

Electronic Supporting Information

CO₂ Reduction to CO on an Iron-Porphyrin Complex with Crown-Ether Appended Cation-Binding Site

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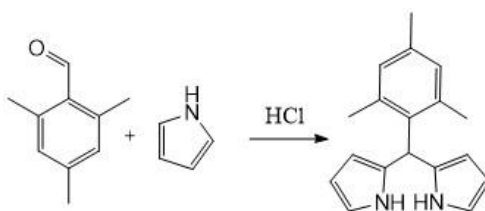
Experimental Details

1. Cyclic voltammetry

Homogeneous cyclic voltammetry (CV) experiments were performed using a standard three-electrode cell in a solution containing 0.25 M of the [(TPP^{Mes}Crown)Fe^{III}(OAc)] and 0.1 M of the corresponding supporting electrolytes (*n*-Bu₄BF₄, NaBF₄, KBF₄) in 10 mL dimethylformamide (DMF) with the water concentration at 0.5 M. A glassy carbon working electrode (WE) was used and polished between each measurement. A double junction non-aqueous Ag/AgCl reference electrode (RE) filled with 2 M LiCl in ethanol as the inner electrolyte and the DMF solution as the outer electrolyte was used. The counter electrode (CE) was a platinum mesh of 2 cm² area. The reference electrode was calibrated against the ferrocene/ferrocenium redox couple. Prior to the measurements, the solution was deoxygenated with argon or saturated with CO₂ for 30 minutes, and during the measurements, the corresponding gas was kept flowing over the head space.

2. Synthesis of [(TPP^{Mes}Crown)Fe^{III}(OAc)] complex

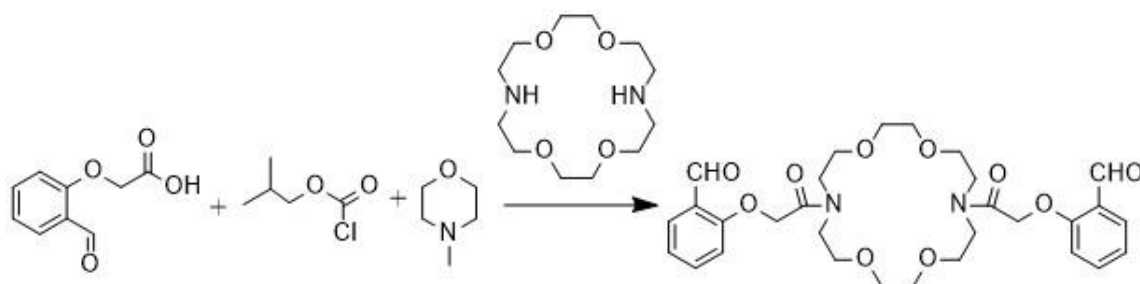
2.1 Synthesis of mesityldipyrromethane



A Schenk flask flushed with nitrogen was filled with 200 mL of water containing 3 mL of concentrated HCl, 2,4,6-trimethylbenzaldehyde (4.00 g, 1 eq, 27.0 mmol), and 1H-pyrrole (5.43 g, 3 eq, 81.0 mmol). A white emulsion was formed and stirred overnight at room temperature under nitrogen shielded from light (covered with Al foil). A black solid was formed, filtered, and washed with 3 × 50 mL water followed by 3 × 50 mL heptane. The solid was then dissolved in dichloromethane (giving a dark green solution) and purified by silica column chromatography using eluent dichloromethane/heptane 60/40. The fraction was evaporated, and a white solid was obtained, followed by washing it with heptane and then pentane. The yield of white solid 2,2'-(mesitylmethylene)bis(1H-pyrrole) was 2.678 g, 37.5%.

¹H NMR (Fig. S1) (400 MHz, CDCl₃) δ 7.93 (s, 2H), 6.86 (s, 2H), 6.68 – 6.63 (m, 2H), 6.20 – 6.14 (m, 2H), 6.00 (s, 2H), 5.92 (s, 1H), 2.28 (s, 3H), 2.06 (s, 6H).

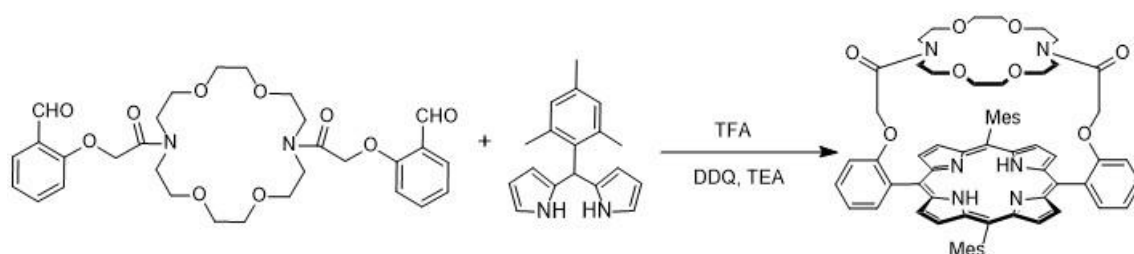
2.2 Synthesis of *N,N*-bisformylphenoxyacetyl-4,13-diaza-18-crown-6-ether



A Schlenk round-bottom flask of 100 mL with a stirring bar was filled with 50 mL of dry THF and 2-(2-formylphenoxy)acetic acid (369.1 mg, 2.15 eq, 2.049 mmol). The reaction mixture was cooled to $-40\text{ }^{\circ}\text{C}$ (in a dry ice bath), and then isobutyl chloroformate (312.4 mg, 2.4 eq, 2.287 mmol) and 4-methylmorpholine (231.3 mg, 2.4 eq, 2.287 mmol) were added slowly. The reaction mixture was stirred at $-40\text{ }^{\circ}\text{C}$ for two hours. A white solid appeared, and 1,4,10,13-tetraoxa-7,16-diazacyclooctadecane (250.0 mg, 1 eq, 952.9 μmol) was added, and stirring at $-40\text{ }^{\circ}\text{C}$ was continued for 15 min. After that, the reaction mixture was gradually heated up by not adding dry ice to the cooling bath and allowed to react overnight. The reaction mixture analysed using electrospray ionisation-mass spectrometry (ESI-MS) showed the mass disubstituted product (*N,N*-bisformylphenoxyacetyl-4,13-diaza-18-crown-6-ether). The reaction mixture was evaporated to dryness and used directly for the next step.

ESI-MS (Fig. S2): m/z $[\text{M}+\text{Na}]^+$, $[\text{C}_{30}\text{H}_{38}\text{N}_2\text{NaO}_{10}]^+$ Calculated: 609.24, Observed: 609.40

2.3 Synthesis of crown-capped dimesityldiphenylporphyrin ($\text{H}_2(\text{TPP}^{\text{Mes}}\text{Crown})$)

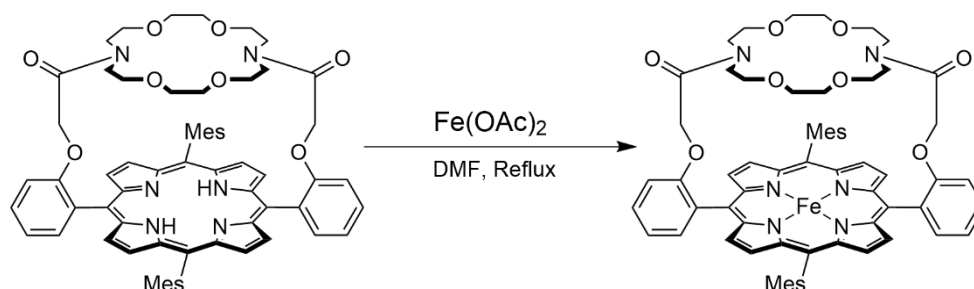


The *N,N*-bisformylphenoxyacetyl 4,13-diaza-18-crown-6-ether residue from the previous step, and the mesityldipyrromethane (504 mg, 2 eq, 1.91 mmol) was dissolved in dichloromethane. The solution was sparged with nitrogen, and trifluoroacetic acid (65.2 mg, 0.6 eq, 572 μmol) was added. The solution was shielded from light and stirred overnight under nitrogen. Further, 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) (541 mg, 2.5 eq, 2.38 mmol) was added to the solution and left under stirring. After 1.5 hours, 3 mL triethylamine was added, and the solution was stirred for another 30 minutes. The reaction mixture was concentrated and purified over silica column chromatography. Two pre-fractions were collected using 1% methanol in dichloromethane as the eluent, and then methanol was increased to 2.5%, and a purple fraction containing the product was collected. The fraction was concentrated and further purified on a 60H silica column using 1.5% methanol in dichloromethane as the eluent. Finally, the purified fraction was concentrated and then precipitated with heptane. The solid was centrifuged and washed with pentane (four times) and dried to the yield crown-capped dimesityldiphenylporphyrin (290 mg, 270 μmol , 28% yield).

^1H NMR (Fig. S3) (400 MHz, CDCl_3) δ 8.76-8.69 (m, 8H), 8.18-8.16 (dd, $J = 7.5, 1.7$ Hz, 2H), 7.82-7.78 (m, 2H), 7.48-7.44 (td, $J = 7.5, 1.0$ Hz, 2H), 7.41-7.39 (d, $J = 8.3$ Hz, 2H), 7.32 (s, 2H), 7.24 (s, 2H), 4.65 (s, 4H), 2.92 (s, 3H), 2.69-2.59 (m, 14H), 2.02 (s, 6H), 1.94 (t, $J = 4.8$ Hz, 4H), 1.66 (s, 6H), 1.53 (s, 2H), -0.04 (t, $J = 4.7$ Hz, 4H), -0.48 (s, 3H), -2.59 (s, 2H).

2.4 Synthesis of Fe(III)(crown-capped dimesityldiphenylporphyrin)OAc

([(TPP^{Mes}Crown)Fe^{III}(OAc)])



A round bottom flask was filled with 25 mL of deoxygenated dimethylformamide (DMF) containing H₂(TPP^{Mes}Crown) (100 mg, 1 eq, 93.2 μmol) and diacetoxyiron (89.1 mg, 5.5 eq, 512 μmol). The reaction mixture was shielded from light and brought to reflux (160 °C) under nitrogen for 3 hours. After cooling down, acetic acid was added and stirred for another one hour in the open air. Water (50 mL) was added to the reaction mixture and extracted with dichloromethane (5 × 35 mL). The combined dichloromethane layers were washed with water (5 × 50 mL). The dichloromethane layer was concentrated, and heptane was added. The dichloromethane was evaporated to yield the solid product. The solid was isolated by centrifuge and washed with pentane (4 × pentane/centrifuge), and dried to obtain [(TPP^{Mes}Crown)Fe^{III}(OAc)] (59.5 mg, 50.2 μmol, 53.8 % yield).

ESI-MS (TOF) (Fig. S4): [M+(Na⁺)]⁺, [(TPP^{Mes}Crown)Fe^{III}(OAc)(Na)]⁺ m/z calculated 1208.4317, m/z observed 1208.4306; [M-(OAc)]⁺, [(TPP^{Mes}Crown)Fe^{III}]⁺ m/z calculated 1126.4292, m/z observed 1126.4299.

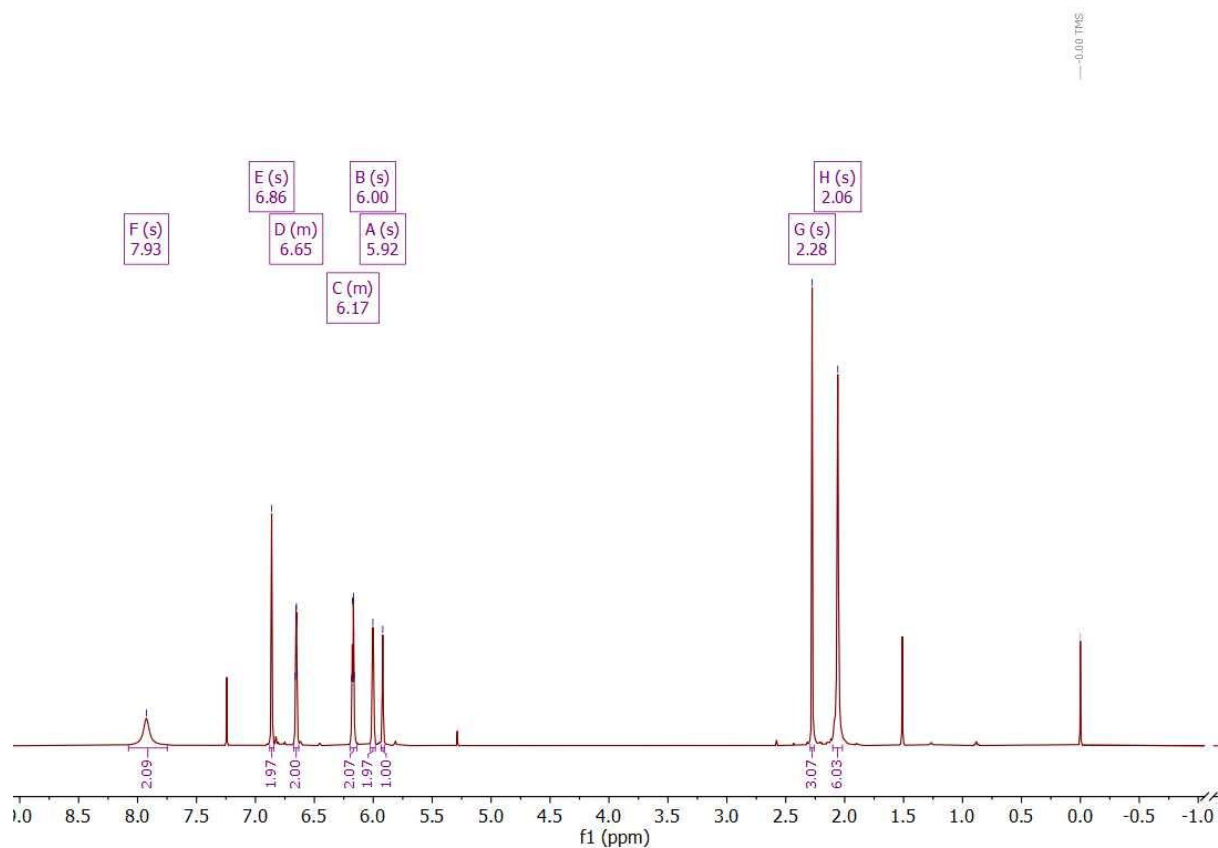


Fig. S1. ^1H NMR spectrum of mesityldipyrromethane (400 MHz, CDCl_3).

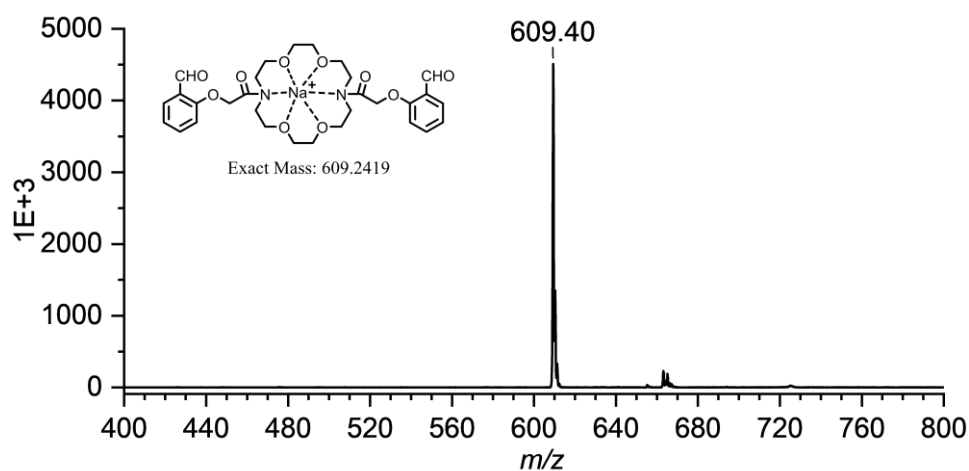


Fig. S2. ESI-MS (Thermo Finnigan LCQ Deca) mass spectrum of *N,N*-bisformylphenoxyacetyl-4,13-diaza-18-crown-6-ether $[\text{M}+\text{Na}]^+ = m/z$ 609.40.

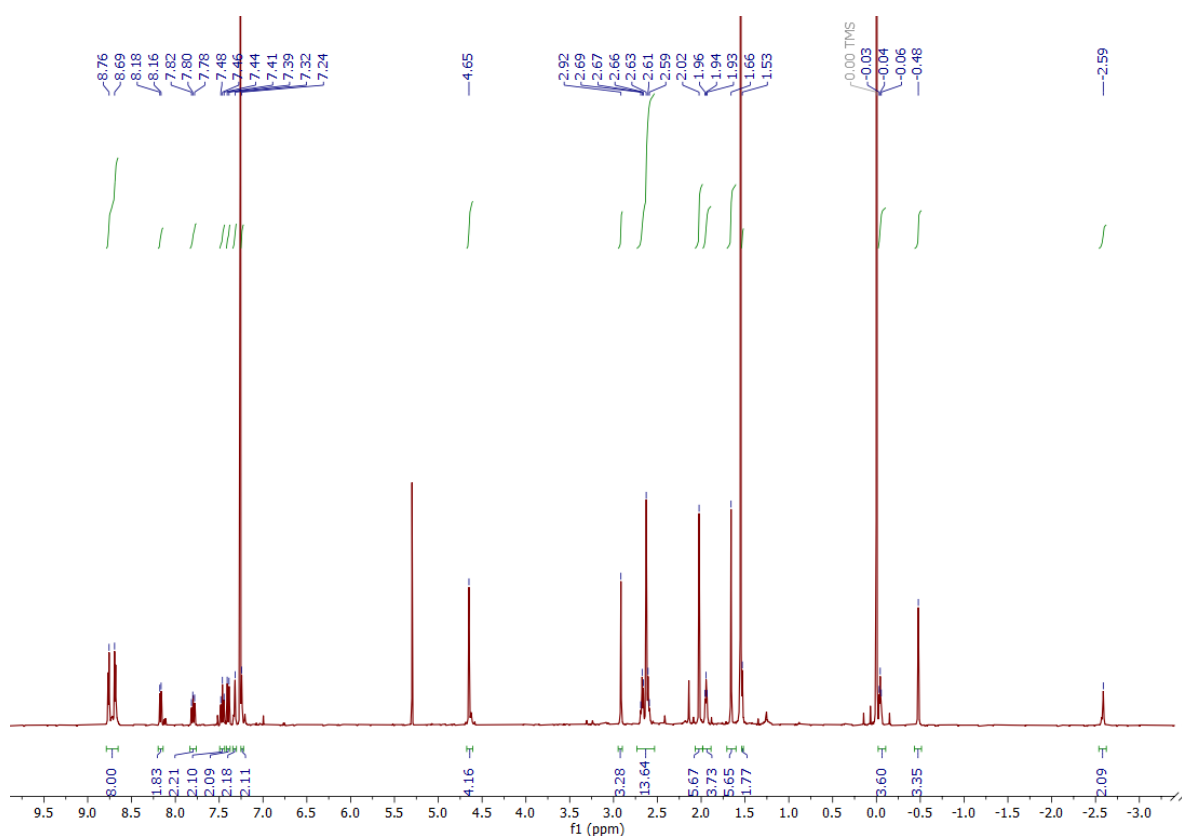


Fig. S3. ^1H NMR spectrum of $\text{H}_2(\text{TPP}^{\text{Mes}}\text{Crown})$ (400 MHz, CDCl_3).

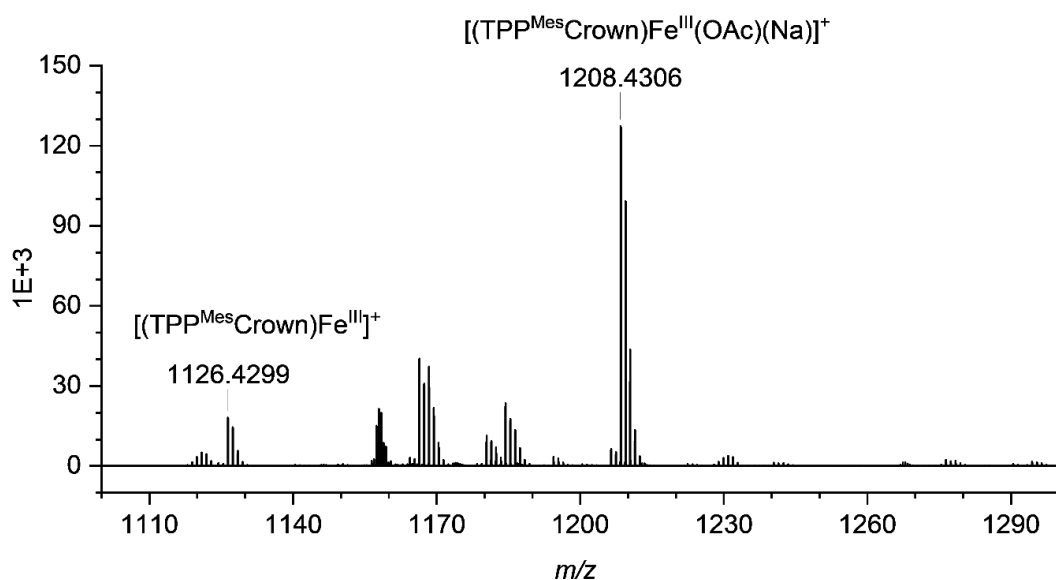


Fig. S4. ESI-MS (Bruker, timsTOF) mass spectrum of $[(\text{TPP}^{\text{Mes}}\text{Crown})\text{Fe}^{\text{III}}(\text{OAc})]$ in the presence of NaBF_4 salt, detected as $[(\text{TPP}^{\text{Mes}}\text{Crown})\text{Fe}^{\text{III}}(\text{OAc})(\text{Na})]^+$: m/z 1208.4306 and $[(\text{TPP}^{\text{Mes}}\text{Crown})\text{Fe}^{\text{III}}]^+$: m/z 1126.4299.

Table S1: Absolute energies and free energies (in au) for UB3LYP-GD3BJ/BS1 optimized geometries for CO₂ reduction on an iron-porphyrin center with/without nearby K⁺ using H₃O⁺, phenol or acetate as a proton source.

	E [au, BS1]	ZPE	G	E [au,BS2]
H₃O⁺				
² CAT _{H3O+}	-4587.404689	1.066504	-4586.435419	-4591.188919
³ CAT _{H3O+}	-4587.490629	1.062391	-4586.525911	-4591.278140
³ RC1 _{H3O+}	-4852.772171	1.114180	-4851.760795	-4856.868489
³ IM1 _{H3O+}	-4852.800085	1.115876	-4851.789252	-4856.903592
³ RC2 _{H3O+}	-4853.223192	1.126182	-4852.202849	-4857.320692
³ IM2 _{H3O+}	-4853.290896	1.125608	-4852.274494	-4857.396762
⁴ CAT _{H3O+}	-4587.391863	1.066022	-4586.423664	-4591.176653
⁵ CAT _{H3O+}	-4587.471954	1.063349	-4586.506096	-4591.259860
⁵ RC1 _{H3O+}	-4852.764580	1.112011	-4851.755962	-4856.857424
⁵ IM1 _{H3O+}	-4852.788577	1.114669	-4851.781143	-4856.889837
⁵ RC2 _{H3O+}	-4853.225846	1.124544	-4852.209623	-4857.323323
⁵ IM2 _{H3O+}	-4853.283947	1.123434	-4852.270961	-4857.386909
² CAT _{H3O+,K+}	-5187.265604	1.067524	-5186.298284	-5191.110762
³ CAT _{H3O+,K+}	-5187.354082	1.065355	-5186.391690	-5191.203501
³ RC1 _{H3O+,K+}	-5452.626611	1.116194	-5451.614907	-5456.782012
³ IM1 _{H3O+,K+}	-5452.648184	1.116736	-5451.639015	-5456.810510
³ RC2 _{H3O+,K+}	-5453.068123	1.126790	-5452.049449	-5457.225416
³ TS2 _{H3O+,K+}	-5453.076019	1.126001	-5452.057176	-5457.231028
³ IM2 _{H3O+,K+}	-5453.140882	1.126912	-5452.123957	-5457.308372
⁴ CAT _{H3O+,K+}	-5187.261996	1.067565	-5186.294064	-5191.10681
⁵ CAT _{H3O+,K+}	-5187.350117	1.064721	-5186.385416	-5191.197633
⁵ RC1 _{H3O+,K+}	-5452.613576	1.113642	-5451.606889	-5456.768711
⁵ IM1 _{H3O+,K+}	-5452.651480	1.115433	-5451.643982	-5456.812878
⁵ RC2 _{H3O+,K+}	-5453.069007	1.125570	-5452.050611	-5457.225974
⁵ TS2 _{H3O+,K+}	-5453.086164	1.124552	-5452.067475	-5457.241761
⁵ IM2 _{H3O+,K+}	-5453.137093	1.125293	-5452.122943	-5457.302426
phenol				
³ RC1 _{phenol,K+}	-5683.105971	1.185644	-5682.031202	-5687.507107
⁵ RC1 _{phenol,K+}	-5683.092219	1.183377	-5682.023243	-5687.492791
³ RC1 _{phenol, 6W, K+}	-6065.094394	1.313519	-6063.903983	-6069.958867
⁵ RC1 _{phenol, 6W, K+}	-6065.037907	1.310238	-6063.853744	-6069.902873
acetate				
³ RC1 _{acetate,K+}	-5604.752623	1.142108	-5603.720928	-5609.087443
⁵ RC1 _{acetate,K+}	-5604.739781	1.140133	-5603.710740	-5609.072379
⁵ TS1 _{acetate,K+}	-5604.718308	1.135460	-5603.692740	-5609.054274
⁵ IM1 _{acetate,K+}	-5604.735224	1.140103	-5603.705841	-5609.075897
⁵ RC2 _{acetate,K+}	-5605.217797	1.153260	-5604.177196	-5609.549445
⁵ TS2 _{acetate,K+}	-5605.221445	1.147683	-5604.188925	-5609.553966
⁵ IM2 _{acetate,K+}	-5605.241660	1.149963	-5604.206575	-5609.575401
³ RC1 _{Ac, 6W, K+}	-5986.705409	1.267449	-5985.558433	-5991.501598
³ TS1 _{acetate, 6W, K+}	-5986.703255	1.264086	-5985.558928	-5991.498899
³ IM1 _{acetate, 6W, K+}	-5986.707065	1.268557	-5985.558978	-5991.505482
³ RC2 _{acetate, 6W, K+}	-5987.170947	1.282746	-5986.010089	-5991.962601
³ IM2 _{acetate, 6W, K+}	-5987.211491	1.280719	-5986.054804	-5992.014555
⁵ RC1 _{acetate, 6W, K+}	-5986.684029	1.266321	-5985.538967	-5991.482361
⁵ TS1 _{acetate, 6W, K+}	-5986.649671	1.262808	-5985.507400	-5991.445074
⁵ IM1 _{acetate, 6W, K+}	-5986.652342	1.267019	-5985.506514	-5991.450036
⁵ RC2 _{acetate, 6W, K+}	-5987.116616	1.279820	-5985.959074	-5991.909516

Table S2: Relative (free) energies (in kcal mol⁻¹) of the CO₂ reduction on an iron-porphyrin center with/without nearby K⁺ using H₃O⁺, phenol or acetate as a proton source as obtained with UB3LYP-GD3BJ in Gaussian-09.

