0.7830	0.5090	0.1799	-13.727	-4.017	2.936	3.9909	19.95
23.	C22	C	0.6401	0.3784	0.2262	-11.971	-2.954	1.158	4.0343	6.96
24.	H18	H	0.3930	0.8760	0.3730	-16.579	1.057	3.171	4.1071	20.54
25.	H6	H	0.9570	0.5680	0.2390	-16.541	-4.943	2.922	4.1821	20.91
26.	H20	H	0.7030	0.8030	0.4460	-19.490	-1.213	2.082	4.1869	20.93
27.	H43	H	0.9700	0.3750	0.2160	-14.537	-5.654	1.642	4.2731	21.37
28.	H60	H	0.3480	0.7850	0.2760	-14.013	0.668	3.526	4.3843	21.92
29.	C25	C	0.5492	0.6498	0.1776	-13.061	-1.807	3.830	4.4159	7.61
30.	C1	C	0.8940	0.7263	0.3264	-18.702	-3.573	3.100	4.4492	7.67
31.	H34	H	0.9400	0.1450	0.4518	-15.428	-4.728	-3.051	4.4911	22.46
32.	H21	H	0.9050	0.6450	0.4680	-20.006	-3.107	0.778	4.4977	22.49
33.	O19	O	0.5125	0.4175	0.6379	-16.994	0.370	-3.545	4.5918	1.77
34.	O17	O	0.2457	0.5480	0.5291	-14.479	2.247	-1.514	4.5918	1.77
35.	O16	O	0.4215	0.3299	0.5607	-14.352	0.463	-3.451	4.5943	1.77
36.	O13	O	0.3350	0.6373	0.6064	-17.123	2.172	-1.597	4.5983	1.77
37.	C16	C	0.9914	0.1390	0.4038	-15.132	-5.412	-2.471	4.6233	7.97
38.	H51	H	0.6360	0.2260	0.2890	-11.394	-2.968	-0.828	4.6452	23.23
39.	W5	W	0.3494	0.4796	0.6041	-15.746	1.649	-2.834	4.6504	2.74
40.	O18	O	0.7876	0.3624	0.6180	-18.490	-2.074	-3.431	4.6606	1.79
41.	O18	O	0.2124	0.6376	0.3820	-12.991	1.950	0.914	4.6629	1.79
42.	O12	O	0.4079	0.8319	0.5490	-18.739	1.770	0.748	4.6652	1.79
43.	O12	O	0.5921	0.1681	0.4510	-12.742	-1.894	-3.266	4.6695	1.80
44.	C12	C	1.1054	0.3900	0.3879	-18.189	-5.778	-0.109	4.7163	8.13
45.	H25	H	1.0800	0.4670	0.4020	-18.889	-5.306	0.320	4.7361	23.68
46.	C6	C	0.6094	0.9182	0.3246	-18.096	-0.826	4.343	4.7627	8.21
47.	H4	H	0.8360	0.7620	0.2250	-17.143	-3.563	4.521	4.7819	23.91
48.	H23	H	0.7240	0.7030	0.5710	-20.472	-0.962	-0.184	4.8317	24.16
49.	H56	H	0.5770	0.7120	0.1540	-13.542	-1.999	4.647	4.8595	24.30
50.	H2	H	0.9830	0.6790	0.3340	-19.107	-4.363	2.731	4.8903	24.45
51.	H15	H	0.5080	0.9420	0.4300	-18.939	0.609	3.170	4.9069	24.53
52.	C17	C	0.7797	0.5250	0.1279	-13.127	-4.229	3.676	4.9118	8.47
53.	C23	C	0.6084	0.2689	0.2454	-10.958	-2.873	0.004	4.9121	8.47
54.	C9	C	0.7766	0.8200	0.4434	-20.223	-1.773	2.338	4.9224	8.49
55.	H57	H	0.3740	0.6250	0.2140	-11.882	-0.274	2.990	4.9234	24.62
56.	H36	H	1.0700	0.1490	0.4000	-15.825	-6.035	-2.252	4.9771	24.89

Bond search from target site: W6:
... Found 55 atoms within 0.00 - 5.00 Å of this site.