	$\Delta E(\text{BS1})$	$\Delta E+\text{ZPE}(\text{BS1})$	$\Delta G(\text{BS1})$	$\Delta E(\text{BS2})$	$\Delta E+\text{ZPE}(\text{BS2})$	$\Delta G(\text{BS2})$
H₃O⁺						
² CAT _{H3O+}	53.93	56.51	56.78	55.99	58.57	58.84
³ CAT _{H3O+}	0.00	0.00	0.00	0.00	0.00	0.00
³ RC1 _{H3O+}	0.00	0.00	0.00	0.00	0.00	0.00
³ IM1 _{H3O+}	-17.52	-16.45	-17.86	-22.03	-20.96	-22.37
³ RC2 _{H3O+}	-17.52	-16.45	-17.86	-22.03	-20.96	-22.37
³ IM2 _{H3O+}	-60.00	-59.30	-62.82	-69.76	-69.06	-72.58
⁴ CAT _{H3O+}	55.02	55.34	54.76	59.16	59.47	58.89
⁵ CAT _{H3O+}	4.76	3.40	3.03	6.94	5.58	5.21
⁵ RC1 _{H3O+}	4.76	3.40	3.03	6.94	5.58	5.21
⁵ IM1 _{H3O+}	-10.30	-9.99	-12.77	-13.40	-13.09	-15.87
⁵ RC2 _{H3O+}	-10.30	-9.99	-12.77	-13.40	-13.09	-15.87
⁵ IM2 _{H3O+}	-46.75	-47.14	-51.26	-53.30	-53.69	-57.80
² CAT _{H3O+,K+}	55.52	56.88	58.61	58.19	59.56	61.29
³ CAT _{H3O+,K+}	0.00	0.00	0.00	0.00	0.00	0.00
³ RC1 _{H3O+,K+}	0.00	0.00	0.00	0.00	0.00	0.00
³ IM1 _{H3O+,K+}	-13.54	-13.20	-15.13	-17.88	-17.54	-19.47
³ RC2 _{H3O+,K+}	-13.54	-13.20	-15.13	-17.88	-17.54	-19.47
³ TS2 _{H3O+,K+}	-18.49	-18.65	-19.98	-21.40	-21.56	-22.89
³ IM2 _{H3O+,K+}	-59.19	-58.78	-61.88	-69.94	-69.52	-72.63
⁴ CAT _{H3O+,K+}	63.48	63.66	62.36	65.34	65.52	64.22
⁵ CAT _{H3O+,K+}	8.18	6.58	5.03	8.35	6.75	5.20
⁵ RC1 _{H3O+,K+}	8.18	6.58	5.03	8.35	6.75	5.20
⁵ IM1 _{H3O+,K+}	-15.61	-16.08	-18.24	-19.37	-19.85	-22.01
⁵ RC2 _{H3O+,K+}	-15.61	-16.08	-18.24	-19.37	-19.85	-22.01
⁵ TS2 _{H3O+,K+}	-26.37	-27.49	-28.83	-29.28	-30.39	-31.73
⁵ IM2 _{H3O+,K+}	-58.33	-58.98	-63.63	-67.34	-68.00	-72.65
phenol						
³ RC1 _{phenol,K+}	0.00	0.00	0.00	0.00	0.00	0.00
⁵ RC1 _{phenol,K+}	8.63	7.21	4.99	8.98	7.56	5.35
³ RC1 _{phenol, 6W, K+}	0.00	0.00	0.00	0.00	0.00	0.00
⁵ RC1 _{phenol, 6W, K+}	35.45	33.39	31.53	35.14	33.08	31.22
acetate						
³ RC1 _{acetate,K+}	0.00	0.00	0.00	0.00	0.00	0.00
⁵ RC1 _{acetate,K+}	8.06	6.82	6.39	9.45	8.21	7.79
⁵ TS1 _{acetate,K+}	21.53	17.36	17.69	20.81	16.64	16.97
⁵ IM1 _{acetate,K+}	10.92	9.66	9.47	7.24	5.99	5.79
⁵ RC2 _{acetate,K+}	10.92	9.66	9.47	7.24	5.99	5.79
⁵ TS2 _{acetate,K+}	8.63	3.87	2.11	4.41	-0.35	-2.11
⁵ IM2 _{acetate,K+}	-4.06	-7.38	-8.97	-9.04	-12.37	-13.96
³ RC1 _{acetate, 6W, K+}	0.00	0.00	0.00	0.00	0.00	0.00
³ TS1 _{acetate, 6W, K+}	1.35	-0.76	-0.31	1.69	-0.42	0.03
³ IM1 _{acetate, 6W, K+}	-1.04	-0.34	-0.34	-2.44	-1.74	-1.74
³ RC2 _{acetate, 6W, K+}	-1.04	-0.34	-0.34	-2.44	-1.74	-1.74
³ IM2 _{acetate, 6W, K+}	-26.48	-27.06	-28.40	-35.04	-35.62	-36.96
⁵ RC1 _{acetate, 6W, K+}	13.42	12.71	12.22	12.07	11.36	10.87
⁵ TS1 _{acetate, 6W, K+}	34.98	32.06	32.02	35.47	32.56	32.52
⁵ IM1 _{acetate, 6W, K+}	33.30	33.03	32.58	32.36	32.09	31.64
⁵ RC2 _{acetate, 6W, K+}	33.30	33.03	32.58	32.36	32.09	31.64

Table S3: Group spin densities (a) and charges (b) of UB3LYP-GD3BJ/BS1 optimized geometries for the CO₂ reduction on an iron-porphyrin center with/without nearby K⁺ using H₃O⁺, phenol or acetate as a proton source as obtained in Gaussian-09.

a Spin densities

	H ₃ O ⁺	CO ₂ (H)	Fe	Lig	total
H₃O⁺					
² CAT _{H3O+}			1.99	-0.99	1.00
³ CAT _{H3O+}			2.00	0.00	2.00
³ RC1 _{H3O+}	0.00	-0.18	1.26	0.92	2.00
³ IM1 _{H3O+}	0.00	0.15	2.27	-0.42	2.00
³ RC2 _{H3O+}	0.00	0.15	2.31	-0.47	2.00
³ IM2 _{H3O+}	0.00	0.03	2.07	-0.10	2.00
⁴ CAT _{H3O+}			2.17	0.83	3.00
⁵ CAT _{H3O+}			2.15	1.85	4.00
⁵ RC1 _{H3O+}	0.00	-0.51	3.40	1.11	4.00
⁵ IM1 _{H3O+}	0.00	0.35	2.64	1.01	4.00
⁵ RC2 _{H3O+}	0.00	0.08	3.87	0.04	4.00
⁵ IM2 _{H3O+}	0.00	0.00	3.81	0.19	4.00
² CAT _{H3O+,K+}			1.98	-0.98	1.00
³ CAT _{H3O+,K+}			1.99	0.01	2.00
³ RC1 _{H3O+,K+}	0.01	-0.16	1.27	0.89	2.00
³ IM1 _{H3O+,K+}	0.00	0.12	2.09	-0.21	2.00
³ RC2 _{H3O+,K+}	0.00	0.13	2.20	-0.33	2.00
³ TS2 _{H3O+,K+}	0.01	-0.06	1.53	0.52	2.00
³ IM2 _{H3O+,K+}	0.00	0.05	2.06	-0.11	2.00
⁴ CAT _{H3O+,K+}			2.04	0.96	3.00
⁵ CAT _{H3O+,K+}			2.05	1.95	4.00
⁵ RC1 _{H3O+,K+}	0.01	-0.49	3.40	1.08	4.00
⁵ IM1 _{H3O+,K+}	0.00	0.06	3.83	0.11	4.00
⁵ RC2 _{H3O+,K+}	0.00	0.06	3.85	0.09	4.00
⁵ TS2 _{H3O+,K+}	0.00	0.02	3.83	0.15	4.00
⁵ IM2 _{H3O+,K+}	0.00	-0.02	3.81	0.21	4.00
acetate					
⁵ RC1 _{acetate,K+}	0.00	-0.44	3.31	1.13	4.00
⁵ TS1 _{acetate,K+}	0.00	-0.34	3.21	1.13	4.00
⁵ IM1 _{acetate,K+}	0.00	0.06	3.85	0.09	4.00
⁵ RC2 _{acetate,K+}	0.00	0.05	3.84	0.11	4.00
⁵ TS2 _{acetate,K+}	0.00	0.02	3.80	0.18	4.00
⁵ IM2 _{acetate,K+}	0.00	0.00	3.80	0.20	4.00
³ RC1 _{acetate, 6W, K+}	0.00	-0.17	1.25	0.91	2.00
³ TS1 _{acetate, 6W, K+}	0.00	-0.14	1.21	0.93	2.00
³ IM1 _{acetate, 6W, K+}	0.00	-0.12	1.18	0.94	2.00
³ RC2 _{acetate, 6W, K+}	0.00	-0.15	1.24	0.91	2.00
³ IM2 _{acetate, 6W, K+}	0.00	0.04	2.06	-0.10	2.00
⁵ RC1 _{acetate, 6W, K+}	0.00	0.41	2.56	1.03	4.00
⁵ TS1 _{acetate, 6W, K+}	0.00	-0.21	1.40	2.80	4.00
⁵ IM1 _{acetate, 6W, K+}	0.00	-0.16	1.29	2.86	4.00

b Charges

	H ₃ O ⁺	CO ₂ (H)	Fe	Lig	total
H₃O⁺:					
² CAT _{H3O+}			0.55	-1.55	-1.00
³ CAT _{H3O+}			0.48	-2.48	-2.00
³ RC1 _{H3O+}	0.72	-0.53	0.45	-1.65	-1.00
³ IM1 _{H3O+}	0.22	-0.56	0.56	-1.22	-1.00
³ RC2 _{H3O+}	0.74	-0.32	0.57	-0.99	0.00
³ IM2 _{H3O+}	0.22	-0.09	0.60	-0.73	0.00
⁴ CAT _{H3O+}			0.70	-1.70	-1.00
⁵ CAT _{H3O+}			0.65	-2.65	-2.00

⁵ RC1 _{H3O+}	0.72	-0.50	0.61	-1.82	-1.00
⁵ IM1 _{H3O+}	0.25	-0.47	0.62	-1.39	-1.00
⁵ RC2 _{H3O+}	0.74	-0.39	0.67	-1.03	0.00
⁵ IM2 _{H3O+}	0.27	-0.07	0.72	-0.92	0.00
² CAT _{H3O+,K+}			0.55	-0.55	0.00
³ CAT _{H3O+,K+}			0.48	-1.48	-1.00
³ RC1 _{H3O+,K+}	0.65	-0.51	0.47	-0.61	0.00
³ IM1 _{H3O+,K+}	0.27	-0.55	0.55	-0.26	0.00
³ RC2 _{H3O+,K+}	0.78	-0.31	0.59	-0.05	1.00
³ TS2 _{H3O+,K+}	0.69	-0.11	0.49	-0.07	1.00
³ IM2 _{H3O+,K+}	0.26	-0.07	0.61	0.20	1.00
⁴ CAT _{H3O+,K+}			0.58	-0.58	0.00
⁵ CAT _{H3O+,K+}			0.52	-1.52	-1.00
⁵ RC1 _{H3O+,K+}	0.67	-0.48	0.62	-0.81	0.00
⁵ IM1 _{H3O+,K+}	0.28	-0.58	0.66	-0.36	0.00
⁵ RC2 _{H3O+,K+}	0.77	-0.32	0.68	-0.13	1.00
⁵ TS2 _{H3O+,K+}	0.65	-0.28	0.68	-0.05	1.00
⁵ IM2 _{H3O+,K+}	0.26	-0.05	0.72	0.07	1.00
Acetate:					
⁵ RC1 _{acetate,K+}	-0.10	-0.46	0.57	-1.02	-1.00
⁵ TS1 _{acetate,K+}	-0.38	-0.33	0.57	-0.86	-1.00
⁵ IM1 _{acetate,K+}	-0.49	-0.64	0.65	-0.52	-1.00
⁵ RC2 _{acetate,K+}	-0.01	-0.32	0.66	-0.32	0.00
⁵ TS2 _{acetate,K+}	-0.07	-0.30	0.67	-0.30	0.00
⁵ IM2 _{acetate,K+}	-0.36	-0.06	0.70	-0.28	0.00
³ RC1 _{acetate, 6W, K+}	-0.03	-0.50	0.44	-0.91	-1.00
³ TS1 _{acetate, 6W, K+}	-0.15	-0.43	0.44	-0.87	-1.00
³ IM1 _{acetate, 6W, K+}	-0.34	-0.29	0.44	-0.82	-1.00
³ RC2 _{acetate, 6W, K+}	0.05	-0.02	0.46	-0.49	0.00
³ IM2 _{acetate, 6W, K+}	-0.47	-0.11	0.58	-0.01	0.00
⁵ RC1 _{acetate, 6W, K+}	-0.05	-0.66	0.58	-0.87	-1.00
⁵ TS1 _{acetate, 6W, K+}	-0.16	-0.39	0.46	-0.92	-1.00
⁵ IM1 _{acetate, 6W, K+}	-0.33	-0.27	0.46	-0.86	-1.00

Table S4: Absolute energies and free energies (in au) for UB3LYP/BS1 optimized geometries for CO₂ reduction on an iron-porphyrin center with nearby K⁺ using H₃O⁺ as a proton source.

	E [au, BS1]	ZPE	G	E [au,BS2]
³ CAT _{H3O+,K+}	-5186.942526	1.057999	-5185.991308	-5190.801361
³ RC1 _{H3O+,K+}	-5452.216713	1.111464	-5451.211828	-5456.379711
³ IM1 _{H3O+,K+}	-5452.246950	1.112348	-5451.246724	-5456.416558
³ RC2 _{H3O+,K+}	-5452.646236	1.122733	-5451.635105	-5456.810513
³ TS2 _{H3O+,K+}	-5452.657027	1.121953	-5451.646329	-5456.818193
³ IM2 _{H3O+,K+}	-5452.715820	1.122009	-5451.709326	-5456.887664
⁵ CAT _{H3O+,K+}	-5186.934014	1.059161	-5185.981996	-5190.792326
⁵ RC1 _{H3O+,K+}	-5452.210413	1.109122	-5451.210337	-5456.372956
⁵ IM1 _{H3O+,K+}	-5452.253399	1.110935	-5451.254863	-5456.421439
⁵ RC2 _{H3O+,K+}	-5452.650026	1.120547	-5451.644121	-5456.813508
⁵ TS2 _{H3O+,K+}	-5452.665182	1.119849	-5451.657255	-5456.826934
⁵ IM2 _{H3O+,K+}	-5452.712124	1.120077	-5451.708877	-5456.881115

Table S5: Relative (free) energies (in kcal mol⁻¹) of the CO₂ reduction on an iron-porphyrin center with nearby K⁺ using H₃O⁺ as a proton source as obtained with UB3LYP in Gaussian-09.

	$\Delta E(\text{BS1})$	$\Delta E + \text{ZPE}$	$\Delta G(\text{BS1})$	$\Delta E(\text{BS2})$	$\Delta E + \text{ZPE}$	$\Delta G(\text{BS2})$
³ RC1 _{H3O+,K+}	0.00	0.00	0.00	0.00	0.00	0.00
³ IM1 _{H3O+,K+}	-18.97	-18.42	-21.90	-23.12	-22.57	-26.05
³ RC2 _{H3O+,K+}	-18.97	-18.42	-21.90	-23.12	-22.57	-26.05
³ TS2 _{H3O+,K+}	-25.75	-25.68	-28.94	-27.94	-27.88	-31.14
³ IM2 _{H3O+,K+}	-62.64	-62.54	-68.47	-71.54	-71.43	-77.37
⁵ RC1 _{H3O+,K+}	3.95	2.48	0.94	4.24	2.77	1.22
⁵ IM1 _{H3O+,K+}	-23.02	-23.35	-27.00	-26.18	-26.52	-30.17
⁵ RC2 _{H3O+,K+}	-23.02	-23.35	-27.00	-26.18	-26.52	-30.17
⁵ TS2 _{H3O+,K+}	-32.53	-33.30	-35.25	-34.61	-35.38	-37.32
⁵ IM2 _{H3O+,K+}	-61.99	-62.61	-67.64	-68.61	-69.24	-74.26

Table S6: Group spin densities (a) and charges (b) of UB3LYP/BS1 optimized geometries for the CO₂ reduction on an iron-porphyrin center with nearby K⁺ using H₃O⁺ as a proton source as obtained in Gaussian-09.

a Spin densities

	H ₃ O ⁺	CO ₂ (H)	Fe	Lig	total
³ CAT _{H3O+,K+}			2.00	0.00	2.00
³ RC1 _{H3O+,K+}	0.00	-0.21	1.31	0.89	2.00
³ IM1 _{H3O+,K+}	0.00	0.10	2.14	-0.24	2.00
³ RC2 _{H3O+,K+}	0.00	0.12	2.17	-0.28	2.00
³ TS2 _{H3O+,K+}	0.00	-0.08	1.46	0.62	2.00
³ IM2 _{H3O+,K+}	0.00	0.04	2.08	-0.12	2.00
⁵ CAT _{H3O+,K+}			2.05	1.95	4.00
⁵ RC1 _{H3O+,K+}	0.00	-0.54	3.47	1.07	4.00
⁵ IM1 _{H3O+,K+}	0.00	0.04	3.85	0.11	4.00
⁵ RC2 _{H3O+,K+}	0.00	0.05	3.85	0.10	4.00
⁵ TS2 _{H3O+,K+}	0.00	0.01	3.83	0.16	4.00
⁵ IM2 _{H3O+,K+}	0.00	-0.01	3.82	0.20	4.00

b Charges

	H ₃ O ⁺	CO ₂ (H)	Fe	Lig	total
³ CAT _{H3O+,K+}			0.51	-1.51	-1.00
³ RC1 _{H3O+,K+}	0.67	-0.53	0.48	-0.62	0.00
³ IM1 _{H3O+,K+}	0.27	-0.60	0.58	-0.25	0.00
³ RC2 _{H3O+,K+}	0.76	-0.34	0.60	-0.02	1.00
³ TS2 _{H3O+,K+}	0.70	-0.09	0.50	-0.11	1.00
³ IM2 _{H3O+,K+}	0.24	-0.09	0.66	0.19	1.00
⁵ CAT _{H3O+,K+}			0.53	-1.53	-1.00
⁵ RC1 _{H3O+,K+}	0.68	-0.52	0.65	-0.81	0.00
⁵ IM1 _{H3O+,K+}	0.27	-0.62	0.69	-0.34	0.00
⁵ RC2 _{H3O+,K+}	0.76	-0.35	0.70	-0.12	1.00
⁵ TS2 _{H3O+,K+}	0.64	-0.31	0.70	-0.03	1.00
⁵ IM2 _{H3O+,K+}	0.25	-0.05	0.73	0.06	1.00

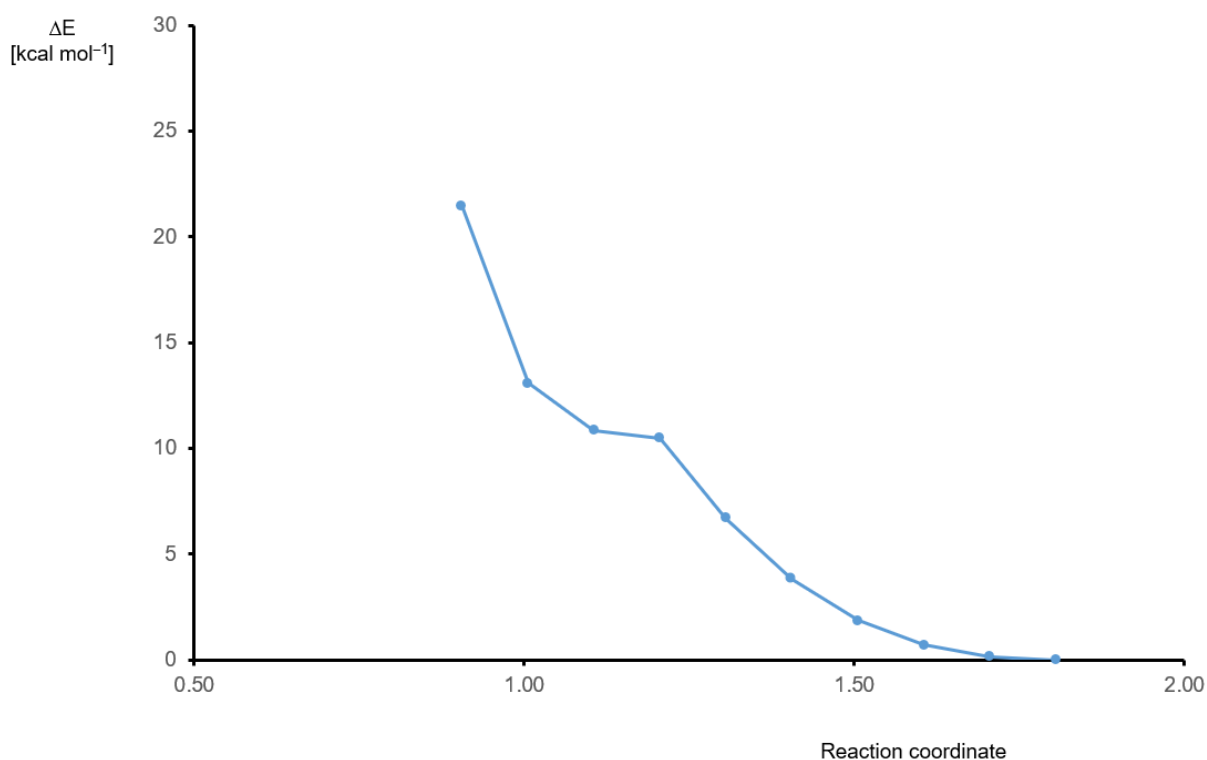


Fig. S5: UB3LYP-GD3BJ /BS1 calculated geometry scan for the O–H distance starting from ${}^3\text{IM1}_{\text{H3O}^+}$ on the right-hand-side to ${}^3\text{RC1}_{\text{H3O}^+}$. As can be seen no proton transfer barrier is encountered for the pathway from ${}^3\text{RC1}_{\text{H3O}^+}$ to ${}^3\text{IM1}_{\text{H3O}^+}$.

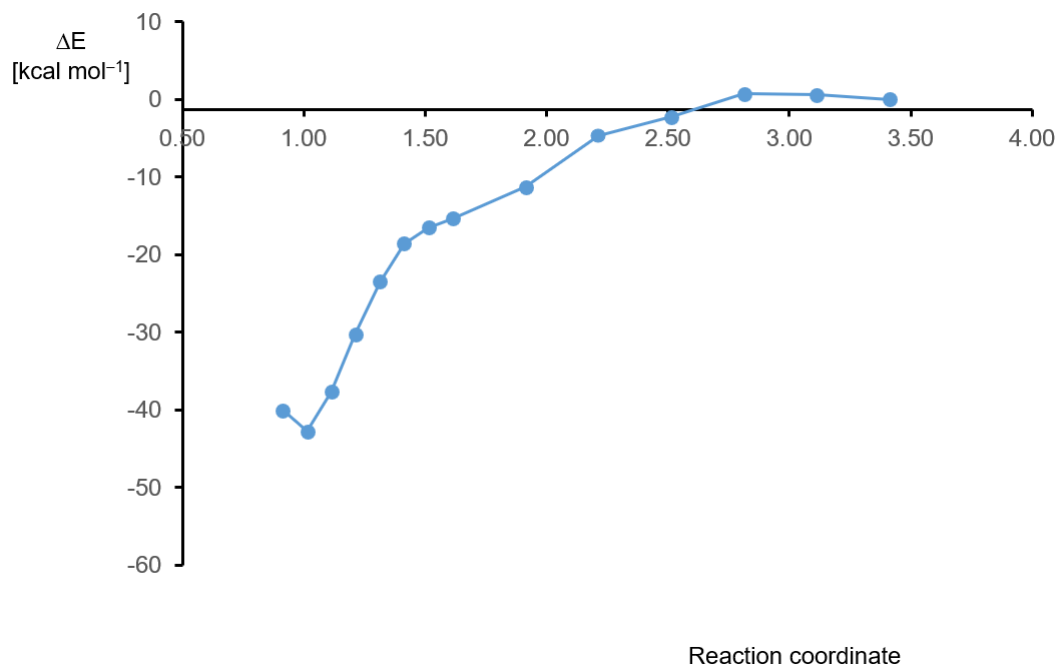


Fig. S6: UB3LYP-GD3BJ /BS1 calculated geometry scan for the O–H distance starting from ${}^3\text{RC2}_{\text{H3O}^+}$ on the right-hand-side to ${}^3\text{IM2}_{\text{H3O}^+}$. As can be seen a negligible proton transfer barrier is encountered for the pathway from ${}^3\text{RC2}_{\text{H3O}^+}$ to ${}^3\text{IM2}_{\text{H3O}^+}$.

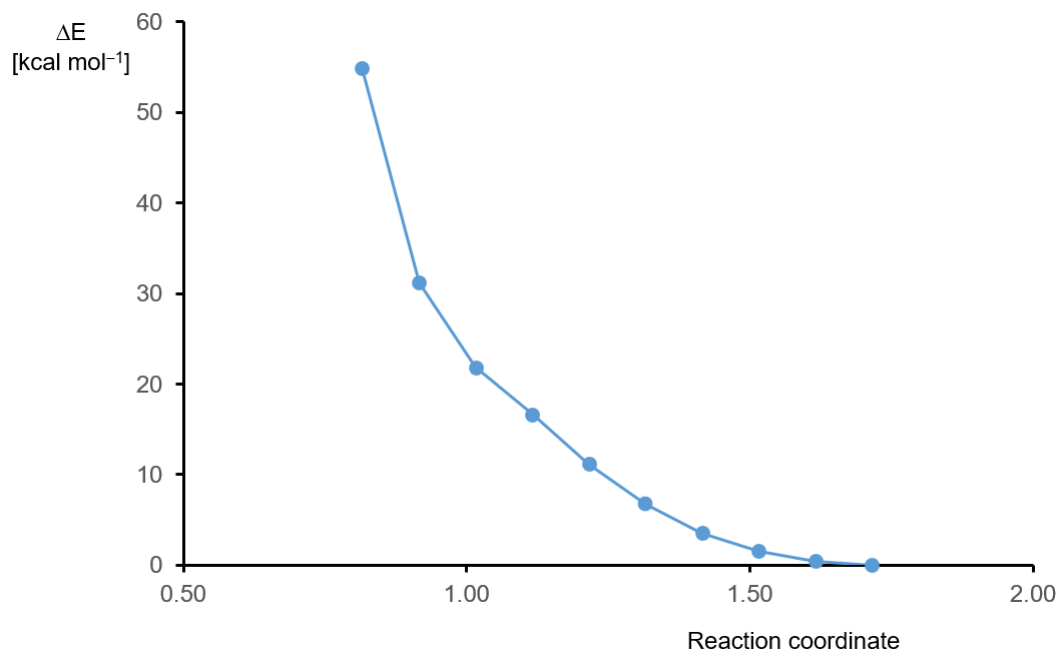


Fig. S7: UB3LYP-GD3BJ /BS1 calculated geometry scan for the O–H distance starting from ${}^5\text{IM1}_{\text{H3O}^+}$ on the right-hand-side to ${}^5\text{RC1}_{\text{H3O}^+}$. As can be seen no proton transfer barrier is encountered for the pathway from ${}^5\text{RC1}_{\text{H3O}^+}$ to ${}^5\text{IM1}_{\text{H3O}^+}$.

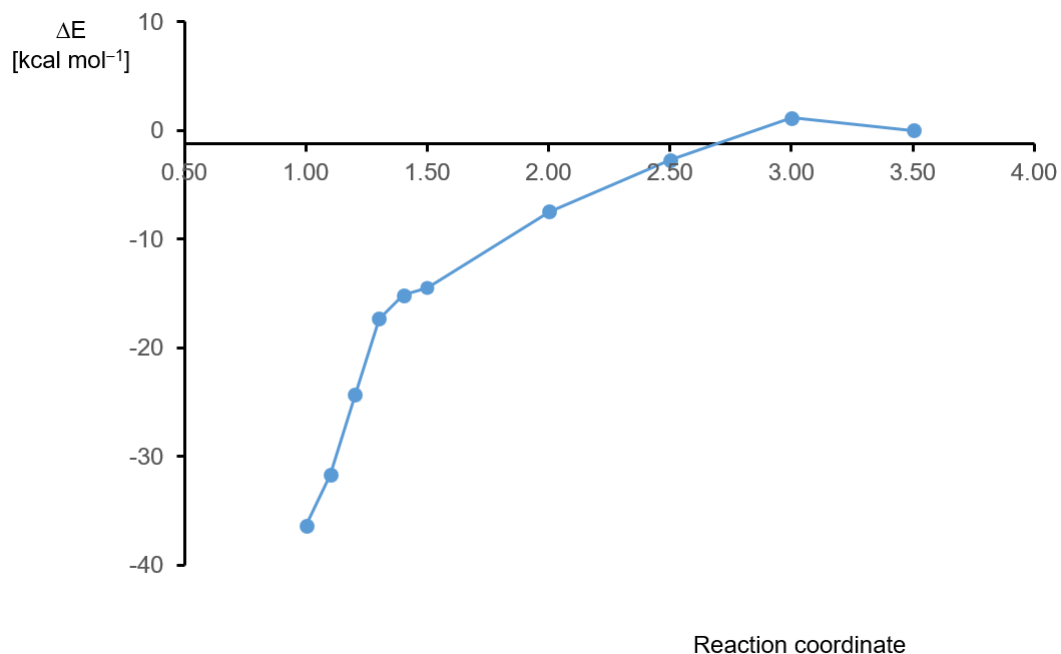


Fig. S8: UB3LYP-GD3BJ /BS1 calculated geometry scan for the O–H distance starting from ${}^5\text{RC2}_{\text{H3O}^+}$ on the right-hand-side to ${}^5\text{IM2}_{\text{H3O}^+}$. As can be seen a negligible proton transfer barrier is encountered for the pathway from ${}^5\text{RC2}_{\text{H3O}^+}$ to ${}^5\text{IM2}_{\text{H3O}^+}$.

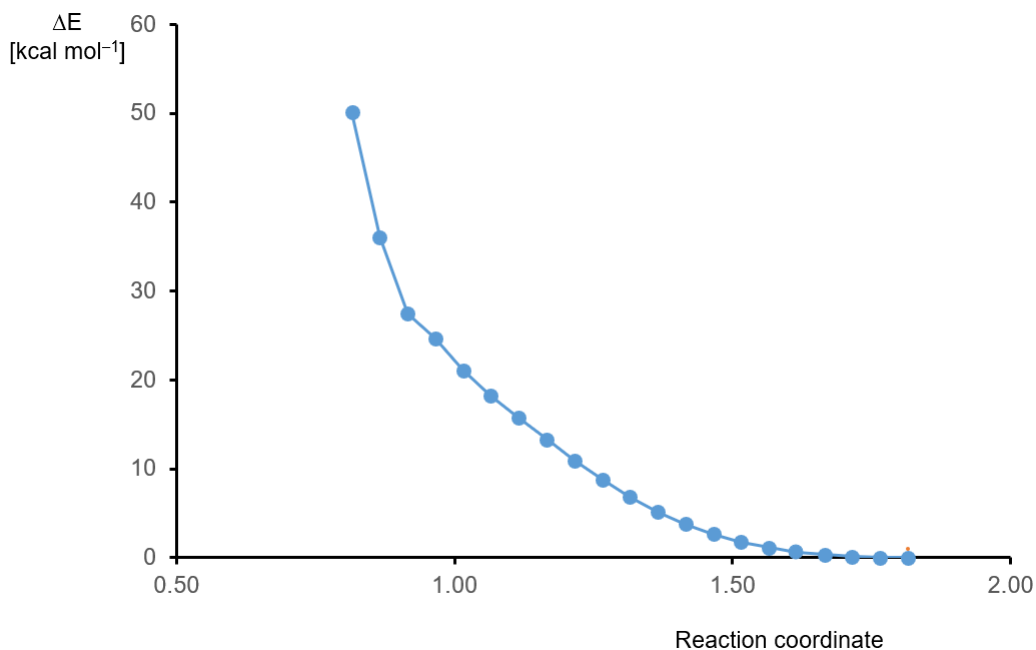


Fig. S9: UB3LYP-GD3BJ /BS1 calculated geometry scan for the O–H distance starting from ${}^3\text{IM1}_{\text{H}_3\text{O}^+, \text{K}^+}$ on the right-hand-side to ${}^3\text{RC1}_{\text{H}_3\text{O}^+, \text{K}^+}$. As can be seen no proton transfer barrier is encountered for the pathway from ${}^3\text{RC1}_{\text{H}_3\text{O}^+, \text{K}^+}$ to ${}^3\text{IM1}_{\text{H}_3\text{O}^+, \text{K}^+}$ (with nearby K^+).

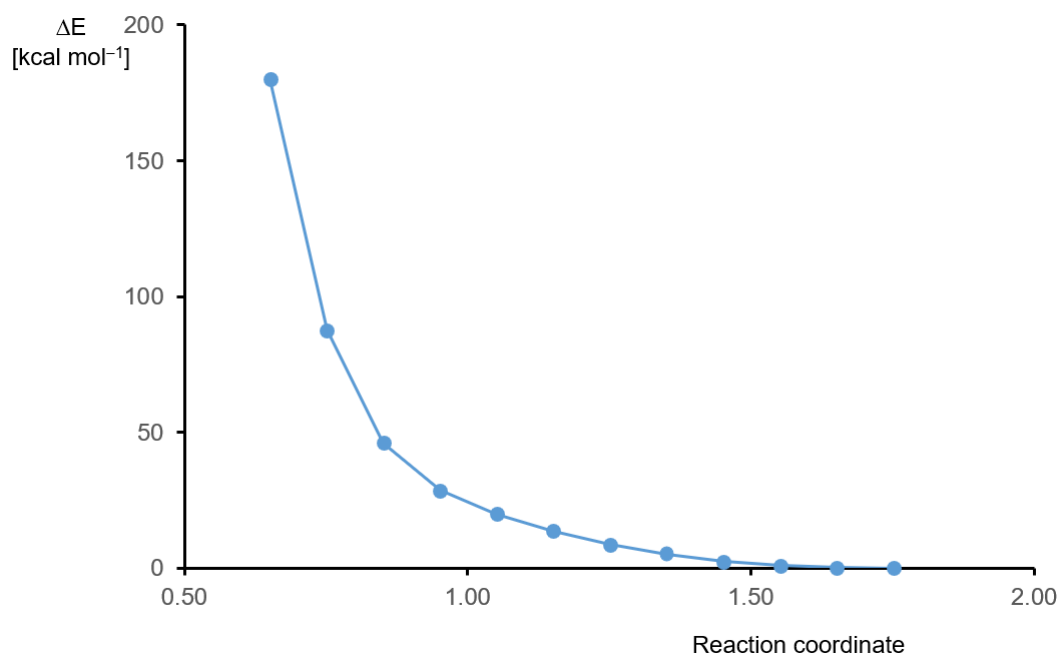


Fig. S10: UB3LYP-GD3BJ /BS1 calculated geometry scan for the O–H distance starting from ${}^5\text{IM1}_{\text{H}_3\text{O}^+, \text{K}^+}$ on the right-hand-side to ${}^5\text{RC1}_{\text{H}_3\text{O}^+, \text{K}^+}$. As can be seen no proton transfer barrier is encountered for the pathway from ${}^5\text{RC1}_{\text{H}_3\text{O}^+, \text{K}^+}$ to ${}^5\text{IM1}_{\text{H}_3\text{O}^+, \text{K}^+}$ (with nearby K^+).

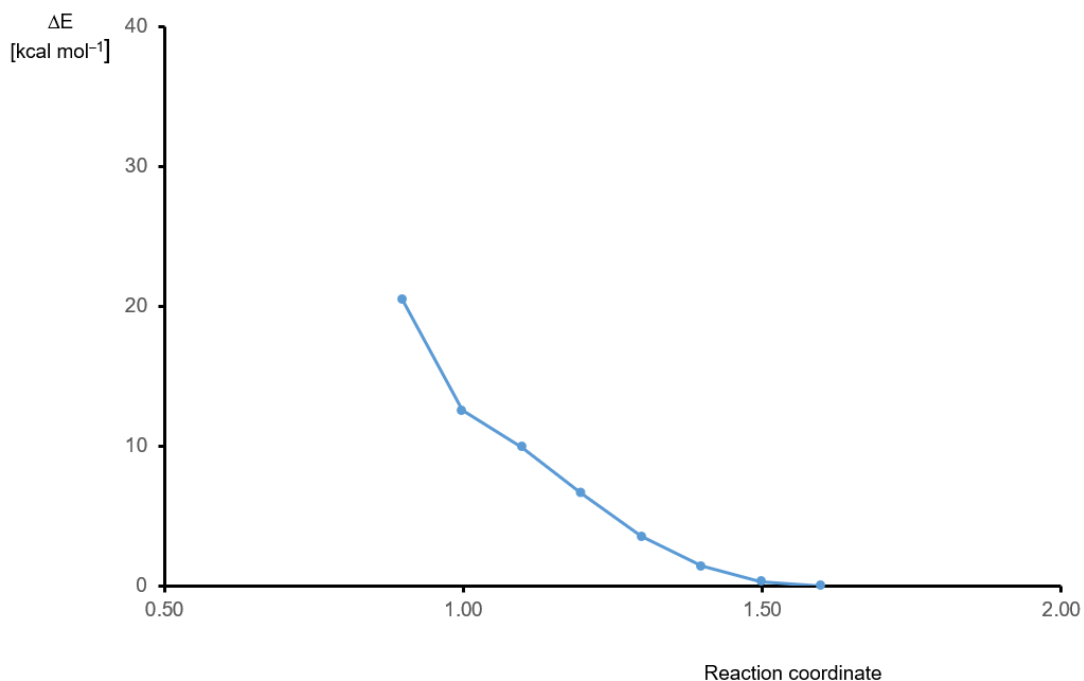


Fig. S11: UB3LYP-GD3BJ /BS1 calculated geometry scan for the O–H distance starting from ${}^3\text{IM1}_{\text{phenol},\text{K}^+}$ on the right-hand-side to ${}^3\text{RC1}_{\text{phenol},\text{K}^+}$. As can be seen no proton transfer barrier is encountered for the pathway from ${}^3\text{RC1}_{\text{phenol},\text{K}^+}$ to ${}^3\text{IM1}_{\text{phenol},\text{K}^+}$ (with nearby K^+).

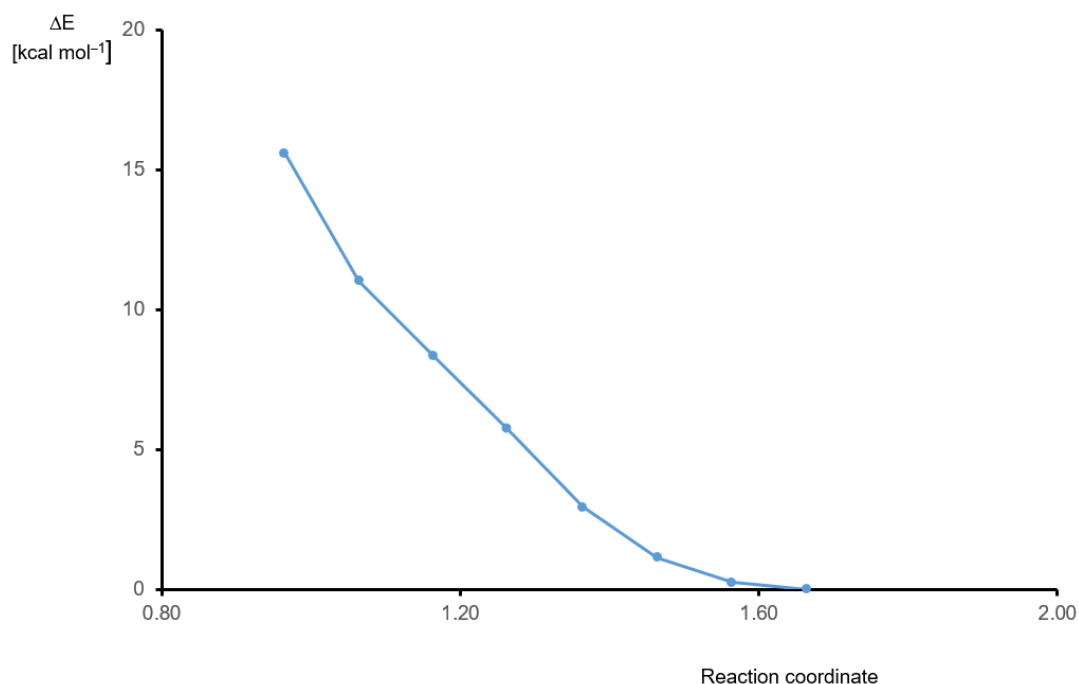


Fig. S12: UB3LYP-GD3BJ /BS1 calculated geometry scan for the O–H distance starting from ${}^5\text{IM1}_{\text{phenol},\text{K}^+}$ on the right-hand-side to ${}^5\text{RC1}_{\text{phenol},\text{K}^+}$. As can be seen no proton transfer barrier is encountered for the pathway from ${}^5\text{RC1}_{\text{phenol},\text{K}^+}$ to ${}^5\text{IM1}_{\text{phenol},\text{K}^+}$ (with nearby K^+).

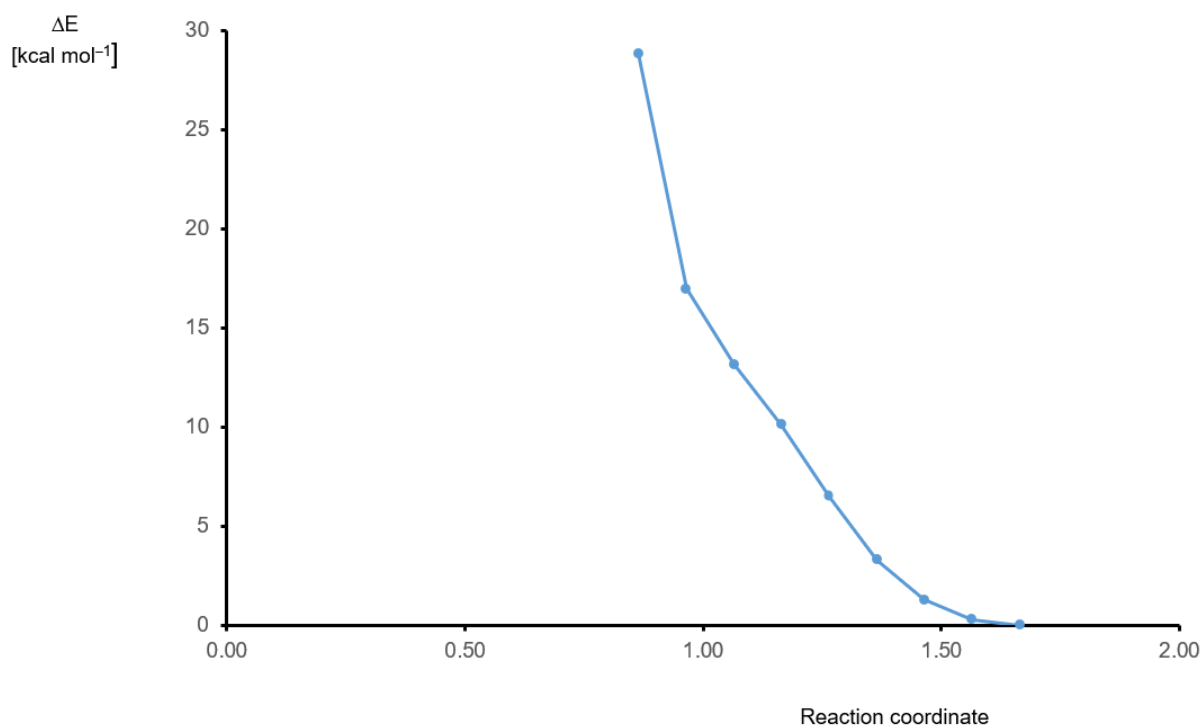


Fig. S13: UB3LYP-GD3BJ /BS1 calculated geometry scan for the O–H distance starting from ${}^3\text{IM1}_{\text{phenol, 6W, K}^+}$ on the right-hand-side to ${}^3\text{RC1}_{\text{phenol, 6W, K}^+}$. As can be seen no proton transfer barrier is encountered for the pathway from ${}^3\text{RC1}_{\text{phenol, 6W, K}^+}$ to ${}^3\text{IM1}_{\text{phenol, 6W, K}^+}$ (with nearby K^+).

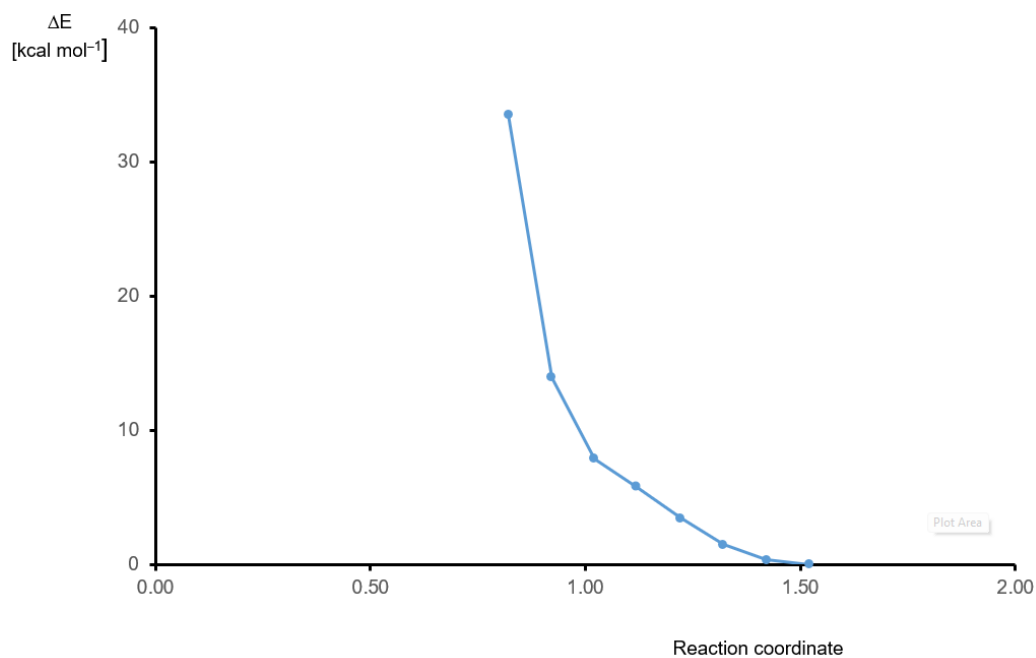


Fig. S14: UB3LYP-GD3BJ /BS1 calculated geometry scan for the O–H distance starting from ${}^3\text{IM1}_{\text{acetate},\text{K}^+}$ on the right-hand-side to ${}^3\text{RC1}_{\text{acetate},\text{K}^+}$. As can be seen no proton transfer barrier is encountered for the pathway from ${}^3\text{RC1}_{\text{acetate},\text{K}^+}$ to ${}^3\text{IM1}_{\text{acetate},\text{K}^+}$ (with nearby K^+).

Cartesian coordinates of optimized geometries:

CO₂ reduction on an iron-porphyrin center			1	1.024033000	-4.771121000	-0.868120000	
with/without nearby K⁺			1	-1.662453000	-4.883425000	-0.866047000	
UB3LYP/GD3BJ:			1	4.426644000	-1.051563000	-2.700947000	
²CAT_{H3O+}:			1	4.319349000	1.657830000	-2.860535000	
6	3.911110000	3.755722000	-1.074495000	1	0.725167000	5.256397000	-1.243103000
6	2.843461000	3.770836000	-1.993041000	1	-1.897141000	5.133514000	-0.636420000
6	2.782592000	4.813368000	-2.932994000	1	-5.587303000	1.400824000	-1.353163000
6	3.755427000	5.817567000	-2.954943000	1	-5.541816000	-1.286150000	-1.737621000
6	4.808882000	5.794680000	-2.035983000	1	2.240009000	-4.402517000	-3.160819000
6	4.881900000	4.759681000	-1.096332000	1	4.087410000	-6.064722000	-3.208477000
6	1.803229000	2.703837000	-1.944282000	1	6.062626000	-5.756008000	-1.697117000
6	2.228640000	1.364380000	-2.122131000	1	6.147235000	-3.819344000	-0.160585000
7	1.471141000	0.239654000	-1.824249000	1	1.963800000	4.830152000	-3.655847000
6	2.319411000	-0.838164000	-1.979478000	1	3.692124000	6.618016000	-3.696452000
6	3.588465000	-0.402267000	-2.460627000	1	5.570065000	6.578593000	-2.052184000
6	3.532041000	0.977261000	-2.547151000	1	5.699504000	4.734879000	-0.371164000
26	-0.517416000	0.171098000	-1.573527000	1	3.975116000	2.955749000	-0.333886000
7	-0.586416000	2.173897000	-1.552937000	1	-4.099832000	4.741198000	-2.137770000
6	-1.670258000	2.950524000	-1.164387000	1	-5.878048000	6.201212000	-1.175567000
6	-1.249554000	4.325728000	-0.966489000	1	-6.819790000	5.675671000	1.079973000
6	0.073562000	4.387478000	-1.277316000	1	-5.960572000	3.733625000	2.365076000
6	0.494630000	3.048594000	-1.640032000	1	-6.605700000	-4.576471000	0.276936000
6	-2.972434000	2.504931000	-0.998884000	1	-6.470594000	-6.400015000	-1.423562000
6	-4.014752000	3.415805000	-0.450703000	1	-4.676967000	-6.331780000	-3.161137000
6	-4.557059000	3.139452000	0.828753000	1	-3.039873000	-4.464875000	-3.185023000
6	-5.561836000	3.947393000	1.372152000	1	6.218582000	-1.956895000	0.784942000
6	-6.036702000	5.047523000	0.648620000	1	5.887943000	-0.943277000	-0.649547000
6	-5.508000000	5.343933000	-0.608955000	1	-4.657250000	1.663327000	3.437081000
6	-4.505757000	4.527900000	-1.146328000	1	-5.877073000	1.413144000	2.153412000
6	2.001345000	-2.182062000	-1.647565000	7	-3.202684000	-0.581931000	2.485750000
6	3.110285000	-3.174211000	-1.628432000	8	-0.119706000	1.480204000	2.470522000
6	3.092312000	-4.286394000	-2.488583000	8	-0.531129000	-2.236572000	2.396358000
6	4.132953000	-5.216760000	-2.521588000	8	2.982375000	2.128397000	2.105455000
6	5.235909000	-5.041954000	-1.683423000	8	2.190970000	-1.479387000	2.932426000
6	5.287762000	-3.944947000	-0.819593000	6	-1.784032000	-2.662722000	2.886552000
6	4.236116000	-3.020839000	-0.783823000	1	-1.853975000	-2.503711000	3.980778000
8	4.240647000	-1.962273000	0.088325000	6	-2.916889000	-1.983323000	2.144139000
6	5.475595000	-1.296267000	0.305761000	1	-1.905328000	-3.747382000	2.707867000
6	5.273024000	-0.054219000	1.175201000	1	-3.837195000	-2.547145000	2.338736000
7	4.790899000	-0.224046000	2.440082000	1	-2.714814000	-2.066985000	1.064476000
8	-4.017933000	2.081608000	1.498248000	6	0.511210000	-3.174785000	2.544051000
6	-4.810441000	1.323123000	2.397928000	1	0.614616000	-3.490600000	3.601375000
6	-4.470771000	-0.161328000	2.224598000	1	0.303273000	-4.077712000	1.937403000
8	-5.356984000	-0.927202000	1.844945000	6	1.795887000	-2.537683000	2.065824000
7	-0.444993000	-1.818254000	-1.516772000	1	2.585046000	-3.302034000	1.989768000
6	0.697217000	-2.601840000	-1.405449000	1	1.649402000	-2.116912000	1.061542000
6	0.325426000	-3.964825000	-1.073080000	6	3.296350000	-1.725578000	3.778159000
6	-1.034460000	-4.021327000	-1.073687000	1	3.191115000	-1.033431000	4.625746000
6	-1.523130000	-2.691359000	-1.374711000	1	3.266927000	-2.749480000	4.193272000
6	-2.870355000	-2.361882000	-1.482976000	6	4.634658000	-1.531654000	3.071505000
6	-3.878598000	-3.460913000	-1.466804000	1	5.435716000	-1.681313000	3.819472000
6	-4.902982000	-3.505378000	-0.500486000	1	4.745914000	-2.311982000	2.314062000
6	-5.823933000	-4.555953000	-0.486913000	6	-2.133636000	0.286802000	2.967935000
6	-5.748281000	-5.580096000	-1.437329000	6	-1.178085000	0.736905000	1.870031000
6	-4.742129000	-5.543009000	-2.407369000	1	-2.569136000	1.172158000	3.446801000
6	-3.819650000	-4.493496000	-2.421011000	1	-1.562559000	-0.242680000	3.741152000
7	-2.512579000	0.094157000	-1.394383000	1	-1.718102000	1.364052000	1.147095000
6	-3.326865000	-1.022146000	-1.544248000	1	-0.769714000	-0.135417000	1.337286000
6	-4.694161000	-0.621588000	-1.598835000	6	0.599446000	2.226797000	1.497714000
6	-4.719996000	0.746453000	-1.401243000	1	-0.073609000	2.985323000	1.064939000
6	-3.365221000	1.167370000	-1.267124000	6	1.818540000	2.932138000	2.053680000
8	5.602847000	1.040309000	0.727608000	1	0.919603000	1.567683000	0.673727000
1	-4.977090000	-2.712982000	0.246027000	1	2.041800000	3.762732000	1.363548000
				1	1.590412000	3.371219000	3.042922000
				6	4.702137000	0.956096000	3.300258000