	Label	Elmt	Fractional Coordinates x	y	z	Orthogonal Coordinates xor[Å]	yor[Å]	zor[Å]	Bond Distance d[Å]	d/(rA+rB)
TARG.	W6	W	0.6669	0.4197	0.5676	-17.319	-1.236	-2.512		
1.	O18	O	0.7876	0.3624	0.6180	-18.490	-2.074	-3.431	1.7079	0.66
2.	O17	O	0.7543	0.4520	0.4709	-17.003	-2.371	-1.003	1.9146	0.74
3.	O14	O	0.5892	0.5882	0.5775	-18.377	-0.138	-1.352	1.9156	0.74
4.	O15	O	0.6768	0.2818	0.5321	-15.628	-1.851	-3.201	1.9267	0.74
5.	O19	O	0.5125	0.4175	0.6379	-16.994	0.370	-3.545	1.9366	0.74
6.	O11	O	0.5000	0.5000	0.5000	-15.741	-0.062	-1.259	2.3327	0.90
7.	W5	W	0.6506	0.5204	0.3959	-15.735	-1.773	0.316	3.2861	1.93
8.	W4	W	0.5546	0.3083	0.4720	-14.026	-1.130	-2.421	3.2962	1.94
9.	W4	W	0.4454	0.6917	0.5280	-17.455	1.006	-0.097	3.2985	1.94
10.	W5	W	0.3494	0.4796	0.6041	-15.746	1.649	-2.834	3.3012	1.94
11.	O16	O	0.5785	0.6701	0.4393	-17.129	-0.587	0.934	3.5120	1.35
12.	O13	O	0.6650	0.3627	0.3936	-14.358	-2.296	-0.920	3.5251	1.36
13.	O13	O	0.3350	0.6373	0.6064	-17.123	2.172	-1.597	3.5338	1.36
14.	O16	O	0.4215	0.3299	0.5607	-14.352	0.463	-3.451	3.5460	1.36
15.	H60	H	0.6520	0.2150	0.7240	-17.468	-0.792	-6.043	3.5614	17.81
16.	H29	H	0.9880	0.1870	0.6240	-18.609	-4.084	-4.689	3.8097	19.05
17.	H22	H	1.0510	0.2610	0.5180	-18.347	-4.970	-2.760	3.8805	19.40
18.	H52	H	0.5890	0.6420	0.7080	-20.688	0.698	-2.459	3.8845	19.42
19.	H48	H	0.4020	0.5650	0.7390	-18.850	2.165	-3.673	3.9065	19.53
20.	H23	H	0.7240	0.7030	0.5710	-20.472	-0.962	-0.184	3.9293	19.65
21.	H18	H	0.6070	0.1240	0.6270	-14.902	-1.181	-5.688	3.9917	19.96
22.	H25	H	0.9200	0.5330	0.5980	-20.896	-2.811	-1.652	4.0020	20.01
23.	H34	H	0.9400	0.1450	0.4518	-15.428	-4.728	-3.051	4.0079	20.04
24.	H57	H	0.6260	0.3750	0.7860	-19.599	0.149	-5.507	4.0108	20.05
25.	H33	H	0.9150	0.0430	0.5910	-16.207	-4.039	-5.556	4.2841	21.42
26.	H55	H	0.4240	0.3740	0.7750	-17.760	1.703	-5.625	4.3030	21.52
27.	C27	C	0.6794	0.1984	0.7716	-18.202	-0.798	-6.708	4.3102	7.43
28.	H59	H	0.7690	0.1910	0.7670	-18.814	-1.557	-6.608	4.3715	21.86
29.	H9	H	0.8430	0.4180	0.7450	-21.231	-1.697	-4.416	4.3745	21.87
30.	H2	H	1.0170	0.3210	0.6660	-20.677	-3.754	-4.063	4.4749	22.37
31.	H21	H	1.0950	0.3550	0.5320	-19.779	-5.010	-2.110	4.5234	22.62
32.	H27	H	1.0260	0.3840	0.3880	-17.475	-5.158	-0.253	4.5288	22.64
33.	C26	C	0.5982	0.3133	0.8118	-19.154	0.355	-6.347	4.5385	7.82
34.	O19	O	0.4875	0.5825	0.3621	-14.487	-0.494	1.028	4.5938	1.77
35.	O15	O	0.3232	0.7182	0.4679	-15.853	1.727	0.683	4.5979	1.77
36.	O14	O	0.4108	0.4118	0.4225	-13.104	0.014	-1.165	4.5981	1.77
37.	C12	C	0.8946	0.6100	0.6121	-21.596	-2.339	-1.223	4.6012	7.93
38.	O17	O	0.2457	0.5480	0.5291	-14.479	2.247	-1.514	4.6038	1.77
39.	H21	H	0.9050	0.6450	0.4680	-20.006	-3.107	0.778	4.6414	23.21
40.	C11	C	0.8044	0.7132	0.5670	-21.179	-1.601	0.042	4.6428	8.00
41.	O12	O	0.4079	0.8319	0.5490	-18.739	1.770	0.748	4.6570	1.79
42.	H35	H	0.9410	0.2010	0.3680	-14.792	-5.045	-1.604	4.6603	23.30
43.	O20	O	0.2405	0.4632	0.6820	-15.772	2.895	-4.018	4.6608	1.79
44.	C10	C	1.1267	0.2791	0.5127	-19.070	-5.558	-2.460	4.6632	8.04
45.	W6	W	0.3331	0.5803	0.4324	-14.162	1.112	-0.005	4.6654	2.74
46.	O20	O	0.7595	0.5368	0.3180	-15.709	-3.019	1.501	4.6772	1.80
47.	O12	O	0.5921	0.1681	0.4510	-12.742	-1.894	-3.266	4.6852	1.80
48.	H26	H	0.8470	0.6150	0.6634	-21.960	-1.671	-1.845	4.7085	23.54
49.	C16	C	0.9914	0.1390	0.4038	-15.132	-5.412	-2.471	4.7137	8.13
50.	C13	C	1.0550	0.1193	0.6446	-18.823	-4.679	-5.404	4.7411	8.17
51.	C22	C	0.3599	0.6216	0.7738	-19.510	2.830	-3.675	4.7634	8.21
52.	C24	C	0.5380	0.7003	0.7437	-21.301	1.443	-2.469	4.7998	8.28
53.	C8	C	0.6321	0.0367	0.6285	-14.320	-1.593	-6.386	4.9113	8.47
54.	C25	C	0.4508	0.3502	0.8224	-18.420	1.683	-6.347	4.9437	8.52
55.	H51	H	0.3640	0.7740	0.7110	-20.087	2.844	-1.689	4.9980	24.99

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