1	4.989362000	0.614327000	4.347743000	8	3.364687000	1.117388000	3.327077000
1	5.435947000	1.639802000	2.960160000	1	0.050537000	-4.453604000	-2.311074000
6	3.334487000	1.572580000	3.378999000	1	4.504013000	0.158484000	-2.641442000
1	3.406071000	2.408339000	4.105585000	1	3.143657000	-2.015077000	-3.474551000
1	2.564619000	0.885285000	3.757820000	1	3.186201000	4.810273000	-0.553094000
8	0.616327000	-0.037517000	4.683247000	1	0.844507000	6.011968000	0.128823000
1	0.368211000	0.674949000	4.062914000	1	-4.240996000	4.530048000	0.122372000
1	0.970698000	-0.689694000	4.046108000	1	-5.520732000	2.185618000	-0.252886000

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6	-1.484208000	6.027793000	1.553980000	1	-1.961367000	-3.522949000	-3.295641000
6	-1.818002000	5.643679000	0.243051000	1	3.935392000	3.853268000	-3.246360000
6	-2.533394000	6.553327000	-0.554122000	1	6.311749000	4.570414000	-3.429511000
6	-2.910469000	7.804495000	-0.056478000	1	7.996603000	3.657789000	-1.805783000
6	-2.572521000	8.172139000	1.249487000	1	7.246851000	2.072677000	-0.022911000
6	-1.856423000	7.278108000	2.053573000	1	-2.794653000	6.270703000	-1.576602000
6	-1.425346000	4.302053000	-0.279408000	1	-3.466996000	8.496514000	-0.693699000
6	-0.043760000	4.043114000	-0.473164000	1	-2.865360000	9.149967000	1.639559000
7	0.488405000	2.867071000	-0.963777000	1	-1.591853000	7.554133000	3.077553000
6	1.853089000	3.080991000	-1.051112000	1	-0.930643000	5.328979000	2.185344000
6	2.184266000	4.390683000	-0.586845000	1	-5.863043000	0.105655000	-2.768107000
6	0.993209000	5.000317000	-0.238835000	1	-8.198074000	-0.656128000	-2.332024000
26	-0.487206000	1.119254000	-1.289033000	1	-8.802526000	-1.551308000	-0.075166000
7	-2.234759000	2.056727000	-0.946645000	1	-7.077993000	-1.689773000	1.703811000
6	-3.473619000	1.442861000	-0.838678000	1	0.652567000	-6.440994000	-3.646393000
6	-4.466741000	2.405313000	-0.405152000	1	1.627520000	-6.173071000	-5.932590000
6	-3.820741000	3.587289000	-0.217524000	1	1.980517000	-3.876444000	-6.853292000
6	-2.418030000	3.361868000	-0.516152000	1	1.368573000	-1.887418000	-5.504742000
6	-3.751974000	0.105422000	-1.065219000	1	3.222811000	2.075391000	1.110862000
6	-5.141863000	-0.375444000	-0.803430000	1	2.966224000	0.482506000	0.378194000
6	-5.505666000	-0.899758000	0.445927000	1	-3.802433000	-1.820581000	3.116186000
6	-6.812901000	-1.310202000	0.716289000	1	-5.322850000	-2.535591000	2.538461000
6	-7.780821000	-1.227481000	-0.285557000	7	-2.370808000	-3.536517000	1.635726000
6	-7.443309000	-0.723513000	-1.545539000	8	-0.633807000	-1.556670000	4.210111000
6	-6.136270000	-0.298393000	-1.790876000	8	0.664572000	-4.068685000	1.215885000
6	2.795874000	2.157813000	-1.559093000	8	2.159136000	-1.794798000	4.035255000
6	4.235657000	2.566738000	-1.556949000	8	3.379983000	-3.389884000	1.379278000
6	4.676903000	3.471844000	-2.540435000	6	-0.392415000	-4.983778000	0.981239000
6	6.007779000	3.872724000	-2.646146000	1	-0.503175000	-5.579973000	1.899568000
6	6.946653000	3.361864000	-1.742034000	6	-1.707317000	-4.336715000	0.590634000
6	6.538191000	2.477409000	-0.748362000	1	-0.114044000	-5.683193000	0.172439000
6	5.193395000	2.078978000	-0.641352000	1	-2.400136000	-5.135196000	0.283814000
8	4.950228000	1.187028000	0.360241000	1	-1.572069000	-3.704227000	-0.302506000
6	3.666333000	1.081735000	0.974020000	6	1.389798000	-3.663141000	0.066096000
6	3.804735000	0.482708000	2.367729000	1	1.785343000	-4.557116000	-0.452067000
7	4.389056000	-0.742716000	2.507378000	1	0.738351000	-3.115335000	-0.636202000
8	-4.534302000	-0.932568000	1.446708000	6	2.520302000	-2.741778000	0.456102000
6	-4.351644000	-2.131859000	2.225327000	1	3.052339000	-2.477222000	-0.476535000
6	-3.646861000	-3.169733000	1.345793000	1	2.114726000	-1.814657000	0.884969000
8	-4.252281000	-3.586658000	0.361753000	6	4.726745000	-2.984682000	1.359665000
7	1.179540000	0.392005000	-2.199483000	1	5.205547000	-3.486630000	2.214050000
6	2.456717000	0.924452000	-2.089490000	1	5.235299000	-3.354092000	0.444951000
6	3.430118000	-0.010160000	-2.613631000	6	4.990165000	-1.478046000	1.397471000
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6	1.333878000	-0.856258000	-2.774220000	1	4.651049000	-1.031348000	0.459850000
6	0.332514000	-1.799088000	-3.008980000	6	-1.717979000	-3.193945000	2.900237000
6	0.676597000	-3.016422000	-3.798792000	6	-1.031684000	-1.836692000	2.882914000
6	0.474672000	-4.319350000	-3.304688000	1	-2.456657000	-3.218750000	3.713676000
6	0.813429000	-5.442866000	-4.061648000	1	-0.969720000	-3.951615000	3.154604000
6	1.361734000	-5.294371000	-5.340048000	1	-1.720290000	-1.060777000	2.507256000
6	1.561950000	-4.008762000	-5.852288000	1	-0.173934000	-1.852729000	2.196092000
6	1.219602000	-2.887540000	-5.092399000	6	0.235248000	-0.442758000	4.360266000
7	-1.479999000	-0.542275000	-1.842688000	1	-0.226808000	0.285389000	5.052565000
6	-1.000075000	-1.638009000	-2.543838000	6	1.571011000	-0.868986000	4.933473000
6	-2.052256000	-2.587608000	-2.752052000	1	0.381553000	0.063638000	3.393870000
6	-3.181690000	-2.079107000	-2.143000000	1	2.206913000	0.023940000	5.044174000
6	-2.819913000	-0.808958000	-1.607804000	1	1.435722000	-1.344627000	5.925267000
				6	4.564327000	-1.243600000	3.865755000

6	-3.321010000	-0.288480000	0.293213000	6	3.068276000	-4.303220000	-2.469793000
1	-3.089987000	0.062487000	1.313303000	6	4.104502000	-5.238664000	-2.499761000
1	-2.514918000	0.055328000	-0.378869000	6	5.209253000	-5.065981000	-1.663569000
6	-4.906873000	1.509115000	0.240416000	6	5.266030000	-3.965156000	-0.804556000
1	-5.898633000	1.704278000	-0.193054000	6	4.218519000	-3.036504000	-0.771439000
1	-5.013955000	1.576817000	1.341372000	8	4.229668000	-1.975749000	0.098523000
6	-3.918411000	2.605457000	-0.167570000	6	5.466963000	-1.312816000	0.308718000
1	-4.364011000	3.571586000	0.129478000	6	5.272020000	-0.070841000	1.179594000
1	-3.007605000	2.500469000	0.427201000	7	4.788925000	-0.239433000	2.444373000
6	-1.804683000	-3.212695000	-3.521919000	8	-4.002931000	2.081412000	1.515998000
6	-2.004384000	-1.696154000	-3.555112000	6	-4.804174000	1.316611000	2.401497000
1	-1.050463000	-3.499963000	-4.269423000	6	-4.469438000	-0.168141000	2.221925000
1	-2.736527000	-3.704746000	-3.833986000	8	-5.363331000	-0.932749000	1.858366000
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1	-2.766469000	-1.401453000	-2.824636000	6	0.676268000	-2.610185000	-1.407468000
6	-2.350902000	0.064447000	-5.121713000	6	0.294717000	-3.977034000	-1.087594000
1	-2.058639000	0.207279000	-6.175888000	6	-1.064315000	-4.026721000	-1.098818000
6	-3.685921000	0.758295000	-4.914286000	6	-1.542813000	-2.687701000	-1.392037000
1	-1.594635000	0.559393000	-4.487826000	6	-2.886550000	-2.343658000	-1.493977000
1	-3.543687000	1.830615000	-5.127690000	6	-3.904318000	-3.433586000	-1.487514000
1	-4.446135000	0.356598000	-5.612278000	6	-4.931001000	-3.477719000	-0.523193000
6	-4.635068000	2.754236000	-2.566190000	6	-5.859277000	-4.521786000	-0.517474000
1	-5.481423000	3.285073000	-2.102008000	6	-5.789718000	-5.540812000	-1.474141000
1	-4.259832000	3.377522000	-3.387702000	6	-4.781938000	-5.504306000	-2.442396000
6	-5.146617000	1.418058000	-3.107490000	6	-3.852505000	-4.460698000	-2.448402000
1	-5.885111000	1.620643000	-3.905585000	7	-2.513440000	0.114703000	-1.380903000
1	-5.653727000	0.849439000	-2.320114000	6	-3.335097000	-0.997029000	-1.540754000
8	-5.644349000	-1.649618000	-2.860108000	6	-4.695888000	-0.585586000	-1.593752000
1	-5.066952000	-1.032204000	-3.346650000	6	-4.711619000	0.785389000	-1.387973000
1	-5.183306000	-1.662773000	-2.000673000	6	-3.357693000	1.196256000	-1.249806000
6	0.503859000	-0.077176000	-0.329354000	8	5.607042000	1.022625000	0.733119000
8	-0.012922000	-0.849375000	-0.984052000	1	-5.000300000	-2.690099000	0.228765000
1	1.875067000	1.941209000	-2.084527000	1	0.987470000	-4.788529000	-0.882862000
8	3.027331000	-0.461725000	-2.661905000	1	-1.698808000	-4.886568000	-0.901747000
1	2.734046000	-1.341555000	-2.350203000	1	4.415175000	-1.073176000	-2.693298000
1	2.029069000	2.031080000	-1.133666000	1	4.321365000	1.637134000	-2.869540000
1	2.244527000	1.052104000	-2.295734000	1	0.754803000	5.273687000	-1.258698000
1	3.923969000	-0.386349000	-2.299345000	1	-1.862147000	5.166049000	-0.629484000
				1	-5.575178000	1.444766000	-1.338121000
				1	-5.549369000	-1.241915000	-1.736166000
				1	2.216164000	-4.417873000	-3.142457000
				1	4.054491000	-6.088741000	-3.183852000
				1	6.032940000	-5.783586000	-1.675137000
				1	6.126390000	-3.840417000	-0.146435000
				1	1.985867000	4.829711000	-3.668012000
				1	3.724684000	6.607168000	-3.712106000
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				1	5.727386000	4.711550000	-0.391089000
				1	3.992018000	2.943460000	-0.350410000
				1	-4.064236000	4.796464000	-2.080207000
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6	3.931600000	3.743626000	-1.091027000				
6	2.861290000	3.764628000	-2.006809000				
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1	-1.913825000	-3.760427000	2.689333000	6	5.227305000	-5.055203000	-1.687911000
1	-3.839099000	-2.551965000	2.308696000	6	5.287465000	-3.968487000	-0.811085000
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1	0.600008000	-3.507155000	3.607622000	6	5.507368000	-1.346967000	0.356884000
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1	4.745397000	-2.327647000	2.320942000	6	-1.075942000	-4.008003000	-1.162422000
6	-2.124105000	0.275870000	2.938189000	6	-1.542642000	-2.683310000	-1.450892000
6	-1.165170000	0.715541000	1.838053000	6	-2.905533000	-2.321735000	-1.566447000
1	-2.553154000	1.167510000	3.410519000	6	-3.918844000	-3.408873000	-1.573003000
1	-1.553790000	-0.250899000	3.713866000	6	-4.967559000	-3.456588000	-0.627664000
1	-1.700530000	1.343800000	1.112464000	6	-5.899705000	-4.497626000	-0.633751000
1	-0.763135000	-0.167729000	1.315584000	6	-5.815062000	-5.525955000	-1.579584000
6	0.608230000	2.220573000	1.479035000	6	-4.782237000	-5.496639000	-2.523822000
1	-0.068597000	2.983330000	1.059854000	6	-3.853247000	-4.453764000	-2.519184000
6	1.824034000	2.920644000	2.048066000	7	-2.518851000	0.133417000	-1.405051000
1	0.935118000	1.579655000	0.643436000	6	-3.342482000	-0.978217000	-1.573797000
1	2.052750000	3.755353000	1.364593000	6	-4.707713000	-0.555681000	-1.614295000
1	1.589486000	3.353409000	3.038490000	6	-4.720790000	0.806445000	-1.368336000
6	4.701256000	0.941443000	3.303504000	6	-3.364483000	1.221333000	-1.234242000
1	4.997602000	0.649453000	4.323379000	8	5.682933000	0.981847000	0.805624000
1	5.427967000	1.675643000	2.931753000	1	-5.045294000	-2.671297000	0.125954000
6	3.331820000	1.603986000	3.372942000	1	0.991127000	-4.775307000	-0.927453000
1	3.405069000	2.428887000	4.111165000	1	-1.709963000	-4.873681000	-0.988356000
1	2.564158000	0.909796000	3.743497000	1	4.453483000	-1.032995000	-2.603028000
8	0.617813000	-0.033003000	4.695222000	1	4.349761000	1.667386000	-2.809155000
1	0.370244000	0.688505000	4.087072000	1	0.757457000	5.297152000	-1.194526000
1	0.976587000	-0.674615000	4.049753000	1	-1.870493000	5.175459000	-0.548248000
				1	-5.585154000	1.464306000	-1.298810000
				1	-5.564324000	-1.205081000	-1.772634000
				1	2.231174000	-4.368266000	-3.144863000
				1	4.061759000	-6.043104000	-3.223899000
				1	6.048023000	-5.776024000	-1.713772000
				1	6.148075000	-3.858476000	-0.150088000
				1	1.885067000	4.892046000	-3.629890000
				1	3.588952000	6.694599000	-3.744439000
				1	5.559343000	6.657755000	-2.207425000
				1	5.791680000	4.795843000	-0.554920000
				1	4.083517000	3.006746000	-0.440603000
				1	-4.066565000	4.837140000	-1.971853000
				1	-5.818322000	6.286080000	-0.949759000
				1	-6.767675000	5.686133000	1.286114000
				1	-5.932450000	3.680798000	2.489089000
				1	-6.695921000	-4.510743000	0.116156000
				1	-6.544491000	-6.339908000	-1.581205000
				1	-4.704959000	-6.287315000	-3.275398000
				1	-3.055167000	-4.436788000	-3.264574000
				1	6.244900000	-2.017187000	0.833581000
				1	5.925920000	-0.991973000	-0.595269000
				1	-4.666572000	1.596986000	3.495292000
				1	-5.882265000	1.373011000	2.204696000
				7	-3.204332000	-0.627720000	2.445735000
				8	-0.109275000	1.416356000	2.409391000
				8	-0.533248000	-2.286870000	2.387930000
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				8	2.184124000	-1.542233000	2.937028000
				6	-1.807596000	-2.725864000	2.808063000
⁵CAT_{H3O+}:							
6	3.975947000	3.808493000	-1.173903000				
6	2.856082000	3.810687000	-2.033342000				
6	2.742182000	4.872171000	-2.952853000				
6	3.701417000	5.886832000	-3.015965000				
6	4.807214000	5.866249000	-2.158802000				
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6	1.827341000	2.741385000	-1.946298000				
6	2.248341000	1.400291000	-2.081697000				
7	1.484627000	0.272785000	-1.781466000				
6	2.336045000	-0.820386000	-1.911864000				
6	3.611407000	-0.382566000	-2.376571000				
6	3.556610000	0.996437000	-2.488171000				
26	-0.518031000	0.205674000	-1.573366000				
7	-0.578121000	2.240278000	-1.537518000				
6	-1.655266000	3.012082000	-1.110955000				
6	-1.233416000	4.367142000	-0.899008000				
6	0.102706000	4.430399000	-1.237411000				
6	0.504799000	3.108122000	-1.626892000				
6	-2.967612000	2.542464000	-0.939042000				
6	-3.996096000	3.437757000	-0.346613000				
6	-4.542574000	3.125779000	0.925914000				
6	-5.533870000	3.927321000	1.503431000				
6	-5.994723000	5.064211000	0.827844000				
6	-5.461251000	5.401148000	-0.417519000				
6	-4.473887000	4.589524000	-0.988932000				
6	2.009609000	-2.161361000	-1.612686000				
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1	-1.922963000	-2.608567000	3.904178000	6	5.173364000	2.178808000	-2.918214000
6	-2.909431000	-2.012132000	2.049110000	6	6.559111000	2.247267000	-3.056605000
1	-1.922183000	-3.802649000	2.582203000	6	7.369372000	1.558390000	-2.146902000
1	-3.838593000	-2.577087000	2.186918000	6	6.783058000	0.829342000	-1.116159000
1	-2.670955000	-2.049745000	0.973267000	6	5.385232000	0.766194000	-0.976708000
6	0.499827000	-3.233923000	2.543700000	8	4.957765000	-0.021109000	0.053566000
1	0.587654000	-3.554265000	3.601616000	6	3.742928000	0.248105000	0.754497000
1	0.291611000	-4.131957000	1.930010000	6	3.890813000	0.031106000	2.261107000
6	1.796014000	-2.610730000	2.077725000	7	4.428098000	-1.127995000	2.741128000
1	2.581061000	-3.381960000	2.029782000	8	-4.433637000	-0.241599000	1.616681000
1	1.672139000	-2.209150000	1.062151000	6	-4.421742000	-1.428033000	2.429339000
6	3.278741000	-1.780336000	3.798006000	6	-3.997821000	-2.620048000	1.565759000
1	3.161412000	-1.084501000	4.641157000	8	-4.763390000	-2.978775000	0.675475000
1	3.246568000	-2.802402000	4.217897000	7	1.070463000	-0.021669000	-2.357841000
6	4.627001000	-1.588138000	3.110346000	6	2.428575000	0.226941000	-2.318108000
1	5.416259000	-1.743758000	3.869957000	6	3.137601000	-0.924266000	-2.854395000
1	4.745226000	-2.365987000	2.351421000	6	2.198784000	-1.849105000	-3.204456000
6	-2.123517000	0.236244000	2.908321000	6	0.894010000	-1.290312000	-2.871043000
6	-1.171032000	0.681264000	1.804907000	6	-0.319926000	-1.987797000	-2.963314000
1	-2.546939000	1.126828000	3.387163000	6	-0.314775000	-3.313709000	-3.642351000
1	-1.547816000	-0.294935000	3.677284000	6	-0.794797000	-4.467611000	-2.992747000
1	-1.708272000	1.309795000	1.080848000	6	-0.782678000	-5.712189000	-3.624421000
1	-0.766015000	-0.197626000	1.277289000	6	-0.292105000	-5.836015000	-4.929455000
6	0.614919000	2.172214000	1.444312000	6	0.181076000	-4.699927000	-5.593346000
1	-0.050165000	2.941201000	1.018848000	6	0.165428000	-3.454933000	-4.958222000
6	1.836945000	2.859038000	2.013271000	7	-1.759360000	-0.347064000	-1.747349000
1	0.929732000	1.523960000	0.609938000	6	-1.569733000	-1.525085000	-2.441011000
1	2.085543000	3.675493000	1.315151000	6	-2.830337000	-2.199088000	-2.578742000
1	1.601427000	3.313910000	2.993810000	6	-3.780310000	-1.419862000	-1.942496000
6	4.695412000	0.900545000	3.343543000	6	-3.100212000	-0.261922000	-1.450588000
1	4.972157000	0.610422000	4.369602000	8	3.504436000	0.933444000	3.006762000
1	5.428338000	1.634521000	2.984104000	1	-1.168096000	-4.373204000	-1.974158000
6	3.322906000	1.560380000	3.383186000	1	4.218538000	-1.008566000	-2.943035000
1	3.387840000	2.404084000	4.101055000	1	2.372274000	-2.839993000	-3.615736000
1	2.554121000	0.874085000	3.765865000	1	4.093042000	3.996705000	-1.103705000
8	0.604682000	-0.052627000	4.674211000	1	2.130587000	5.736321000	-0.429249000
1	0.357948000	0.656874000	4.050437000	1	-3.176404000	5.327254000	0.239159000
1	0.965772000	-0.704881000	4.040700000	1	-4.938546000	3.301791000	0.117705000
				1	-4.842612000	-1.619430000	-1.836608000
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				1	7.391273000	0.292431000	-0.385317000
				1	-1.680876000	6.639839000	-1.773921000
				1	-1.805907000	8.994752000	-0.986159000
				1	-0.762062000	9.643689000	1.187555000
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				1	0.512412000	5.559850000	1.766701000
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				1	-8.889407000	0.021731000	0.581663000
				1	-7.048375000	-0.649085000	2.096077000
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				1	-0.281572000	-6.809659000	-5.425336000
				1	0.558176000	-4.780620000	-6.616137000
				1	0.524013000	-2.570390000	-5.488746000
				1	3.457212000	1.298274000	0.643263000
				1	2.918911000	-0.363623000	0.371947000
				1	-3.758733000	-1.203306000	3.267072000
				1	-5.422247000	-1.634890000	2.828629000
				7	-2.795060000	-3.213062000	1.798537000
				8	-0.462086000	-1.513194000	4.099058000
				8	-0.201456000	-3.713242000	0.372631000
				8	2.264139000	-1.886784000	4.531882000
				8	2.396666000	-2.749423000	1.381387000
				6	-1.015881000	-4.768033000	0.838240000
⁵RC1 H3O+:							
6	0.008850000	6.316442000	1.160954000				
6	-0.576345000	5.933159000	-0.059672000				
6	-1.226497000	6.920374000	-0.820875000				
6	-1.295744000	8.244322000	-0.376770000				
6	-0.709948000	8.609285000	0.839181000				
6	-0.056506000	7.638461000	1.606986000				
6	-0.517115000	4.516550000	-0.526878000				
6	0.779433000	3.977187000	-0.799520000				
7	1.027317000	2.686425000	-1.211515000				
6	2.386547000	2.561190000	-1.385122000				
6	3.024539000	3.801561000	-1.055753000				
6	2.018472000	4.691875000	-0.709145000				
26	-0.334670000	1.106066000	-1.257318000				
7	-1.886827000	2.499164000	-1.014143000				
6	-3.189432000	2.139193000	-0.725622000				
6	-3.895429000	3.294089000	-0.190833000				
6	-3.001017000	4.319812000	-0.129738000				
6	-1.721603000	3.810304000	-0.608855000				
6	-3.748662000	0.869879000	-0.871067000				
6	-5.171475000	0.667083000	-0.461426000				
6	-5.495122000	0.044756000	0.756385000				
6	-6.817793000	-0.182706000	1.138195000				
6	-7.854043000	0.203472000	0.285165000				
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6	-6.234955000	1.057234000	-1.290189000				
6	3.052028000	1.387944000	-1.857277000				
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1	-0.637997000	-5.130739000	1.810793000	6	5.316868000	-1.584089000	-0.497497000
6	-2.469161000	-4.337325000	0.905223000	6	6.537630000	-2.189678000	-0.809784000
1	-0.987079000	-5.625197000	0.138476000	6	7.516389000	-2.326402000	0.176119000
1	-3.062688000	-5.222920000	1.198245000	6	7.281880000	-1.851317000	1.470264000
1	-2.808729000	-4.051001000	-0.099088000	6	6.064605000	-1.232717000	1.766148000
6	1.070821000	-4.109941000	-0.115604000	6	-2.423725000	2.564092000	1.472053000
1	1.453095000	-4.977962000	0.454073000	6	-3.789439000	3.178145000	1.475577000
1	0.992867000	-4.412086000	-1.174969000	6	-4.063837000	4.161102000	2.446508000
6	2.032393000	-2.948525000	0.021647000	6	-5.315388000	4.759973000	2.576371000
1	2.923363000	-3.119088000	-0.603755000	6	-6.347458000	4.371078000	1.714931000
1	1.542851000	-2.028290000	-0.323247000	6	-6.105657000	3.409651000	0.738715000
6	3.613506000	-3.323090000	1.822655000	6	-4.840157000	2.810148000	0.605256000
1	3.410883000	-3.778873000	2.799827000	8	-4.770380000	1.874918000	-0.382331000
1	3.940957000	-4.134640000	1.148096000	6	-3.532945000	1.537891000	-1.004510000
6	4.733270000	-2.285046000	1.904552000	6	-3.810212000	0.848387000	-2.334908000
1	5.634280000	-2.776089000	2.308549000	7	-4.523057000	-0.315393000	-2.329977000
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6	-1.995312000	-2.938178000	2.995471000	6	3.930898000	-2.479960000	-2.281062000
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1	-1.329513000	-3.786261000	3.186886000	7	-1.087519000	0.575903000	2.161508000
1	-1.729536000	-0.810868000	2.610673000	6	-2.275636000	1.276217000	2.042071000
1	-0.404092000	-1.833069000	2.039225000	6	-3.347190000	0.528746000	2.605715000
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1	-0.066527000	0.496571000	4.482939000	6	-1.403666000	-0.603879000	2.809917000
6	1.607021000	-0.733989000	5.034609000	6	-0.498450000	-1.660776000	3.103525000
1	0.819045000	-0.207901000	3.113794000	6	-0.992123000	-2.771639000	-2.969192000
1	2.281868000	0.136901000	5.027995000	6	-1.023772000	-4.111115000	3.541986000
1	1.268257000	-0.919278000	6.072752000	6	-1.491907000	-5.126307000	4.381210000
6	4.626105000	-1.234489000	4.182995000	6	-1.943204000	-4.824649000	5.668917000
1	5.624667000	-1.661922000	4.375477000	6	-1.919020000	-3.496931000	6.110326000
1	4.614534000	-0.212007000	4.576973000	6	-1.449904000	-2.485632000	5.270183000
6	3.597217000	-2.099624000	4.933449000	7	1.438400000	-0.672029000	1.905059000
1	3.724372000	-1.924517000	6.018955000	6	0.806336000	-1.678271000	2.628250000
1	3.795875000	-3.166363000	4.755308000	6	1.727268000	-2.783052000	2.819677000
8	1.011415000	-4.139394000	3.413600000	6	2.880386000	-2.470371000	2.170673000
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6	-0.140339000	0.850836000	0.704149000	1	-0.683389000	-4.363100000	2.538710000
8	0.734197000	-0.011953000	0.726513000	1	-4.384034000	0.852836000	2.646032000
8	-0.713893000	1.476391000	1.621596000	1	-3.318096000	-1.468389000	3.581007000
8	-3.016764000	1.703776000	2.355211000	1	-2.438199000	5.177610000	0.354756000
1	-3.598178000	0.905776000	2.042122000	1	0.034073000	6.036272000	-0.300031000
1	-2.114205000	1.654601000	1.976569000	1	4.889789000	3.932582000	-0.093429000
1	-2.960471000	1.717116000	3.326205000	1	5.837275000	1.413096000	0.346676000
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				1	1.507254000	-3.688242000	3.377327000
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				1	-7.339122000	4.822465000	1.796838000
				1	-6.887970000	3.098528000	0.043514000
				1	3.548623000	5.961803000	1.517957000
				1	4.522370000	8.046593000	0.572193000
				1	4.146628000	8.625504000	-1.826383000
				1	2.793798000	7.101445000	-3.268023000
				1	1.830835000	5.013488000	-2.312358000
				1	5.871866000	-0.850741000	2.771313000
				1	8.045341000	-1.957554000	2.243975000
				1	8.467625000	-2.803111000	-0.071955000
				1	6.722172000	-2.557157000	-1.820464000
				1	-1.508532000	-6.157945000	4.021157000
				1	-2.311222000	-5.617370000	6.324577000
				1	-2.262934000	-3.247766000	7.117329000
				1	-1.430086000	-1.452336000	5.622691000
				1	-2.959272000	2.442832000	-1.239479000
				1	-2.913178000	0.895855000	-0.368919000
				1	3.359985000	-2.026648000	-3.095338000
5IM1 Н30+:							
6	2.417624000	5.685050000	-1.681199000				
6	2.617282000	5.350408000	-0.331523000				
6	3.384657000	6.213720000	0.467622000				
6	3.931684000	7.384147000	-0.065449000				
6	3.720145000	7.710022000	-1.409344000				
6	2.960693000	6.856704000	-2.216088000				
6	2.041997000	4.093227000	0.231925000				
6	0.674098000	4.001816000	0.425526000				
7	-0.023325000	2.925619000	0.961170000				
6	-1.360657000	3.306405000	0.990650000				
6	-1.497253000	4.642317000	0.449422000				
6	-0.250594000	5.074418000	0.117817000				
26	0.678121000	1.075883000	1.281720000				
7	2.556381000	1.749097000	0.885562000				
6	3.701520000	0.977532000	0.836665000				
6	4.817155000	1.772651000	0.453042000				
6	4.332939000	3.056330000	0.225013000				
6	2.931673000	3.017595000	0.480819000				
6	3.768009000	-0.412406000	1.094918000				
6	5.063031000	-1.092239000	0.795399000				

1	-1.169510000	-6.426523000	3.666792000	6	-1.467212000	6.711315000	2.230845000
1	-2.202003000	-6.090061000	5.916516000	6	-1.479737000	4.167329000	-0.570187000
1	-2.422043000	-3.777971000	6.835883000	6	-0.150804000	3.933408000	-0.980429000
1	-1.626786000	-1.833648000	5.517210000	7	0.345536000	2.754082000	-1.494531000
1	-2.961859000	2.358241000	-1.100498000	6	1.692066000	2.928182000	-1.713625000
1	-2.879869000	0.755157000	-0.338327000	6	2.062678000	4.271171000	-1.325357000
1	3.502623000	-1.759722000	-3.051258000	6	0.925848000	4.891204000	-0.877382000
1	4.946555000	-2.716222000	-2.638422000	26	-0.713850000	0.993408000	-1.753309000
7	2.036978000	-3.613901000	-1.785125000	7	-2.462881000	1.988967000	-1.203535000
8	0.338772000	-1.687989000	-4.444566000	6	-3.679279000	1.388435000	-1.024056000
8	-0.987545000	-3.986429000	-1.312361000	6	-4.598737000	2.335352000	-0.417734000
8	-2.447773000	-1.702072000	-4.161943000	6	-3.899874000	3.492290000	-0.212495000
8	-3.608272000	-3.082298000	-1.305467000	6	-2.548495000	3.259522000	-0.696800000
6	-0.009230000	-5.006103000	-1.216756000	6	-3.992631000	0.047346000	-1.320069000
1	0.011419000	-5.511910000	-2.192717000	6	-5.302063000	-0.465675000	-0.814397000
6	1.364656000	-4.505493000	-0.821515000	6	-5.423341000	-0.785069000	0.553138000
1	-0.313841000	-5.758735000	-0.467532000	6	-6.618915000	-1.304041000	1.058186000
1	2.009160000	-5.382666000	-0.645733000	6	-7.701460000	-1.513547000	0.200509000
1	1.312947000	-3.981358000	0.145806000	6	-7.599682000	-1.199092000	-1.157430000
6	-1.620851000	-3.633083000	-0.095385000	6	-6.402578000	-0.675977000	-1.653745000
1	-2.066328000	-4.535939000	0.363733000	6	2.589991000	1.946572000	-2.187646000
1	-0.892421000	-3.207754000	0.616985000	6	4.035362000	2.329886000	-2.244782000
6	-2.683979000	-2.590887000	-0.348747000	6	4.475965000	3.204983000	-3.253099000
1	-3.178970000	-2.386956000	0.618953000	6	5.814350000	3.576968000	-3.373268000
1	-2.213699000	-1.655742000	-0.692926000	6	6.750965000	3.069504000	-2.466278000
6	-4.908541000	-2.553565000	-1.227314000	6	6.337958000	2.209956000	-1.450927000
1	-5.471332000	-3.007431000	-2.056614000	6	4.990492000	1.838013000	-1.330948000
1	-5.406806000	-2.872052000	-0.288418000	8	4.720507000	0.940728000	-0.335906000
6	-5.017545000	-1.029339000	-1.264556000	6	3.545225000	1.022580000	0.463933000
1	-6.094974000	-0.784436000	-1.218022000	6	3.862858000	0.760074000	1.939403000
1	-4.575545000	-0.620814000	-0.352029000	7	4.509283000	-0.386284000	2.295962000
6	1.469085000	-3.271019000	-3.093810000	8	-4.348955000	-0.495854000	1.360647000
6	0.767331000	-1.919300000	-3.114962000	6	-3.943751000	-1.375340000	2.400629000
1	2.257681000	-3.298989000	-3.860206000	6	-3.204054000	-2.566976000	1.783734000
1	0.734479000	-4.029149000	-3.385855000	8	-3.652641000	-3.059314000	0.751830000
1	1.446833000	-1.114069000	-2.777813000	7	0.982073000	0.111300000	-2.610796000
1	-0.078503000	-1.933059000	-2.415744000	6	2.246549000	0.643565000	-2.593561000
6	-0.446271000	-0.514206000	-4.615374000	6	3.192782000	-0.360475000	-3.048251000
1	0.043431000	0.144390000	-5.356780000	6	2.475100000	-1.489490000	-3.323206000
6	-1.840974000	-0.843557000	-5.111093000	6	1.078193000	-1.184567000	-3.049429000
1	-0.525065000	0.034173000	-3.665705000	6	0.008949000	-2.099039000	-3.174185000
1	-2.404713000	0.099363000	-5.205448000	6	0.340431000	-3.468205000	-3.675108000
1	-1.806179000	-1.343345000	-6.099780000	6	0.209802000	-4.591104000	-2.840660000
6	-4.737219000	-0.851535000	-3.756263000	6	0.535889000	-5.867895000	-3.303764000
1	-5.772500000	-1.231171000	-3.754064000	6	0.995455000	-6.043279000	-4.612858000
1	-4.704463000	0.017346000	-4.425124000	6	1.125664000	-4.933864000	-5.454223000
6	-3.827618000	-1.962977000	-4.297068000	6	0.801594000	-3.656938000	-4.988541000
1	-4.095127000	-2.139039000	-5.357238000	7	-1.829765000	-0.668488000	-2.306236000
1	-3.988475000	-2.899598000	-3.750802000	6	-1.337141000	-1.842995000	-2.824782000
8	-1.703614000	-4.369315000	-3.933045000	6	-2.410497000	-2.815349000	-2.878424000
1	-1.730006000	-3.426736000	-4.188885000	6	-3.514020000	-2.230037000	-2.319652000
1	-1.716853000	-4.274346000	-2.961223000	6	-3.143989000	-0.879941000	-1.958223000
6	0.074728000	0.642231000	-0.775618000	8	3.499767000	1.596932000	2.764092000
8	-0.891825000	0.020936000	-1.203025000	1	-0.147223000	-4.458841000	-1.818097000
8	0.790693000	1.313334000	-1.766505000	1	4.266230000	-0.216030000	-3.140440000
8	3.997382000	1.173442000	-2.184591000	1	2.853807000	-2.443781000	-3.678276000
1	4.211582000	0.166635000	-1.875860000	1	3.063256000	4.690005000	-1.386707000
1	1.527864000	1.758284000	-1.322589000	1	0.826640000	5.909193000	-0.510315000
1	4.244854000	1.768642000	-1.409874000	1	-4.260584000	4.418925000	0.226217000
1	4.536199000	1.422187000	-2.958784000	1	-5.640207000	2.133817000	-0.179161000
				1	-4.491821000	-2.673544000	-2.158897000
				1	-2.328786000	-3.823552000	-3.274237000
				1	3.737258000	3.586067000	-3.961727000
				1	6.124824000	4.253821000	-4.171808000
				1	7.804205000	3.348730000	-2.544062000
				1	7.045598000	1.807296000	-0.723905000
				1	-2.870359000	6.401717000	-1.383455000
⁵IM2 H3O+:							
6	-1.234677000	5.552217000	1.487261000				
6	-1.737242000	5.433700000	0.179921000				
6	-2.477879000	6.490369000	-0.367911000				
6	-2.708130000	7.651163000	0.376992000				
6	-2.203725000	7.764070000	1.676460000				

1	-0.470529000	-5.106573000	-1.661618000	8	-1.380288000	-0.718662000	4.402254000
1	2.051538000	-5.071062000	-0.735547000	1	-1.032155000	-1.249303000	3.661169000
1	5.884804000	-1.415921000	-0.881788000	1	-1.707472000	0.077941000	3.950119000
1	5.948288000	1.299569000	-1.189243000				
1	-1.673611000	4.685064000	-3.211053000	³RC1 H3O+,K+:			
1	-3.443001000	6.435516000	-3.191088000	6	2.385704000	4.995257000	-1.734917000
1	-5.457630000	6.126742000	-1.729606000	6	1.149315000	4.803719000	-2.379389000
1	-5.666106000	4.115063000	-0.330277000	6	0.608753000	5.872554000	-3.116214000
1	-1.476919000	-4.673912000	-4.070907000	6	1.286751000	7.089554000	-3.217675000
1	-3.259013000	-6.398017000	-4.238868000	6	2.518738000	7.264136000	-2.577444000
1	-5.304374000	-6.228815000	-2.815851000	6	3.065025000	6.212433000	-1.835055000
1	-5.539802000	-4.314010000	-1.224224000	6	0.423411000	3.508214000	-2.259201000
1	-3.762196000	-2.597428000	-1.064441000	6	1.050422000	2.346712000	-2.685131000
1	4.529473000	-4.646180000	-1.920872000	7	0.595141000	1.050007000	-2.499169000
1	6.224897000	-6.088355000	-0.797239000	6	1.626177000	0.217142000	-2.882875000
1	6.871058000	-5.625178000	1.572476000	6	2.716546000	1.003738000	-3.430107000
1	5.754708000	-3.779197000	2.824195000	6	2.356202000	2.311420000	-3.327508000
1	6.735917000	4.518746000	1.191938000	26	-1.186248000	0.495113000	-1.772946000
1	6.939974000	6.381546000	-0.459444000	7	-1.684198000	2.426002000	-1.463327000
1	5.458853000	6.408517000	-2.471292000	6	-2.750244000	2.848457000	-0.698806000
1	3.804847000	4.586015000	-2.822871000	6	-2.571890000	4.215285000	-0.313136000
1	-5.216693000	2.546070000	1.289787000	6	-1.377650000	4.638387000	-0.916417000
1	-5.941088000	1.985336000	-0.234614000	6	-0.839816000	3.521613000	-1.600241000
1	4.347985000	-1.624952000	3.739776000	6	-3.844625000	2.038024000	-0.308197000
1	5.557119000	-1.256372000	2.476870000	6	-4.751328000	2.507277000	0.776436000
7	2.570645000	0.235613000	2.366971000	6	-4.562651000	2.006645000	2.083691000
19	-1.837020000	0.170885000	0.770725000	6	-5.394860000	2.387323000	3.138766000
8	-0.381428000	-1.833083000	2.042882000	6	-6.445549000	3.277439000	2.898999000
8	-0.231756000	1.986717000	2.472041000	6	-6.646971000	3.797183000	1.617858000
8	-3.212729000	-2.148579000	1.902260000	6	-5.800125000	3.415253000	0.573533000
8	-2.921003000	1.303463000	3.100837000	6	1.644180000	-1.166742000	-2.766375000
6	1.149662000	2.321752000	2.606848000	6	2.913923000	-1.911239000	-2.989990000
1	1.451366000	2.258105000	3.669508000	6	3.055995000	-2.763252000	-4.101110000
6	2.032747000	1.438680000	1.740949000	6	4.215071000	-3.508260000	-4.314600000
1	1.281555000	3.370904000	2.284680000	6	5.268234000	-3.425964000	-3.397932000
1	2.891480000	2.024752000	1.407819000	6	5.152445000	-2.592927000	-2.285579000
1	1.482506000	1.162450000	0.828787000	6	3.989637000	-1.837702000	-2.085494000
6	-1.051310000	2.827259000	3.264277000	8	3.890142000	-1.036797000	-0.954648000
1	-0.904132000	2.600922000	4.337874000	6	4.786721000	0.074561000	-0.942059000
1	-0.779784000	3.888386000	3.104299000	6	4.849570000	0.748384000	0.426551000
6	-2.506244000	2.654471000	2.889559000	7	5.311667000	0.032546000	1.499878000
1	-3.115299000	3.345625000	3.492982000	8	-3.463499000	1.179479000	2.299427000
1	-2.656867000	2.907594000	1.827173000	6	-3.595531000	0.048692000	3.184270000
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1	-3.757571000	0.122999000	4.514261000	8	-3.810361000	-1.696815000	1.596552000
1	-4.078369000	1.853458000	4.745672000	7	-0.786480000	-1.400141000	-2.346965000
6	-5.344109000	0.921533000	3.262538000	6	0.483472000	-1.925581000	-2.484115000
1	-6.090007000	0.555378000	3.984842000	6	0.445620000	-3.350372000	-2.386760000
1	-5.697674000	1.904470000	2.934965000	6	-0.882612000	-3.700418000	-2.227533000
6	1.614717000	-0.764892000	2.818210000	6	-1.631101000	-2.484856000	-2.202715000
6	0.991106000	-1.607146000	1.704327000	6	-3.031184000	-2.421490000	-1.990745000
1	2.082360000	-1.410517000	3.571480000	6	-3.782987000	-3.708896000	-1.964617000
1	0.802065000	-0.234965000	3.334832000	6	-4.365500000	-4.158771000	-0.765255000
1	1.506316000	-2.568038000	1.592051000	6	-5.047446000	-5.378149000	-0.721540000
1	1.060384000	-1.093050000	0.733100000	6	-5.156956000	-6.167085000	-1.871678000
6	-1.000614000	-2.917435000	1.363108000	6	-4.576913000	-5.730225000	-3.067708000
1	-0.350313000	-3.807635000	1.396527000	6	-3.891877000	-4.512897000	-3.111450000
6	-2.307374000	-3.232506000	2.043198000	7	-3.079103000	-0.020748000	-1.415183000
1	-1.156496000	-2.674986000	0.297786000	6	-3.687601000	-1.251024000	-1.651706000
1	-2.737853000	-4.148246000	1.595909000	6	-5.091209000	-1.177296000	-1.292530000
1	-2.116787000	-3.433388000	3.113348000	6	-5.291746000	0.037054000	-0.716477000
6	-5.488106000	-1.426963000	2.400374000	6	-4.031922000	0.750775000	-0.794097000
1	-6.252939000	-1.530016000	3.185584000	8	4.523969000	1.929066000	0.515006000
1	-5.871191000	-1.882778000	1.479475000	1	-4.265280000	-3.538621000	0.128474000
6	-4.260095000	-2.203288000	2.855521000	1	1.305722000	-4.011691000	-2.446931000
1	-4.590365000	-3.248884000	2.997920000	1	-1.300664000	-4.698021000	-2.122234000
1	-3.879982000	-1.846580000	3.828770000	1	3.621501000	0.589127000	-3.868513000

6	-5.228288000	-1.070288000	-0.912797000	1	1.225547000	2.546474000	3.107925000
6	-5.319073000	0.184746000	-0.400614000	1	3.361126000	3.115282000	4.359148000
6	-4.047235000	0.832229000	-0.656816000	1	3.254748000	1.529988000	5.181949000
8	4.241491000	1.676600000	-0.141644000	6	5.698280000	0.933249000	2.045085000
1	-4.266769000	-3.436663000	0.487397000	1	6.738693000	0.642231000	2.265018000
1	0.795070000	-4.296826000	-2.802204000	1	5.715596000	1.911159000	1.549488000
1	-1.792608000	-4.830706000	-2.247015000	6	4.962541000	1.092066000	3.366266000
1	3.312684000	0.157799000	-4.244110000	1	5.485977000	1.888721000	3.926318000
1	2.800309000	2.797948000	-4.007094000	1	4.997548000	0.183111000	3.990415000
1	-0.865145000	5.613573000	-1.308559000	8	2.884660000	-1.125083000	5.284377000
1	-3.160867000	4.959556000	-0.031669000	1	2.207032000	-0.523433000	4.927503000
1	-6.171870000	0.659688000	0.078461000	1	3.360809000	-1.467672000	4.508077000
1	-5.992262000	-1.842399000	-0.932037000	6	-0.259156000	-0.008594000	-0.049881000
1	1.734034000	-3.188285000	-5.058794000	8	0.212576000	-1.124089000	0.184284000
1	3.732049000	-4.601598000	-5.489462000	8	0.369423000	0.993401000	0.693664000
1	5.682772000	-4.495847000	-3.920126000	8	-0.975309000	3.091661000	1.727673000
1	5.610638000	-2.958618000	-1.971398000	1	-1.758982000	2.554365000	1.948592000
1	-0.214608000	5.544383000	-3.964840000	1	-0.152126000	1.824955000	0.721028000
1	1.152673000	7.602951000	-4.231656000	1	-1.316960000	3.759676000	1.109387000
1	3.376921000	7.780673000	-3.113353000				
1	4.219795000	5.880876000	-1.730489000				
1	2.849992000	3.823864000	-1.470048000				
1	-5.802189000	4.045320000	-0.392989000				
1	-7.167422000	4.878606000	1.522778000				
1	-6.734413000	4.002041000	3.821428000				
1	-4.926286000	2.346183000	4.204768000				
1	-5.591864000	-5.527649000	0.836544000				
1	-6.212851000	-6.949859000	-1.118009000				
1	-5.502296000	-6.277108000	-3.413135000				
1	-4.179737000	-4.196101000	-3.748071000				
1	5.625857000	-0.757098000	-1.516669000				
1	4.400762000	0.367674000	-2.174563000				
1	-2.904449000	0.711443000	4.202944000				
1	-4.429809000	0.125328000	3.497122000				
7	-1.606501000	-1.416944000	3.167329000				
19	2.190718000	-0.534086000	1.839555000				
8	1.030513000	0.738384000	4.111317000				
8	1.226056000	-2.923249000	2.910298000				
8	3.613904000	1.450978000	3.138585000				
8	4.118806000	-2.242415000	2.893468000				
6	-0.059797000	-3.445788000	3.227488000				
1	-0.199439000	-3.490954000	4.323982000				
6	-1.172481000	-2.682018000	2.542292000				
1	-0.115618000	-4.485621000	2.857597000				
1	-2.050808000	-3.342958000	2.507267000				
1	-0.875864000	-2.478138000	1.502463000				
6	2.279426000	-3.756891000	3.367125000				
1	2.455343000	-3.596730000	4.445705000				
1	2.006739000	-4.817567000	3.218450000				
6	3.551499000	-3.518342000	2.584718000				
1	4.269972000	-4.310388000	2.856065000				
1	3.347194000	-3.596893000	1.501490000				
6	5.476605000	-2.074492000	2.487068000				
1	5.979376000	-1.497550000	3.274358000				
1	5.975966000	-3.055880000	2.442186000				
6	5.641050000	-1.405943000	1.124389000				
1	6.716573000	-1.442902000	0.870124000				
1	5.097405000	-1.997585000	0.379288000				
6	-0.839180000	-0.780445000	4.238031000				
6	-0.376326000	0.646371000	3.918477000				
1	-1.403382000	-0.805886000	5.183112000				
1	0.061616000	-1.379025000	4.405619000				
1	-0.873047000	1.387214000	4.568211000				
1	-0.607450000	0.889028000	2.872515000				
6	1.507188000	2.080524000	4.067759000				
1	1.042534000	2.669059000	4.880064000				
6	3.002126000	2.074410000	4.255086000				
				³RC2 H30+,K+:			
6				6	2.118630000	5.429997000	-1.093948000
6				6	0.869235000	5.276712000	-1.721996000
6				6	0.224782000	6.417480000	-2.229894000
6				6	0.818738000	7.677639000	-2.124466000
6				6	2.063644000	7.817651000	-1.502655000
6				6	2.710549000	6.690302000	-0.985434000
6				6	0.232093000	3.933356000	-1.816047000
6				6	0.916794000	2.909049000	-2.474970000
7				7	0.574372000	1.562845000	-2.426863000
6				6	1.653965000	0.870321000	-2.936025000
6				6	2.660743000	1.800636000	-3.403613000
6				6	2.198066000	3.056597000	-3.138953000
26				6	-1.142154000	0.764066000	-1.781835000
7				7	-1.764703000	2.595315000	-1.188964000
6				6	-2.807061000	2.774094000	-0.310366000
6				6	-2.669946000	4.045864000	0.359688000
6				6	-1.545975000	4.648070000	-0.176507000
6				6	-0.988113000	3.730569000	-1.127358000
6				6	-3.867456000	1.872370000	-0.119604000
6				6	-4.870756000	2.111189000	0.959803000
6				6	-4.743563000	1.432206000	2.188583000
6				6	-5.682593000	1.579842000	3.209087000
6				6	-6.788002000	2.410149000	3.006283000
6				6	-6.932107000	3.105549000	1.803101000
6				6	-5.975663000	2.958132000	0.795407000
6				6	1.789585000	-0.519814000	-2.941444000
6				6	3.119853000	-1.111995000	-3.260183000
6				6	3.367938000	-1.708281000	-4.507091000
6				6	4.609723000	-2.268831000	-4.808604000
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6				6	5.399682000	-1.673596000	-2.600704000
6				6	4.152577000	-1.108630000	-2.307606000
8				8	3.906198000	-0.585006000	-1.049644000
6				6	4.621707000	0.605830000	-0.735005000
6				6	4.622021000	0.929652000	0.759736000
7				7	5.105587000	0.005632000	1.657147000
8				8	-3.582929000	0.679662000	2.391339000
6				6	-3.638658000	-0.608843000	3.052438000
6				6	-3.037645000	-1.644742000	2.091316000
8				8	-3.650969000	-1.830514000	1.044603000
7				7	-0.588450000	-1.013968000	-2.511896000
6				6	0.720065000	-1.397703000	-2.704682000
6				6	0.807807000	-2.835038000	-2.764887000
6				6	-0.475245000	-3.310755000	-2.668005000
6				6	-1.338845000	-2.166562000	-2.521079000
6				6	-2.740664000	-2.225811000	-2.386073000

6	-3.123878000	2.495093000	-0.747815000	1	5.339918000	-0.951679000	-1.265099000
6	-4.100627000	3.420757000	-0.111135000	1	-4.584197000	1.434631000	3.721958000
6	-4.559917000	3.149715000	1.202062000	1	-5.718640000	1.182142000	2.365128000
6	-5.558741000	3.926477000	1.797994000	7	-2.766006000	-0.382649000	2.334061000
6	-6.102054000	5.012570000	1.102615000	19	1.736007000	-0.262808000	0.963768000
6	-5.638623000	5.323824000	-0.178259000	8	0.218293000	1.684619000	2.260803000
6	-4.650670000	4.529316000	-0.771507000	8	0.023068000	-2.137163000	2.409335000
6	1.664796000	-2.313086000	-1.717856000	8	3.032819000	2.021971000	2.145332000
6	2.755121000	-3.313946000	-1.638529000	8	2.727955000	-1.591398000	3.241771000
6	2.693015000	-4.520222000	-2.369440000	6	-1.359645000	-2.487121000	2.479559000
6	3.684202000	-5.497662000	-2.288524000	1	-1.692099000	-2.502182000	3.534897000
6	4.789296000	-5.296683000	-1.455773000	6	-2.222425000	-1.552255000	1.651068000
6	4.889914000	-4.110581000	-0.725541000	1	-1.474319000	-3.509304000	2.076054000
6	3.896112000	-3.130298000	-0.821051000	1	-3.077031000	-2.114037000	1.268804000
8	3.999693000	-1.974519000	-0.058903000	1	-1.651306000	-1.227660000	0.769131000
6	5.221157000	-1.256639000	-0.218657000	6	0.824342000	-3.065035000	3.115685000
6	5.218302000	0.026432000	0.605039000	1	0.658131000	-2.962979000	4.205182000
7	5.039400000	-0.070917000	1.961220000	1	0.550236000	-4.098230000	2.828886000
8	-3.934211000	2.140659000	1.874901000	6	2.289278000	-2.877080000	2.800538000
6	-4.656149000	1.197723000	2.644797000	1	2.856283000	-3.665760000	3.321751000
6	-4.118781000	-0.207888000	2.347559000	1	2.474327000	-2.992382000	1.718705000
8	-4.916881000	-1.109309000	2.103858000	6	4.051228000	-1.518545000	3.757951000
7	-0.787411000	-1.911878000	-1.586729000	1	4.060468000	-0.683668000	4.471016000
6	0.340396000	-2.719637000	-1.438424000	1	4.281439000	-2.434902000	4.327335000
6	-0.060936000	-4.040208000	-1.066058000	6	5.122583000	-1.337771000	2.689988000
6	-1.445372000	-4.062028000	-1.075493000	1	6.104362000	-1.404337000	3.193360000
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6	-3.244537000	-2.349989000	-1.450997000	6	-1.808084000	0.565603000	2.884700000
6	-4.276632000	-3.419007000	-1.389846000	6	-1.127633000	1.449348000	1.841059000
6	-5.202286000	-3.491196000	-0.327612000	1	-2.292744000	1.180448000	3.653018000
6	-6.147583000	-4.519286000	-0.267911000	1	-1.028495000	-0.013150000	3.400792000
6	-6.192729000	-5.503357000	-1.261955000	1	-1.649437000	2.405067000	1.727920000
6	-5.276995000	-5.449452000	-2.318950000	1	-1.136472000	0.964770000	0.852338000
6	-4.333423000	-4.420963000	-2.378978000	6	0.824454000	2.821557000	1.656946000
7	-2.774044000	0.083756000	-1.270527000	1	0.163457000	3.699672000	1.753217000
6	-3.639664000	-1.002106000	-1.390344000	6	2.128168000	3.096265000	2.358812000
6	-4.993877000	-0.547878000	-1.280041000	1	0.976764000	2.655318000	0.576677000
6	-4.948573000	0.799768000	-0.992786000	1	2.559536000	4.040902000	1.978911000
6	-3.570881000	1.184272000	-0.988224000	1	1.930744000	3.220663000	3.437879000
8	5.400593000	1.097885000	0.037830000	6	5.217573000	1.159942000	2.735005000
1	-5.165166000	-2.737451000	0.461877000	1	5.845190000	0.937298000	3.612800000
1	0.609765000	-4.865067000	-0.840991000	1	5.762498000	1.863301000	2.094364000
1	-2.095613000	-4.903952000	-0.851361000	6	3.940748000	1.830764000	3.219614000
1	3.979076000	-1.310805000	-3.086344000	1	4.237268000	2.803185000	3.651976000
1	3.916552000	1.386632000	-3.395797000	1	3.430255000	1.259023000	4.012047000
1	0.610721000	5.160165000	-1.433271000	8	1.174703000	0.363802000	4.591500000
1	-1.940893000	5.103624000	-0.522146000	1	0.853744000	0.903960000	3.845713000
1	-5.785381000	1.473451000	-0.821157000	1	1.604490000	-0.394777000	4.156613000
1	-5.875999000	-1.175929000	-1.368429000				
1	1.835728000	-4.673910000	-3.026854000	⁵RC1 H3O+,K+:			
1	3.597977000	-6.412057000	-2.880367000	6	2.531755000	4.638524000	-2.050320000
1	5.571751000	-6.054208000	-1.372189000	6	1.292543000	4.486698000	-2.701553000
1	5.744074000	-3.953028000	-0.064647000	6	0.817539000	5.553172000	-3.486447000
1	1.411966000	4.709361000	-3.944787000	6	1.558803000	6.728837000	-3.624778000
1	3.116883000	6.475146000	-4.312652000	6	2.791059000	6.864637000	-2.975581000
1	5.286130000	6.402863000	-3.073816000	6	3.274038000	5.814561000	-2.188224000
1	5.716691000	4.539740000	-1.461868000	6	0.506777000	3.230255000	-2.545564000
1	4.013838000	2.785390000	-1.096652000	6	1.120164000	2.030508000	-2.906809000
1	-4.309961000	4.749457000	-1.785837000	7	0.632960000	0.755338000	-2.681402000
1	-6.056655000	6.173462000	-0.723286000	6	1.593347000	-0.138494000	-3.095357000
1	-6.880638000	5.619314000	1.571386000	6	2.704655000	0.597301000	-3.680717000
1	-5.893007000	3.694578000	2.811469000	6	2.411863000	1.923359000	-3.576389000
1	-6.850242000	-4.557891000	0.569295000	26	-1.172021000	0.241114000	-1.833640000
1	-6.932529000	-6.306362000	-1.212502000	7	-1.681830000	2.295232000	-1.771742000
1	-5.301716000	-6.209833000	-3.104311000	6	-2.771504000	2.782630000	-1.091569000
1	-3.622064000	-4.383143000	-3.207259000	6	-2.585460000	4.181060000	-0.829812000
1	6.089567000	-1.870359000	0.075027000	6	-1.344842000	4.528176000	-1.390539000

6	1.431326000	0.092020000	-3.235710000	1	-6.029606000	3.842427000	-0.530937000
6	2.531845000	0.851348000	-3.805569000	1	-7.440555000	4.612652000	1.379065000
6	2.244561000	2.172890000	-3.610403000	1	-6.962875000	3.774448000	3.683161000
26	-1.273649000	0.374504000	-1.755464000	1	-5.072986000	2.217832000	0.077636000
7	-1.770440000	2.415857000	-1.622059000	1	-5.306610000	-5.666309000	0.846866000
6	-2.832259000	2.854961000	-0.875083000	1	-5.817451000	-7.187124000	-1.065063000
6	-2.664669000	4.265027000	-0.592748000	1	-5.125936000	-6.545142000	-3.375007000
6	-1.479838000	4.648898000	-1.176321000	1	-3.932871000	-4.397899000	-3.766879000
6	-0.915117000	3.473503000	-1.806947000	1	5.633583000	-0.645245000	-1.504574000
6	-3.907878000	2.057777000	-0.422317000	1	4.416716000	0.486269000	-2.166092000
6	-4.767404000	2.593903000	0.676221000	1	-2.915328000	0.759743000	4.089122000
6	-4.506079000	2.137318000	1.990072000	1	-4.422514000	0.057575000	3.458115000
6	-5.291578000	2.560717000	3.065479000	7	-1.589674000	-1.417695000	3.172549000
6	-6.350834000	3.446771000	2.839779000	19	2.158915000	-0.557014000	1.944473000
6	-6.615959000	3.918272000	1.552793000	8	0.989238000	0.689722000	4.204109000
6	-5.822196000	3.491233000	0.482304000	8	1.242042000	-2.931049000	2.987393000
6	1.359708000	-1.314509000	-3.188722000	8	3.572805000	1.421866000	3.208187000
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6	2.712257000	-2.900102000	-4.603230000	6	-0.043857000	-3.452874000	3.299984000
6	3.851875000	-3.661809000	-4.861912000	1	-0.193482000	-3.486768000	4.395403000
6	4.921922000	-3.630059000	-3.962774000	6	-1.151361000	-2.703361000	2.591467000
6	4.845842000	-2.829513000	-2.822778000	1	-0.095263000	-4.497115000	2.942024000
6	3.706827000	-2.053035000	-2.576258000	1	-2.029198000	-3.366562000	2.567375000
8	3.644909000	-1.285203000	-1.424735000	1	-0.849914000	-2.527729000	1.548412000
6	4.615777000	-0.242860000	-1.370389000	6	2.299240000	-3.763229000	3.439173000
6	4.565356000	0.556928000	-0.065956000	1	2.487496000	-3.593749000	4.513944000
7	5.090965000	-0.000954000	1.080077000	1	2.023544000	-4.824569000	3.302177000
8	-3.414131000	1.314723000	2.148447000	6	3.561325000	-3.532414000	2.637627000
6	-3.393331000	0.342843000	3.193601000	1	4.287029000	-4.316115000	2.914382000
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7	-1.042334000	-1.551470000	-2.610395000	1	5.997781000	-1.503185000	3.237905000
6	0.201085000	-2.064335000	-2.885145000	1	5.967128000	-3.049128000	2.384854000
6	0.150451000	-3.510991000	-2.808841000	6	5.586727000	-1.382000000	1.103012000
6	-1.136789000	-3.847312000	-2.486916000	1	6.655791000	-1.410839000	0.820493000
6	-1.875236000	-2.607265000	-2.345418000	1	5.027024000	-1.964903000	0.361974000
6	-3.218993000	-2.526395000	-1.900321000	6	-0.910815000	-0.807423000	4.316781000
6	-3.949365000	-3.810391000	-1.688152000	6	-0.428429000	0.630860000	4.088304000
6	-4.344054000	-4.180884000	-0.388952000	1	-1.551088000	-0.858393000	5.211041000
6	-5.010930000	-5.388433000	-0.168009000	1	-0.025726000	-1.409989000	4.544565000
6	-5.294976000	-6.243274000	-1.238802000	1	-0.871501000	1.315490000	4.832871000
6	-4.905095000	-5.884249000	-2.533172000	1	-0.711950000	0.976706000	3.085207000
6	-4.235104000	-4.677865000	-2.755175000	6	1.475724000	2.029228000	4.175342000
7	-3.274126000	-0.112093000	-1.416236000	1	1.024017000	2.607871000	5.001797000
6	-3.868965000	-1.342187000	-1.506687000	6	2.973235000	2.021120000	4.344143000
6	-5.231966000	-1.254905000	-0.998031000	1	1.184778000	2.510487000	3.225183000
6	-5.396175000	0.012299000	-0.523356000	1	3.329824000	3.061225000	4.463112000
6	-4.155460000	0.723521000	-0.789280000	1	3.238422000	1.459880000	5.257019000
8	4.147572000	1.708895000	-0.091353000	6	5.640433000	0.942339000	2.067296000
1	-4.109850000	-3.510538000	0.441543000	1	6.687963000	0.659343000	2.263572000
1	0.987798000	-4.184757000	-2.969402000	1	5.638669000	1.929702000	1.590524000
1	-1.540331000	-4.844500000	-2.332477000	6	4.928365000	1.070479000	3.404649000
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1	2.833535000	3.031113000	-3.922921000	1	4.983899000	0.151294000	4.011889000
1	-1.030857000	5.638386000	-1.160494000	8	2.908269000	-1.153338000	5.344046000
1	-3.360291000	4.885586000	-0.032144000	1	2.202587000	-0.578011000	4.998783000
1	-6.278808000	0.444074000	-0.056821000	1	3.383138000	-1.481082000	4.560745000
1	-5.956410000	-2.065067000	-0.992377000	6	-0.226924000	-0.020863000	0.016523000
1	1.869434000	-2.926111000	-5.296952000	8	0.249982000	-1.143414000	0.216118000
1	3.902863000	-4.281157000	-5.759907000	8	0.331199000	0.949818000	0.842702000
1	5.815669000	-4.231427000	-4.143373000	8	-1.114168000	3.014471000	1.710073000
1	5.672308000	-2.811418000	-2.109802000	1	-1.915711000	2.478446000	1.867166000
1	-0.284751000	5.721045000	-3.743707000	1	-0.202100000	1.778236000	0.868854000
1	1.042869000	7.818575000	-3.854849000	1	-1.408318000	3.695960000	1.081768000
1	3.245528000	7.968336000	-2.690495000				
1	4.106792000	6.000262000	-1.418753000				
1	2.775795000	3.904771000	-1.311910000				
				5RC2 H3O+,K+:			
				6	2.238327000	5.236764000	-1.185494000

6	1.011810000	5.132687000	-1.867794000	1	4.686495000	-3.133477000	-5.800242000
6	0.442264000	6.298137000	-2.409741000	1	6.452156000	-3.198534000	-4.026721000
6	1.083551000	7.532471000	-2.280850000	1	6.046237000	-2.094180000	-1.840459000
6	2.303367000	7.623101000	-1.602869000	1	-0.507610000	6.228791000	-2.944211000
6	2.877613000	6.471437000	-1.054479000	1	0.629832000	8.426686000	-2.714784000
6	0.320993000	3.817549000	-1.990126000	1	2.804201000	8.588628000	-1.500316000
6	1.032554000	2.757281000	-2.593285000	1	3.825991000	6.535068000	-0.515637000
7	0.644113000	1.438154000	-2.581469000	1	2.684317000	4.343024000	-0.743216000
6	1.688294000	0.687673000	-3.051455000	1	-6.115979000	3.550697000	-0.538604000
6	2.761507000	1.574877000	-3.468469000	1	-7.802231000	3.997937000	1.242698000
6	2.354531000	2.851362000	-3.195847000	1	-7.538583000	2.942545000	3.491960000
26	-1.124046000	0.635432000	-1.807656000	1	-5.578566000	1.490196000	3.960311000
7	-1.787857000	2.606181000	-1.459880000	1	-5.034842000	-5.915130000	-0.157621000
6	-2.861886000	2.823607000	-0.635927000	1	-5.096867000	-7.296384000	-2.235477000
6	-2.722654000	4.128864000	-0.013183000	1	-4.095102000	-6.408505000	-4.341291000
6	-1.550718000	4.674296000	-0.498425000	1	-3.037214000	-4.158478000	-4.365290000
6	-0.966072000	3.701743000	-1.392877000	1	5.706093000	0.148116000	-1.198559000
6	-3.913374000	1.912578000	-0.383469000	1	4.279874000	1.186266000	-1.484597000
6	-4.912339000	2.252047000	0.676563000	1	-3.223653000	-0.000302000	4.027750000
6	-4.787120000	1.675497000	1.956737000	1	-4.734508000	-0.505891000	3.233327000
6	-5.713407000	1.923200000	2.968434000	7	-1.941373000	-2.041097000	2.738990000
6	-6.807946000	2.751099000	2.703506000	19	2.008161000	-0.698508000	1.747979000
6	-6.952097000	3.344190000	1.447183000	8	0.649705000	-0.140408000	4.228277000
6	-6.005915000	3.098130000	0.448903000	8	0.971330000	-3.308675000	2.035786000
6	1.741924000	-0.721712000	-3.079403000	8	3.312507000	0.760765000	3.719170000
6	3.062006000	-1.365202000	-3.353644000	8	3.862897000	-2.644304000	2.429372000
6	3.308696000	-2.003090000	-4.580827000	6	-0.284342000	-3.939548000	2.272220000
6	4.517615000	-2.651289000	-4.835159000	1	-0.363656000	-4.252159000	3.330231000
6	5.505543000	-2.684517000	-3.846331000	6	-1.464185000	-3.100832000	1.833030000
6	5.280369000	-2.063440000	-2.617478000	1	-0.324630000	-4.864269000	1.668708000
6	4.069997000	-1.403051000	-2.373343000	1	-2.302837000	-3.792235000	1.664923000
8	3.852298000	-0.811200000	-1.137842000	1	-1.236066000	-2.636246000	0.862582000
6	4.661130000	0.339782000	-0.899038000	6	2.042622000	-4.228059000	2.185798000
6	4.659824000	0.805247000	0.556721000	1	2.181057000	-4.485230000	3.251551000
7	5.119543000	-0.036691000	1.541314000	1	1.807499000	-5.160542000	1.640058000
8	-3.632549000	0.920461000	2.207229000	6	3.335213000	-3.692733000	1.612994000
6	-3.682345000	-0.248668000	3.064982000	1	4.057115000	-4.525655000	1.578597000
6	-3.070408000	-1.431934000	2.298668000	1	3.179432000	-3.338587000	0.577328000
8	-3.667036000	-1.801994000	1.291881000	6	5.266780000	-2.419676000	2.312714000
7	-0.645605000	-1.223934000	-2.641376000	1	5.623892000	-2.126292000	3.308336000
6	0.655063000	1.597802000	-2.867214000	1	5.775193000	-3.362703000	2.053736000
6	0.734872000	-3.046762000	-2.902279000	6	5.642765000	-1.377093000	1.263257000
6	-0.537203000	-3.518290000	-2.719746000	1	6.746280000	-1.347062000	1.207977000
6	-1.399676000	-2.363038000	-2.552307000	1	5.264353000	-1.709140000	0.293327000
6	-2.787995000	-2.416401000	-2.273058000	6	-1.208730000	-1.662045000	3.946199000
6	-3.440112000	-3.756967000	-2.280293000	6	-0.754384000	-0.197157000	4.007254000
6	-4.011167000	-4.264252000	-1.097935000	1	-1.798251000	-1.917576000	4.840409000
6	-4.601480000	-5.530296000	-1.084207000	1	-0.304121000	-2.276686000	3.993721000
6	-4.633867000	-6.306734000	-2.247709000	1	-1.258433000	0.340927000	4.829103000
6	-4.069672000	-5.810114000	-3.427334000	1	-0.975828000	0.296369000	3.052442000
6	-3.474633000	-4.545896000	-3.442517000	6	1.105431000	1.175832000	4.519425000
7	-3.063595000	-0.068996000	-1.579667000	1	0.541916000	1.588851000	5.375289000
6	-3.563002000	-1.311648000	-1.869059000	6	2.569163000	1.122870000	4.869185000
6	-4.978157000	-1.347347000	-1.528199000	1	0.936680000	1.835404000	3.648025000
6	-5.272670000	-0.157934000	-0.930659000	1	2.892468000	2.112844000	5.240935000
6	-4.056044000	0.636275000	-0.958650000	1	2.724825000	0.385282000	5.676522000
8	4.316396000	1.959114000	0.793088000	6	5.534581000	0.594179000	2.801330000
1	-3.973110000	-3.653797000	-0.193090000	1	6.546947000	0.235049000	3.048212000
1	1.640895000	-3.627997000	-3.051553000	1	5.590141000	1.672447000	2.611697000
1	-0.857043000	-4.556175000	-2.680360000	6	4.641798000	0.372816000	4.012330000
1	3.695093000	1.259191000	-3.928720000	1	5.053896000	0.992123000	4.829491000
1	2.898506000	3.772796000	-3.385549000	1	4.643103000	-0.671930000	4.365761000
1	-1.127086000	5.643458000	-0.248323000	8	2.426812000	-2.291158000	4.922525000
1	-3.450492000	4.603966000	0.642863000	1	1.796926000	-1.577669000	4.717920000
1	-6.225919000	0.167768000	-0.520883000	1	2.952764000	-2.409530000	4.112289000
1	-5.646103000	-2.187898000	-1.695858000	6	-0.292107000	0.465393000	0.113767000
1	2.527269000	-1.981531000	-5.343316000	8	-0.505234000	-0.390683000	0.967200000

1	5.693736000	1.310021000	3.057056000	6	-1.630046000	-5.763047000	-3.577325000
6	4.701095000	-0.213411000	4.174675000	6	-1.375075000	-4.391852000	-3.500770000
1	5.102398000	0.228529000	5.104463000	7	-2.139490000	-0.145523000	-1.262645000
1	4.671610000	-1.306100000	4.321130000	6	-2.220993000	-1.470578000	-1.623764000
8	2.387532000	-2.991941000	4.380389000	6	-3.560860000	-1.952294000	-1.357527000
1	1.810039000	-2.208842000	4.377997000	6	-4.255191000	-0.920173000	-0.794002000
1	2.866202000	-2.957299000	3.533453000	6	-3.358231000	0.209631000	-0.731833000
6	-0.423548000	0.543518000	0.191466000	8	4.460488000	0.918244000	1.119831000
8	-0.481329000	-0.368536000	0.975375000	1	-1.777589000	-3.946464000	-0.147966000
8	0.275938000	1.728096000	0.861387000	1	3.059245000	-1.912175000	-4.061689000
8	-1.570936000	2.501873000	2.320502000	1	1.158065000	-3.628718000	-3.244048000
1	-2.286033000	1.779964000	2.326576000	1	3.668408000	3.408454000	-3.894830000
1	0.458031000	2.404871000	0.183739000	1	2.221949000	5.460094000	-2.933558000
1	-0.715833000	2.181633000	1.748785000	1	-2.295507000	5.897986000	-0.095030000
1	-1.949850000	3.263963000	1.814572000	1	-4.184408000	4.162722000	0.749431000

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6	1.049045000	6.503914000	-0.643644000	1	3.357896000	1.605760000	-5.892552000
6	0.024516000	6.054500000	-1.492427000	1	5.668124000	1.334452000	-6.774470000
6	-0.764140000	7.001641000	-2.164041000	1	7.410926000	0.235764000	-5.345639000
6	-0.531488000	8.369236000	-1.993487000	1	6.804314000	-0.547672000	-3.047884000
6	0.492011000	8.807270000	-1.147295000	1	-1.562216000	6.659828000	-2.826903000
6	1.281645000	7.870823000	-0.472108000	1	-1.151002000	9.094903000	-2.525828000
6	-0.225611000	4.589510000	-1.665211000	1	0.673766000	9.876254000	-1.013743000
6	0.733757000	3.850928000	-2.390671000	1	2.080597000	8.205550000	0.193785000
7	0.721573000	2.491655000	-2.616311000	1	1.661462000	5.771057000	-0.113451000
6	1.911959000	2.157990000	-3.219496000	1	-6.250445000	1.911418000	-0.989344000
6	2.686536000	3.363261000	-3.432344000	1	-8.321160000	1.841152000	0.400750000
6	1.952178000	4.407629000	-2.939662000	1	-8.143488000	1.392448000	2.854139000
26	-0.544188000	1.126025000	-1.648250000	1	-5.922256000	1.070155000	3.902235000
7	-1.762720000	2.744134000	-1.066259000	1	-2.250549000	-6.384785000	-0.282781000
6	-2.929778000	2.640563000	-0.354198000	1	-2.146306000	-7.557805000	-2.482458000
6	-3.300188000	3.948197000	0.153377000	1	-1.591743000	-6.267274000	-4.545774000
6	-2.341164000	4.827124000	-0.273971000	1	-1.150227000	-3.828311000	-4.408343000
6	-1.379024000	4.059687000	-1.048968000	1	3.670091000	1.270683000	-1.144197000
6	-3.682194000	1.465982000	-0.182133000	1	2.663876000	-0.200854000	-1.092419000
6	-4.922352000	1.519385000	0.653551000	1	-2.434678000	0.719385000	4.170092000
6	-4.840237000	1.284031000	2.040430000	1	-4.092548000	0.126676000	4.309846000
6	-5.994321000	1.239089000	2.826960000	7	-2.186967000	-1.984485000	3.743231000
6	-7.245260000	1.429676000	2.233791000	19	1.065890000	-1.397924000	1.970758000
6	-7.345044000	1.682918000	0.863646000	8	0.724605000	-1.290139000	4.802731000
6	-6.185067000	1.728795000	0.085485000	8	-0.318718000	-3.806488000	2.101700000
6	2.361782000	0.849272000	-3.505266000	8	3.387688000	-1.220628000	3.554190000
6	3.766244000	0.695070000	-3.990044000	8	2.497663000	-3.705297000	1.266930000
6	4.128088000	1.140685000	-5.273432000	6	-1.090726000	-4.225402000	3.222521000
6	5.421438000	0.984317000	-5.770150000	1	-0.454771000	-4.218304000	4.123171000
6	6.392440000	0.367936000	-4.973483000	6	-2.347757000	-3.400826000	3.388975000
6	6.063125000	-0.073332000	-3.693717000	1	-1.424850000	-5.266945000	3.072747000
6	4.762202000	0.085489000	-3.194434000	1	-2.951728000	-3.888352000	4.175325000
8	4.552561000	-0.438336000	-1.947668000	1	-2.922910000	-3.429695000	2.457552000
6	3.691254000	0.183812000	-1.002545000	6	0.417411000	-4.880629000	1.529559000
6	4.226820000	-0.051255000	0.406845000	1	0.929767000	-5.454998000	2.319732000
7	4.417549000	-1.344218000	0.827819000	1	-0.266014000	-5.564589000	0.998863000
8	-3.577611000	1.200893000	2.584849000	6	1.445815000	-4.364449000	0.554922000
6	-3.257362000	0.273795000	3.605420000	1	1.852531000	-5.225731000	0.000821000
6	-2.910969000	-1.091275000	2.997853000	1	0.986523000	-3.680611000	-0.181617000
8	-3.358351000	-1.365257000	1.893117000	6	3.789770000	-3.775642000	0.665312000
7	0.399881000	-0.418801000	-2.694301000	1	4.505940000	-4.050260000	1.451655000
6	1.636497000	-0.336965000	-3.278357000	1	3.808470000	-4.589513000	-0.076273000
6	2.110847000	-1.673307000	-3.587945000	6	4.216552000	-2.501681000	-0.049659000
6	1.140965000	-2.544609000	-3.178465000	1	5.152244000	-2.731058000	-0.589630000
6	0.053098000	-1.746126000	-2.637241000	1	3.466047000	-2.255864000	-0.809739000
6	-1.177752000	-2.253290000	-2.168373000	6	-1.696844000	-1.679654000	5.090351000
6	-1.425790000	-3.720275000	-2.266785000	6	-0.518430000	-0.723702000	5.208332000
6	-1.745070000	-4.457241000	-1.112101000	1	-2.509364000	-1.267198000	5.711818000
6	-2.003054000	-5.827647000	-1.189585000	1	-1.413778000	-2.629956000	5.562479000
6	-1.944222000	-6.485961000	-2.422014000	1	-0.447951000	-0.437455000	6.272943000

1	3.218712000	-5.408060000	2.705374000	6	-3.456612000	5.634254000	0.200699000
6	4.169660000	-3.869844000	1.567548000	6	0.510577000	-2.311308000	-2.542666000
1	5.114759000	-4.428290000	1.702444000	6	1.292769000	-3.573600000	-2.622680000
1	3.743980000	-4.173632000	0.609362000	6	0.914515000	-4.582970000	-3.532225000
6	-1.770144000	-0.557748000	3.716557000	6	1.599300000	-5.793279000	-3.632792000
6	-0.827316000	0.594367000	3.352906000	6	2.704454000	-6.029934000	-2.810918000
1	-2.119316000	-0.452068000	4.756564000	6	3.108028000	-5.049739000	-1.903206000
1	-1.169495000	-1.471978000	3.691765000	6	2.417831000	-3.833965000	-1.811072000
1	-1.049613000	1.504259000	3.937410000	8	2.811253000	-2.901503000	-0.861455000
1	-0.912924000	0.830793000	2.287126000	6	4.147420000	-2.424270000	-0.982174000
6	1.463921000	1.214279000	3.514751000	6	4.754743000	-1.880940000	0.308169000
1	1.183479000	2.078917000	4.145392000	7	4.470830000	-2.476033000	1.519777000
6	2.812588000	0.710774000	3.966421000	8	-3.131088000	2.463284000	1.968390000
1	1.490481000	1.551019000	2.467703000	6	-3.659453000	1.778360000	3.098406000
1	3.531875000	1.549833000	3.953014000	6	-3.859014000	0.326273000	2.645701000
1	2.726380000	0.341259000	5.003607000	8	-4.900018000	0.064084000	2.043861000
6	5.096387000	-1.870052000	2.730829000	7	-1.771350000	-1.381608000	-2.266284000
1	5.683322000	-2.653301000	3.239090000	6	-0.860202000	-2.414097000	-2.248076000
1	5.798313000	-1.100641000	2.391614000	6	-1.547263000	-3.645663000	-1.883998000
6	4.138560000	-1.252726000	3.743966000	6	-2.868690000	-3.336819000	-1.723639000
1	4.763779000	-0.742252000	4.498118000	6	-3.006310000	-1.907589000	-1.939523000
1	3.530984000	-2.003175000	4.276825000	6	-4.186754000	-1.185353000	-1.708340000
8	1.026920000	-2.347149000	4.835149000	6	-5.440885000	-1.969229000	-1.521982000
1	0.877088000	-1.451990000	4.477818000	6	-6.156008000	-1.909277000	-0.309781000
1	1.240920000	-2.888427000	4.054721000	6	-7.310554000	-2.674717000	-0.127918000
6	-0.401316000	0.402735000	-0.136546000	6	-7.777414000	-3.510805000	-1.149457000
8	-0.974045000	-0.520445000	0.466382000	6	-7.075982000	-3.577920000	-3.357093000
8	0.579319000	1.072459000	0.285780000	6	-5.918838000	-2.814546000	-2.539465000
6	3.566760000	2.154623000	0.670177000	7	-3.133883000	1.039487000	-1.406240000
6	4.890623000	2.093140000	1.137915000	6	-4.245168000	0.223859000	-1.508826000
6	5.393897000	3.116640000	1.942848000	6	-5.415778000	0.989982000	-1.194393000
6	4.597264000	4.215089000	2.291908000	6	-4.983748000	2.252276000	-0.822079000
6	3.284029000	4.278022000	1.812765000	6	-3.558469000	2.255587000	-0.952519000
6	2.766899000	3.262186000	1.005231000	8	5.499811000	-0.915841000	0.198126000
1	5.489529000	1.222027000	0.871922000	1	-5.783057000	-1.268666000	0.491753000
1	6.423340000	3.053073000	2.306811000	1	-1.078373000	-4.618322000	-1.757157000
1	4.996555000	5.011580000	2.924081000	1	-3.673584000	-4.009552000	-1.437008000
1	2.648484000	5.131276000	2.066387000	1	3.037220000	-1.818209000	-3.905112000
1	1.747549000	3.312864000	0.623171000	1	3.593954000	0.823617000	-4.131448000
8	3.102535000	1.147264000	-0.098509000	1	1.475744000	5.120768000	-1.629499000
1	2.105416000	1.206471000	-0.169688000	1	-0.803315000	5.534956000	-0.277730000
				1	-5.588090000	3.096238000	-0.493865000
				1	-6.438192000	0.620812000	-1.214625000
				1	0.057907000	-4.389745000	-4.180583000
				1	1.275621000	-6.546069000	-4.355112000
				1	3.252697000	-6.972735000	-2.869660000
				1	3.966452000	-5.238248000	-1.256069000
				1	1.807388000	4.710869000	-4.381121000
				1	3.837131000	6.079759000	-4.807908000
				1	6.017582000	5.442469000	-3.770317000
				1	6.137709000	3.423560000	-2.300559000
				1	4.097697000	2.066521000	-1.882157000
				1	-3.299384000	6.021529000	-0.808485000
				1	-4.114704000	7.538814000	0.992627000
				1	-4.492198000	6.627177000	3.292837000
				1	-4.032732000	4.244616000	3.773506000
				1	-7.847170000	-2.624823000	0.823509000
				1	-8.681465000	-4.107506000	-1.003962000
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				1	-5.373417000	-2.867573000	-3.484478000
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				7	-2.878034000	-0.594460000	2.839367000
				19	1.469461000	-1.260462000	1.284134000
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⁵RC1 phenol.K+:							
6	4.050134000	2.937767000	-2.533917000				
6	2.810131000	3.287795000	-3.103617000				
6	2.759123000	4.429502000	-3.924841000				
6	3.901754000	5.198876000	-4.163837000				
6	5.123839000	4.841074000	-3.586278000				
6	5.191191000	3.706058000	-2.769015000				
6	1.582042000	2.494408000	-2.817671000				
6	1.642581000	1.082455000	-3.046413000				
7	0.701968000	0.170997000	-2.607644000				
6	1.183812000	-1.089577000	-2.867531000				
6	2.444372000	-0.982653000	-3.538158000				
6	2.723655000	0.372099000	-3.661856000				
26	-1.162373000	0.600129000	-1.838849000				
7	-0.759596000	2.655653000	-1.993223000				
6	-1.419057000	3.539058000	-1.157787000				
6	-0.555070000	4.683569000	-0.906974000				
6	0.600563000	4.476815000	-1.602010000				
6	0.497869000	3.170223000	-2.237166000				
6	-2.698005000	3.354501000	-0.622439000				
6	-3.200333000	4.275972000	0.433286000				
6	-3.425594000	3.777077000	1.748533000				
6	-3.885471000	4.625679000	2.762384000				
6	-4.134145000	5.977068000	2.490857000				
6	-3.919098000	6.486464000	1.210513000				

8	-0.984501000	-3.134224000	2.152495000	6	4.003592000	2.319753000	-0.261689000
8	3.309610000	-0.317443000	3.125669000	7	2.792756000	2.503835000	0.384596000
8	1.849202000	-3.725888000	2.483907000	6	2.187379000	3.596246000	-0.225202000
6	-2.327886000	-3.086545000	2.615435000	6	3.044828000	4.105703000	-1.277334000
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1	-2.867737000	-3.962537000	2.210420000	7	3.391038000	-0.076341000	1.392022000
1	-4.156642000	-2.109535000	2.212777000	6	3.423533000	-1.393923000	1.823269000
1	-2.868228000	-1.720455000	1.063015000	6	4.653425000	-2.006730000	1.452777000
6	-0.443656000	-4.434501000	2.255111000	6	5.389661000	-1.047527000	0.781319000
1	-0.413306000	-4.766081000	3.311232000	6	4.582416000	0.131039000	0.720032000
1	-1.074375000	-5.153638000	1.696524000	6	2.400001000	-2.026706000	2.563517000
6	0.948872000	-4.484079000	1.672960000	6	2.415591000	-3.514632000	2.682059000
1	1.275273000	-5.535812000	1.636500000	6	1.749528000	-4.282277000	1.697652000
1	0.948558000	-4.098947000	0.638335000	6	1.687883000	-5.676606000	1.810614000
6	3.144236000	-4.277917000	2.685963000	6	2.308134000	-6.315592000	2.890017000
1	3.479439000	-3.937406000	3.674187000	6	2.984574000	-5.574988000	3.860432000
1	3.080412000	-5.378180000	2.728585000	6	3.027898000	-4.179958000	3.748280000
6	4.148779000	-3.906001000	1.604996000	6	0.982523000	4.163342000	0.149307000
1	5.076815000	-4.469990000	1.812438000	6	0.361400000	5.224155000	-0.693564000
1	3.767131000	-4.247335000	0.641317000	6	0.865743000	6.529251000	-0.783411000
6	-1.746688000	-0.413359000	3.748091000	6	0.232385000	7.501365000	-1.565288000
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1	-2.111416000	-0.325280000	4.784716000	6	-1.443618000	5.877075000	-2.214828000
1	-1.152648000	-1.331083000	3.712168000	6	-0.804961000	4.915551000	-1.426574000
1	-0.927673000	1.584199000	4.122949000	8	-1.251810000	3.623551000	-1.362151000
1	-0.916553000	1.096851000	2.406689000	6	-2.618467000	3.356797000	-1.098709000
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1	1.268505000	2.087770000	4.247348000	7	-4.426828000	2.029019000	-2.153912000
6	2.861912000	0.690062000	4.019672000	8	1.221428000	-3.578672000	0.658983000
1	1.607812000	1.673814000	2.546662000	6	0.352180000	-4.173347000	-0.272096000
1	3.606674000	1.505349000	4.073234000	6	-1.061542000	-4.291763000	0.300982000
1	2.735922000	0.268510000	5.032702000	8	-1.262557000	-4.024989000	1.488326000
6	5.113097000	-1.884124000	2.699967000	7	0.563894000	2.644317000	2.076234000
1	5.714116000	-2.657040000	3.207559000	6	0.282143000	3.768343000	1.320531000
1	5.802003000	-1.115250000	2.333595000	6	-0.788391000	4.498492000	1.902452000
6	4.181469000	-1.257556000	3.730581000	6	-1.175675000	3.801225000	3.041272000
1	4.830121000	-0.759536000	4.473574000	6	-0.346780000	2.637360000	3.114403000
1	3.573899000	-2.000468000	4.273425000	6	-0.580339000	1.544799000	3.996090000
8	1.035826000	-2.277548000	4.805655000	6	-1.716983000	1.671063000	4.953899000
1	0.887172000	-1.379735000	4.455225000	6	-2.892762000	0.922162000	4.763164000
1	1.210295000	-2.815734000	4.013139000	6	-3.970382000	1.050642000	5.643582000
6	-0.498042000	0.523001000	0.004690000	6	-3.897283000	1.936766000	6.723959000
8	-0.970026000	-0.486662000	0.534285000	6	-2.736469000	2.692991000	6.918398000
8	0.333061000	1.351883000	0.429673000	6	-1.657426000	2.560789000	6.039452000
6	3.481326000	2.207524000	0.731417000	7	1.129127000	0.036294000	3.036186000
6	4.809893000	2.079953000	1.165582000	6	0.074972000	0.326220000	3.883682000
6	5.426260000	3.142017000	1.829871000	6	-0.299098000	-0.871682000	4.617784000
6	4.736934000	4.337949000	2.069821000	6	0.466829000	-1.891263000	4.144361000
6	3.414917000	4.459377000	1.628294000	6	1.379167000	-1.320894000	3.175175000
6	2.784579000	3.405523000	0.961832000	8	-2.782672000	2.964641000	-3.443157000
1	5.328254000	1.140726000	0.973058000	1	-2.949012000	0.247934000	3.907147000
1	6.460911000	3.032857000	2.166736000	1	-1.192939000	5.431975000	1.518073000
1	5.225597000	5.164332000	2.590961000	1	-1.959140000	4.061782000	3.748303000
1	2.862234000	5.387114000	1.800475000	1	2.812584000	4.955511000	-1.914277000
1	1.758187000	3.498799000	0.605940000	1	5.058692000	3.468315000	-1.894563000
8	2.902806000	1.163691000	0.092652000	1	6.371374000	-1.156542000	0.328340000
1	1.933988000	1.344819000	-0.025383000	1	4.927996000	-3.035729000	1.672090000
				1	0.453467000	-2.937291000	4.440226000
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3RC1 phenol, 6W, K+:-							
6	6.203928000	1.054753000	-2.205627000				
6	6.184281000	1.254307000	-0.814161000				
6	7.408721000	1.402331000	-0.141477000				
6	8.619776000	1.359884000	-0.838513000				
6	8.626271000	1.166414000	-2.224094000				
6	7.413638000	1.014180000	-2.904562000				
6	4.893589000	1.272229000	-0.062919000				

6	2.870883000	0.718675000	-3.226736000	1	-5.807343000	5.701315000	2.629449000
6	2.695004000	2.090518000	-3.139263000	1	-6.065082000	4.125807000	4.557106000
26	-1.077737000	0.793326000	-1.658155000	1	-5.031050000	1.876123000	4.464231000
7	-1.240118000	2.725781000	-1.195890000	1	-6.661011000	-4.672346000	-0.731624000
6	-2.121904000	3.238505000	-0.260984000	1	-6.999107000	-5.637005000	-3.008937000
6	-1.728729000	4.592481000	0.078378000	1	-5.689696000	-4.739042000	-4.935956000
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6	-0.307346000	3.717617000	-1.454964000	1	5.691357000	-1.347769000	-1.223088000
6	-3.259102000	2.575700000	0.202046000	1	4.612865000	0.064428000	-1.357857000
6	-4.027956000	3.041204000	1.382751000	1	-3.586907000	-0.150600000	4.180763000
6	-4.197527000	2.158394000	2.487981000	1	-5.144011000	-0.110735000	3.301031000
6	-4.925060000	2.553222000	3.615752000	7	-2.540683000	-2.004771000	2.450915000
6	-5.500554000	3.828832000	3.670009000	19	1.769366000	-1.198782000	1.354973000
6	-5.351071000	4.709310000	2.598485000	8	0.420352000	-0.379947000	3.774413000
6	-4.624361000	4.308356000	1.471612000	8	0.108352000	-3.697511000	1.575906000
6	1.408120000	-1.282104000	-2.720494000	8	3.243183000	0.029337000	3.500839000
6	2.519245000	-2.234048000	-2.991252000	8	2.978192000	-3.564808000	2.202120000
6	2.510196000	-3.008252000	-4.169819000	6	-1.242059000	-4.100210000	1.789886000
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6	0.113590000	-1.794574000	-2.617973000	1	4.696012000	-4.725819000	2.191537000
6	-0.230142000	-3.201532000	-2.705881000	6	5.194285000	-2.793358000	1.423732000
6	-1.592546000	-3.281996000	-2.664542000	1	6.257842000	-3.069772000	1.546303000
6	-2.096370000	-1.937394000	-2.491930000	1	4.910235000	-3.022985000	0.394773000
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6	-4.441421000	-2.724384000	-2.461874000	6	-0.957769000	-0.266778000	3.423335000
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6	-6.097303000	-4.278085000	-1.581477000	1	-0.728740000	-2.377203000	3.376780000
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6	-5.550103000	-4.321817000	-3.935334000	1	-1.055323000	0.148878000	2.415155000
6	-4.636029000	-3.282403000	-3.737350000	6	1.049791000	0.864619000	4.045273000
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8	5.458359000	0.724192000	0.799465000	6	5.438546000	-0.861003000	2.981804000
1	-5.032510000	-2.818227000	-0.385581000	1	6.217460000	-1.523135000	3.393981000
1	0.479805000	-4.019539000	-2.793797000	1	5.883710000	0.129157000	2.833465000
1	-2.206902000	-4.178006000	-2.705900000	6	4.320163000	-0.745754000	4.006902000
1	3.722530000	0.179381000	-3.635862000	1	4.757542000	-0.260522000	4.898131000
1	3.392279000	2.866293000	-3.443229000	1	3.925955000	-1.724444000	4.327646000
1	-0.096622000	5.837388000	-0.714327000	8	1.581621000	-2.848570000	4.599591000
1	-2.220786000	5.225563000	0.811570000	1	1.183486000	-1.988213000	4.372066000
1	-5.926963000	1.523659000	0.050207000	1	2.009470000	-3.147712000	3.777767000
1	-6.077799000	-0.715212000	-1.485042000	6	-0.312400000	0.375135000	0.032556000
1	1.693044000	-2.852494000	-4.876652000	8	-0.637143000	-0.780874000	0.353410000
1	3.459429000	-4.523225000	-5.380107000	8	0.465580000	1.120351000	0.693215000
1	5.329778000	-4.876405000	-3.745489000	6	3.108860000	2.678492000	0.895219000
1	5.403879000	-3.533269000	-1.663921000	1	3.245571000	1.896126000	1.657620000
1	0.131285000	5.722953000	-3.608335000	1	4.094095000	3.090870000	0.653977000
1	1.406462000	7.811193000	-4.042988000	1	2.661724000	2.198739000	0.014241000
1	3.706537000	8.089428000	-3.108926000	6	2.210000000	3.759201000	1.445902000
1	4.705574000	6.258142000	-1.734293000	8	2.617638000	4.851011000	1.800533000
1	3.422071000	4.182863000	-1.305242000	8	0.928821000	3.441633000	1.576065000
1	-4.535774000	4.983449000	0.618370000	1	0.699640000	2.559549000	1.126498000

⁵ RC1 acetate, K ⁺ :			
6	2.245254000	5.356614000	-1.794180000
6	0.970099000	5.056483000	-2.310380000
6	0.293500000	6.072604000	-3.013737000
6	0.861162000	7.337609000	-3.186160000
6	2.125994000	7.618824000	-2.660102000
6	2.814569000	6.620022000	-1.962593000
6	0.326869000	3.727221000	-2.111318000
6	1.077757000	2.560341000	-2.468625000
7	0.675028000	1.263020000	-2.219167000
6	1.685850000	0.420417000	-2.615467000
6	2.770727000	1.201592000	-3.134433000
6	2.380979000	2.532556000	-3.065201000
26	-1.137694000	0.644162000	-1.425079000
7	-1.805337000	2.646665000	-1.386343000
6	-2.777505000	2.995956000	-0.461897000
6	-2.548311000	4.368111000	-0.035387000
6	-1.456796000	4.825578000	-0.711863000
6	-0.944143000	3.720066000	-1.510675000
6	-3.789046000	2.150619000	0.004884000
6	-4.642160000	2.523241000	1.161278000
6	-4.652771000	1.684261000	2.315126000
6	-5.457003000	1.994080000	3.417067000
6	-6.264295000	3.138450000	3.401202000
6	-6.265365000	3.977404000	2.286359000
6	-5.461583000	3.662621000	1.184872000
6	1.615212000	-1.009317000	-2.623268000
6	2.843218000	-1.773863000	-2.987931000
6	2.902320000	-2.450900000	-4.222821000
6	4.001106000	-3.223723000	-4.596917000
6	5.086962000	-3.346264000	-3.725009000
6	5.061234000	-2.683670000	-2.497738000
6	3.958339000	-1.897008000	-2.139106000
8	3.949154000	-1.271529000	-0.899450000
6	4.989068000	-0.318340000	-0.705531000
6	5.254550000	0.021276000	0.756976000
7	5.237915000	-0.971871000	1.713268000
8	-3.811257000	0.609076000	2.308891000
6	-4.081151000	-0.539675000	3.107319000
6	-3.625205000	-1.731746000	2.251663000
8	-4.457422000	-2.272965000	1.531316000
7	-0.834158000	-1.250443000	-2.319915000
6	0.432279000	-1.758639000	-2.493591000
6	0.354198000	-3.210850000	-2.572179000
6	-0.968831000	-3.546920000	-2.493479000
6	-1.716014000	-2.314843000	-2.321766000
6	-3.096343000	-2.244136000	-2.080456000
6	-3.898431000	-3.479699000	-2.301006000
6	-4.669567000	-4.043314000	-1.264795000
6	-5.393692000	-5.219582000	-1.474613000
6	-5.370699000	-5.855843000	-2.721211000
6	-4.613078000	-5.304417000	-3.759186000
6	-3.885848000	-4.129451000	-3.549654000
7	-3.109044000	0.048783000	-1.126049000
6	-3.756013000	-1.097023000	-1.559999000
6	-5.157536000	-0.970412000	-1.291035000
6	-5.336010000	0.236475000	-0.635857000
6	-4.047033000	0.850842000	-0.553170000
8	5.486906000	1.192963000	1.025793000
1	-4.682277000	-3.552213000	-0.290179000
1	1.200646000	-3.885837000	-2.671777000
1	-1.397588000	-4.546020000	-2.509241000
1	3.691771000	0.802837000	-3.555502000
1	2.945048000	3.397131000	-3.404960000
1	-0.990022000	5.803004000	-0.621983000
1	-3.143170000	4.908611000	0.696915000
1	-6.265262000	0.667487000	-0.266754000
1	-5.918907000	-1.705041000	-1.540546000
1	2.049076000	-2.356535000	-4.897431000
1	4.009774000	-3.729818000	-5.564879000
1	5.951739000	-3.957034000	-3.993460000
1	5.903228000	-2.783806000	-1.810197000
1	-0.692118000	5.857236000	-3.431824000
1	0.314097000	8.106044000	-3.738498000
1	2.571730000	8.607747000	-2.792103000
1	3.798450000	6.828240000	-1.534448000
1	2.789134000	4.594770000	-1.238917000
1	-5.482469000	4.300988000	0.299113000
1	-6.897119000	4.868359000	2.265038000
1	-6.886523000	3.368977000	4.269295000
1	-5.440502000	1.356094000	4.301964000
1	-5.977060000	-5.647520000	-0.654823000
1	-5.939668000	-6.774916000	-2.882437000
1	-4.591315000	-5.788318000	-4.739130000
1	-3.300146000	-3.698791000	-4.364685000
1	5.935725000	-0.671663000	-1.148132000
1	4.717317000	0.626894000	-1.197207000
1	-3.582859000	-0.458431000	4.086316000
1	-5.161326000	-0.659353000	3.268200000
7	-2.296591000	-2.051389000	2.244225000
19	2.044674000	-1.154445000	1.307954000
8	0.491740000	-0.328685000	3.665609000
8	0.528017000	-3.532658000	1.357197000
8	3.287950000	0.170343000	3.518076000
8	3.355262000	-3.396017000	2.136995000
6	-0.842566000	-3.939295000	1.329638000
1	-1.098508000	-4.471534000	2.265309000
6	-1.782711000	-2.776244000	1.073537000
1	-0.965038000	-4.656876000	0.498546000
1	-2.659658000	-3.164123000	0.549639000
1	-1.291775000	-2.061102000	0.399859000
6	1.401463000	-4.643490000	1.446426000
1	1.351296000	-5.093948000	2.455740000
1	1.099629000	-5.418283000	0.716894000
6	2.829021000	-4.259594000	1.127350000
1	3.428890000	-5.183808000	1.084352000
1	2.885212000	-3.776512000	0.134330000
6	4.773825000	-3.389797000	2.276308000
1	4.981824000	-3.201743000	3.337880000
1	5.172029000	-4.390874000	2.042176000
6	5.495843000	-2.381472000	1.388162000
1	6.578151000	-2.582528000	1.490122000
1	5.223621000	-2.566653000	0.346865000
6	-1.412654000	-1.755620000	3.368640000
6	-0.927190000	-0.309226000	3.516707000
1	-1.893497000	-2.087994000	4.300800000
1	-0.524547000	-2.388354000	3.257880000
1	-1.364690000	0.161018000	4.416209000
1	-1.210057000	0.294875000	2.648240000
6	1.053048000	0.933831000	3.996257000
1	0.456087000	1.417469000	4.791298000
6	2.449056000	0.719951000	4.524785000
1	1.030714000	1.596591000	3.115739000
1	2.860479000	1.682716000	4.880426000
1	2.395252000	0.032840000	5.387362000
6	5.561606000	-0.544916000	3.079095000
1	6.354655000	-1.193851000	3.483840000
1	5.961824000	0.472513000	3.008843000
6	4.393184000	-0.545615000	4.053619000
1	4.750172000	-0.064617000	4.981389000
1	4.055413000	-1.560870000	4.320215000
8	1.779160000	-2.763810000	4.471797000
1	1.360228000	-1.917261000	4.229814000

6	-2.572561000	-2.113832000	2.787453000	6	-2.323940000	4.579789000	0.537506000
1	-2.173630000	-4.118908000	3.328517000	6	-1.436793000	3.960610000	-0.431825000
1	-3.619861000	-2.442382000	2.850866000	6	-4.064533000	1.530766000	-0.352932000
1	-2.290569000	-2.133478000	1.725190000	6	-5.130135000	1.362424000	0.681741000
6	0.337304000	-4.220678000	3.720419000	6	-4.884904000	0.425995000	1.718292000
1	0.548938000	-4.015422000	4.785164000	6	-5.817381000	0.257469000	2.749089000
1	-0.276559000	-5.138524000	3.666545000	6	-7.006695000	0.995974000	2.737849000
6	1.622812000	-4.510648000	2.978534000	6	-7.266909000	1.910568000	1.716735000
1	2.019491000	-5.468484000	3.355295000	6	-6.321302000	2.090949000	0.699670000
1	1.419585000	-4.627358000	1.898531000	6	2.075642000	0.822619000	-3.211940000
6	3.935801000	-3.838238000	2.867091000	6	3.516786000	0.522541000	-3.456120000
1	4.584338000	-3.387275000	3.629703000	6	4.051556000	0.448913000	-4.750312000
1	4.060460000	-4.929894000	2.947427000	6	5.414015000	0.224177000	-4.959343000
6	4.367154000	-3.425581000	1.461839000	6	6.264226000	0.067809000	-3.861254000
1	5.356718000	-3.883217000	1.278939000	6	5.750905000	0.119190000	-2.563140000
1	3.661203000	-3.852603000	0.741435000	6	4.382730000	0.337238000	-2.359705000
6	-1.496625000	-0.244738000	4.171229000	8	3.834335000	0.301200000	-1.094111000
6	-0.598471000	0.875758000	3.628349000	6	4.308441000	1.234523000	-0.133421000
1	-1.945481000	0.053044000	5.131870000	6	4.266978000	0.799993000	1.339834000
1	-0.841529000	-1.092500000	4.393762000	7	4.754303000	-0.423253000	1.742509000
1	-0.803235000	1.832870000	4.138519000	8	-3.696545000	-0.227360000	1.647881000
1	-0.762530000	1.017941000	2.551075000	6	-3.411268000	-1.362358000	2.433920000
6	1.671296000	1.589470000	3.684267000	6	-2.672278000	-2.371168000	1.542280000
1	1.416013000	2.419218000	4.368797000	8	-2.940521000	-2.412600000	0.352082000
6	3.061553000	1.100314000	3.997173000	7	-0.222369000	-0.101299000	-3.291570000
1	1.618695000	1.957908000	2.647124000	6	1.133884000	-0.185531000	-3.497164000
1	3.757068000	1.959424000	4.014792000	6	1.456750000	-1.498169000	-4.024023000
1	3.074294000	0.631930000	4.997130000	6	0.278652000	-2.187956000	-4.120165000
6	5.272553000	-1.192304000	2.173288000	6	-0.772021000	-1.305971000	-3.639422000
1	6.098544000	-1.835084000	2.518701000	6	-2.123022000	-1.687928000	-3.449727000
1	5.706716000	-0.370972000	1.591509000	6	-2.505417000	-3.070336000	-3.862958000
6	4.587269000	-0.602258000	3.396290000	6	-2.882244000	-4.007310000	-2.882047000
1	5.334605000	0.033908000	3.905156000	6	-3.211128000	-5.316270000	-3.242177000
1	4.272096000	-1.372275000	4.121493000	6	-3.171516000	-5.709178000	-4.584634000
8	1.776956000	-1.712160000	5.369808000	6	-2.799154000	-4.784724000	-5.565828000
1	1.388854000	-0.951289000	4.900815000	6	-2.466125000	-3.475493000	-5.206826000
1	2.117980000	-2.300298000	4.674001000	7	-2.851752000	0.235400000	-2.079803000
6	-0.437750000	0.105529000	-0.036414000	6	-3.091516000	-0.932825000	-2.755505000
8	-0.856223000	-0.765953000	0.722972000	6	-4.459441000	-1.354621000	-2.498880000
8	0.711486000	0.740132000	0.468326000	6	-4.979116000	-0.483518000	-1.584663000
6	4.764338000	2.904938000	1.134074000	6	-3.952094000	0.502389000	-1.311107000
1	4.791274000	2.959563000	2.234322000	8	3.890852000	1.643718000	2.146693000
1	5.711303000	3.297373000	0.744670000	1	-2.906958000	-3.694685000	-1.834963000
1	4.619967000	1.854056000	0.850925000	1	2.453742000	-1.848309000	-4.279478000
6	3.629399000	3.759551000	0.645132000	1	0.138205000	-3.209870000	-4.462154000
8	3.717979000	4.911089000	0.281124000	1	3.767633000	3.163084000	-2.934411000
8	2.451614000	3.107343000	0.681054000	1	2.528448000	5.175906000	-1.641297000
1	1.049534000	1.370372000	-0.185420000	1	-2.139896000	5.521056000	1.048760000
1	1.752197000	3.703740000	0.338971000	1	-4.240237000	3.863710000	1.363533000
				1	-5.969283000	-0.496490000	-1.134953000
				1	-4.946002000	-2.219909000	-2.941098000
				1	3.381020000	0.590517000	-5.600684000
				1	5.811505000	0.179596000	-5.975428000
				1	7.332304000	-0.105394000	-4.010476000
				1	6.416911000	-0.020365000	-1.710475000
				1	-1.135461000	6.942498000	1.243842000
				1	-0.407232000	9.076330000	-0.192613000
				1	1.432192000	9.074871000	1.493711000
				1	2.531468000	6.923801000	2.122787000
				1	1.791673000	4.793209000	1.070410000
				1	-6.506428000	2.809190000	-0.102342000
				1	-8.194967000	2.485780000	1.711621000
				1	-7.728132000	0.854458000	3.544536000
				1	-5.618779000	-0.432228000	3.569725000
				1	-3.495451000	-6.035059000	-2.469537000
				1	-3.429331000	-6.733215000	-4.865375000
				1	-2.769748000	-5.083079000	-6.616654000
5TS2 acetate,K+:							
6	1.319428000	5.736948000	0.787706000				
6	0.285733000	5.726100000	-0.165112000				
6	-0.330897000	6.941051000	-0.505075000				
6	0.079536000	8.138781000	0.086841000				
6	1.111601000	8.138672000	1.030562000				
6	1.729603000	6.933374000	1.380500000				
6	-0.154918000	4.437465000	-0.776474000				
6	0.784473000	3.738687000	-1.567857000				
7	0.613345000	2.475431000	-2.079726000				
6	1.799317000	2.089466000	-2.652329000				
6	2.752756000	3.174850000	-2.544394000				
6	2.121123000	4.199203000	-1.888997000				
26	-1.033407000	1.206982000	-1.840432000				
7	-1.993804000	2.786927000	-0.864844000				
6	-3.176106000	2.613252000	-0.192255000				
6	-3.385628000	3.735915000	0.704166000				

1	-2.176264000	-2.754432000	-5.974445000	6	-0.598245000	7.169106000	-3.562801000
1	5.354351000	1.516234000	-0.348392000	6	0.400713000	7.689918000	-2.734337000
1	3.698870000	2.146757000	-0.183279000	6	1.066460000	6.847285000	-1.837014000
1	-2.832780000	-1.056937000	3.311782000	6	-0.605500000	3.509042000	-2.510417000
1	-4.331547000	-1.865603000	2.777181000	6	0.372757000	2.585713000	-2.940981000
7	-1.780273000	-3.233197000	2.138516000	7	0.278835000	1.216492000	-2.877744000
19	1.447310000	-1.176305000	2.108932000	6	1.463330000	0.693445000	-3.331928000
8	0.402343000	-2.550508000	4.385634000	6	2.343172000	1.774697000	-3.716200000
8	1.048405000	-3.696051000	1.090255000	6	1.661927000	2.943241000	-3.491168000
8	3.057095000	-1.188204000	4.236249000	26	-1.252336000	0.126376000	-2.012177000
8	3.609046000	-3.048412000	1.051671000	7	-2.289150000	1.897362000	-1.687368000
6	0.149173000	-4.714488000	1.489409000	6	-3.455421000	1.991877000	-0.984325000
1	0.370478000	-4.947623000	2.541270000	6	-3.779763000	3.390388000	-0.772725000
6	-1.303404000	-4.331814000	1.288793000	6	-2.789341000	4.120818000	-1.366390000
1	0.339428000	-5.637901000	0.916450000	6	-1.838244000	3.172114000	-1.923128000
1	-1.923572000	-5.230701000	1.468294000	6	-4.233189000	0.907413000	-0.530538000
1	-1.462131000	-4.027375000	0.249613000	6	-5.214369000	1.183462000	0.559074000
6	1.732852000	-3.904414000	-0.129895000	6	-4.702765000	1.489313000	1.843357000
1	2.102529000	-4.944937000	-0.173103000	6	-5.569491000	1.630037000	2.932648000
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6	2.910949000	-2.949816000	-0.185755000	6	-7.470866000	1.224967000	1.482565000
1	3.562509000	-3.235202000	-1.029509000	6	-6.600198000	1.069375000	0.399092000
1	2.583770000	-1.911659000	-0.368887000	6	1.782124000	-0.679800000	-3.432828000
6	5.004222000	-2.819414000	1.022625000	6	3.198888000	-1.020755000	-3.760920000
1	5.393452000	-3.200313000	1.975973000	6	3.563562000	-1.548506000	-5.008382000
1	5.476870000	-3.412313000	0.218079000	6	4.891973000	-1.863632000	-5.301691000
6	5.385840000	-1.356974000	0.809477000	6	5.881044000	-1.661605000	-4.334728000
1	6.486278000	-1.281358000	0.885449000	6	5.541242000	-1.147474000	-3.081598000
1	5.100046000	-1.077095000	-0.203638000	6	4.209791000	-0.823300000	-2.800956000
6	-1.763158000	-3.475187000	3.589521000	8	3.834630000	-0.372944000	-1.551545000
6	-1.020267000	-2.512380000	4.506341000	6	4.490275000	0.777030000	-1.028669000
1	-2.796890000	-3.517408000	3.971913000	6	4.594393000	0.926214000	0.496381000
1	-1.355524000	-4.483202000	3.744073000	7	4.950488000	-0.111926000	1.322824000
1	-1.293291000	-2.803427000	5.538199000	8	-3.357610000	1.699891000	1.940799000
1	-1.341836000	-1.473864000	4.350850000	6	-2.609987000	1.228702000	3.038116000
6	0.987965000	-1.694585000	5.371276000	6	-2.418089000	-0.287034000	2.947160000
1	0.616964000	-1.984043000	6.371461000	8	-2.948731000	-0.907772000	2.037406000
6	2.493363000	-1.794889000	5.389453000	7	-0.430921000	-1.623046000	-2.859420000
1	0.673828000	-0.652223000	5.183241000	6	0.884476000	-1.745575000	-3.233828000
1	2.857880000	-1.280070000	6.298621000	6	1.207286000	-3.154036000	-3.387906000
1	2.798725000	-2.852106000	5.450642000	6	0.067368000	-3.856104000	-3.112945000
6	5.146364000	-0.542852000	3.155855000	6	-0.955262000	-2.884502000	-2.761583000
1	6.215380000	-0.816344000	3.179273000	6	-2.243751000	-3.209505000	-2.286005000
1	5.040638000	0.453932000	3.599891000	6	-2.589521000	-4.664328000	-2.223871000
6	4.418949000	-1.539378000	4.046980000	6	-2.610630000	-5.340622000	-0.992941000
1	4.947563000	-1.514395000	5.018283000	6	-2.914985000	-6.702989000	-0.933745000
1	4.470477000	-2.573656000	3.674583000	6	-3.201209000	-7.409855000	-2.106422000
8	2.601955000	-4.348515000	3.502995000	6	-3.179204000	-6.746671000	-3.337315000
1	1.793003000	-3.880979000	3.772584000	6	-2.874213000	-5.383618000	-3.394965000
1	2.770803000	-4.011852000	2.603965000	7	-3.034082000	-0.928110000	-1.692916000
6	-0.254129000	-0.051603000	-0.382980000	6	-3.183883000	-2.293649000	-1.768430000
8	-0.179960000	-1.163346000	-0.041212000	6	-4.411188000	-2.670032000	-1.094750000
8	1.013279000	0.943552000	0.584591000	6	-4.932212000	-1.531666000	-0.544575000
6	-2.142033000	2.063385000	3.737700000	6	-4.063133000	-0.436996000	-0.922400000
1	-1.947441000	3.124875000	3.942564000	8	4.513869000	2.078357000	0.910342000
1	-2.320690000	1.513077000	4.669917000	1	-2.379975000	-4.789203000	-0.078486000
1	-3.046232000	2.008382000	3.112127000	1	2.178682000	-3.550981000	-3.671079000
6	-1.002778000	1.445374000	2.963439000	1	-0.068065000	-4.934415000	-3.128659000
8	-0.645466000	0.278739000	3.153834000	1	3.340721000	1.657404000	-4.132632000
8	-0.463789000	2.225772000	2.075177000	1	2.005880000	3.956177000	-3.681714000
1	1.272986000	1.559899000	-0.115966000	1	-2.692863000	5.202408000	-1.406850000
1	0.222846000	1.670739000	1.427239000	1	-4.657683000	3.756252000	-0.245022000
				1	-5.824669000	-1.443544000	0.068021000
				1	-4.806136000	-3.679806000	-1.022866000
				1	2.784527000	-1.700834000	-5.758303000
				1	5.154060000	-2.265711000	-6.282476000
				1	6.922050000	-1.912962000	-4.549316000
⁵¹M2 acetate, K+:							
6	0.738269000	5.490940000	-1.768703000				
6	-0.261610000	4.960241000	-2.602020000				
6	-0.928248000	5.811875000	-3.495848000				

8	-5.443244000	0.190987000	-0.598825000	6	-5.449600000	-2.073071000	-2.017486000
1	5.017811000	-2.449220000	1.388600000	1	-6.233842000	-2.847046000	-1.969669000
1	0.260388000	-2.486643000	4.788758000	1	-5.950932000	-1.112851000	-2.169284000
1	2.953897000	-2.348087000	4.636940000	6	-4.561309000	-2.363135000	-3.222931000
1	-3.351687000	1.231279000	3.965459000	1	-5.182179000	-2.182680000	-4.119854000
1	-3.150800000	3.775292000	3.115770000	1	-4.235068000	-3.414707000	-3.269315000
1	-0.310061000	5.745796000	-1.001432000	8	-1.874895000	-4.382810000	-3.967735000
1	1.733383000	4.751626000	-2.457456000	1	-1.387957000	-3.538144000	-3.955566000
1	5.776015000	1.569422000	-0.996792000	1	-2.286622000	-4.424754000	-3.086133000
1	6.239719000	0.047526000	1.193278000	6	0.797870000	0.237412000	-0.082115000
1	-1.293244000	-1.207317000	5.901438000	8	0.921627000	-0.997893000	0.051103000
1	-3.095950000	-2.597002000	6.877991000	8	0.408991000	0.790006000	-1.147788000
1	-5.006450000	-3.346777000	5.439309000	6	-3.613611000	1.658777000	-2.750022000
1	-5.064793000	-2.694138000	3.041597000	1	-3.823969000	2.733914000	-2.791823000
1	0.112007000	6.602727000	1.651248000	1	-4.508578000	1.076542000	-2.516865000
1	-1.096601000	8.766205000	1.743494000	1	-3.239672000	1.367147000	-3.742247000
1	-3.583595000	8.823758000	1.509637000	6	-2.530697000	1.364944000	-1.747379000
1	-4.835570000	6.686233000	1.184476000	8	-2.524897000	0.410235000	-0.992695000
1	-3.626830000	4.532377000	1.087821000	8	-1.515112000	2.228945000	-1.787257000
1	4.127379000	4.817925000	-2.241196000	1	-0.703444000	1.785043000	-1.324185000
1	5.177550000	5.046687000	-4.484982000	8	-3.052231000	4.575196000	-1.677727000
1	5.399796000	3.029907000	-5.951933000	1	-2.939365000	5.234945000	-0.977432000
1	4.568428000	0.837058000	-5.177006000	1	-2.264290000	4.003299000	-1.606463000
1	6.852747000	-3.927221000	2.205673000	8	-0.954745000	-3.163880000	1.492550000
1	7.805325000	-3.587153000	4.487613000	1	-1.069276000	-2.303511000	1.922227000
1	6.912156000	-1.767314000	5.942303000	1	0.027360000	-3.266807000	1.469803000
1	5.077881000	-0.299626000	5.117136000	8	-4.769899000	2.884799000	0.028314000
1	-5.195616000	-0.616958000	1.992225000	1	-4.984415000	1.982873000	-0.279138000
1	-4.043910000	0.555284000	1.318327000	1	-4.272859000	3.326627000	-0.683451000
1	3.189256000	-0.941359000	-4.367517000	8	1.772176000	-3.050413000	1.434267000
1	4.825941000	-0.813255000	-3.674012000	1	2.012700000	-2.808602000	2.343707000
7	2.530609000	-2.820930000	-2.574856000	1	1.579355000	-2.176604000	1.000908000
19	-1.441567000	-2.060690000	-1.048809000	8	0.689679000	1.846320000	-3.739990000
8	-0.661443000	-1.816519000	-3.827414000	1	1.0987261000	1.405795000	-2.922343000
8	0.158971000	-4.574995000	-1.355226000	1	-0.091165000	2.322038000	-3.420104000
8	-3.422758000	-1.523986000	-3.228098000				
8	-2.842811000	-4.468024000	-1.225011000				
6	1.459983000	-4.986696000	-1.751989000	3TS1 acetate, 6W, K+:			
1	1.440905000	-5.384439000	-2.784922000	6	-3.229496000	5.462800000	1.033725000
6	2.496483000	-3.901264000	-1.574013000	6	-1.829239000	5.426299000	1.192271000
1	1.778725000	-5.823316000	-1.102751000	6	-1.152040000	6.647434000	1.379778000
1	3.483593000	-4.390848000	-1.581634000	6	-1.843795000	7.859397000	1.410988000
1	2.377059000	-3.471483000	-0.571751000	6	-3.233225000	7.881221000	1.250480000
6	-0.724474000	-5.682882000	-1.285063000	6	-3.919834000	6.678752000	1.061252000
1	-0.967122000	-6.038267000	-2.302171000	6	-1.048679000	4.157050000	1.160931000
1	-0.228591000	-6.513586000	-0.747545000	6	-1.433692000	3.082110000	1.969846000
6	-1.986226000	-5.375016000	-0.514156000	7	-0.752659000	1.863919000	2.051871000
1	-2.517231000	-6.332516000	-0.375979000	6	-1.527052000	1.028125000	2.810979000
1	-1.740095000	-4.949783000	0.470894000	6	-2.730635000	1.712235000	3.219680000
6	-4.193841000	-4.464408000	-0.762108000	6	-2.638573000	2.997357000	2.753527000
1	-4.847937000	-4.608441000	-1.633123000	26	1.064916000	1.471524000	1.404410000
1	-4.355137000	-5.332117000	-0.104024000	7	1.014750000	3.082525000	0.262718000
6	-4.599405000	-3.235476000	0.043957000	6	1.789184000	3.285166000	-0.862602000
1	-5.562071000	-3.493474000	0.524019000	6	1.266021000	4.392809000	-1.608819000
1	-3.864861000	-3.070574000	0.837555000	6	0.217735000	4.913098000	-0.879348000
6	1.539391000	-2.732928000	-3.642709000	6	0.042561000	4.078302000	0.269063000
6	0.703971000	-1.449496000	-3.624404000	6	2.973452000	2.568924000	-1.152776000
1	2.010476000	-2.884694000	-4.627029000	6	3.654217000	2.705924000	-2.464870000
1	0.837968000	-3.560921000	-3.508244000	6	3.866773000	1.555161000	-3.270556000
1	1.007087000	-0.741532000	-4.410493000	6	4.511641000	1.657340000	-4.508445000
1	0.812188000	-0.928082000	-2.659980000	6	4.961986000	2.901643000	-4.964895000
6	-1.465961000	-0.806472000	-4.417002000	6	4.771337000	4.043745000	-4.187442000
1	-1.097302000	-0.574711000	-5.433507000	6	4.126425000	3.933714000	-2.950890000
6	-2.883285000	-1.317701000	-4.519750000	6	-1.139510000	-0.229009000	3.323262000
1	-1.390944000	0.121509000	-3.829570000	6	-2.202784000	-1.084060000	3.909141000
1	-3.494723000	-0.586784000	-5.082894000	6	-2.226813000	-1.430268000	5.274597000
1	-2.878720000	-2.263279000	-5.088850000	6	-3.242295000	-2.214601000	5.822680000
				6	-4.279055000	-2.677249000	5.007065000

6	-4.288586000	-2.347253000	3.650536000	1	1.964198000	-5.798962000	-0.821768000
6	-3.269442000	-1.557204000	3.106776000	1	3.648272000	-4.346860000	-1.328893000
8	-3.260584000	-1.287941000	1.752342000	1	2.492347000	-3.413961000	-0.389520000
6	-4.363349000	-0.564177000	1.231380000	6	-0.536323000	-5.724214000	-1.073561000
6	-4.825928000	-0.876743000	-0.189540000	1	-0.744747000	-6.138252000	-0.475976000
7	-4.681447000	-2.107081000	-0.779099000	1	-0.037870000	-6.513912000	-0.079553000
8	3.382903000	0.372317000	-2.788023000	6	-1.824119000	-5.401926000	-0.353997000
6	3.862471000	-0.847057000	-3.331398000	1	-2.338229000	-6.361794000	-0.174361000
6	3.674676000	-1.937477000	-2.269532000	1	-1.613792000	-4.916053000	0.611008000
8	4.458642000	-1.974517000	-1.322974000	6	-4.045080000	-4.570514000	-0.719578000
7	1.270975000	0.149352000	2.890323000	1	-4.666082000	-4.758373000	-1.606134000
6	0.238803000	-0.543536000	3.485629000	1	-4.208063000	-5.420744000	-0.039384000
6	0.775496000	-1.565769000	4.336838000	6	-4.504202000	-3.326069000	0.030827000
6	2.154821000	-1.460001000	4.277554000	1	-5.474029000	-3.592257000	0.492430000
6	2.454273000	-0.423308000	3.341394000	1	-3.796661000	-3.116081000	0.838177000
6	3.731832000	-0.206227000	2.781630000	6	1.727594000	-2.849855000	-3.522223000
6	4.860487000	-1.017079000	3.326960000	6	0.870342000	-1.584152000	-3.623053000
6	5.380685000	-2.084773000	2.574845000	1	2.239046000	-3.057468000	-4.475880000
6	6.417049000	-2.871886000	3.083202000	1	1.033850000	-3.679264000	-3.359464000
6	6.946128000	-2.605154000	4.350810000	1	1.182365000	-0.936518000	-4.457333000
6	6.430984000	-1.548158000	5.107971000	1	0.946331000	-0.989404000	-2.699506000
6	5.392690000	-0.761453000	4.599767000	6	-1.299749000	-1.015478000	-4.460666000
7	2.992112000	1.295198000	0.961854000	1	-0.920440000	-0.808223000	-5.478625000
6	3.960621000	0.573278000	1.653863000	6	-2.704432000	-1.558318000	-4.566274000
6	5.216102000	0.662689000	0.943427000	1	-1.253037000	-0.068789000	-3.901246000
6	4.976757000	1.361285000	-0.205248000	1	-3.321072000	-0.857211000	-5.160810000
6	3.583930000	1.754964000	-0.180750000	1	-2.673683000	-2.521591000	-5.104565000
8	-5.430458000	0.048022000	-0.739799000	6	-5.313062000	-2.253620000	-2.095376000
1	4.957459000	-2.294146000	1.590034000	1	-6.093968000	-3.031525000	-2.044307000
1	0.196726000	-2.282742000	4.910651000	1	-5.815381000	-1.303988000	-2.301140000
1	2.889010000	-2.067794000	4.800713000	6	-4.387161000	-2.583989000	-3.261707000
1	-3.507088000	1.286516000	3.850658000	1	-4.986634000	-2.449681000	-4.181031000
1	-3.342760000	3.805388000	2.922876000	1	-4.047987000	-3.632386000	-3.255744000
1	-0.404569000	5.764768000	-1.141291000	8	-1.645346000	-4.582296000	-3.850148000
1	1.645630000	4.745040000	-2.563015000	1	-1.178702000	-3.726809000	-3.877561000
1	5.679676000	1.616087000	-0.994814000	1	-2.074761000	-4.583622000	-2.975788000
1	6.153594000	0.223809000	1.274668000	6	0.813954000	0.201270000	-0.027238000
1	-1.438332000	-1.043096000	5.921553000	8	1.107772000	-0.992636000	0.126762000
1	-3.230458000	-2.453323000	6.888585000	8	0.345552000	0.612827000	-1.153147000
1	-5.078804000	-3.295544000	5.420850000	6	-3.489170000	1.471384000	-2.876126000
1	-5.087990000	-2.713404000	3.004081000	1	-3.719622000	2.540043000	-2.958699000
1	-0.068462000	6.636555000	1.510424000	1	-4.387080000	0.880910000	-2.674414000
1	-1.294744000	8.791748000	1.563980000	1	-3.062727000	1.161464000	-3.841265000
1	-3.775858000	8.829247000	1.271055000	6	-2.449042000	1.225721000	-1.806351000
1	-5.004144000	6.682283000	0.925189000	8	-2.522654000	0.294841000	-1.011279000
1	-3.779450000	4.536509000	0.866790000	8	-1.423040000	2.047815000	-1.820941000
1	4.000027000	4.820308000	-2.326849000	1	-0.502873000	1.462879000	-1.311072000
1	5.131283000	5.015615000	-4.532288000	8	-2.949378000	4.358694000	-1.824915000
1	5.462739000	2.967728000	-5.933744000	1	-2.796974000	5.032604000	-1.147397000
1	4.652443000	0.774768000	-5.132497000	1	-2.187121000	3.747010000	-1.747961000
1	6.810732000	-3.700214000	2.488789000	8	-0.900008000	-3.055319000	1.540245000
1	7.756663000	-3.220895000	4.748185000	1	-1.044907000	-2.188420000	1.947232000
1	6.839797000	-1.333794000	6.098514000	1	0.079477000	-3.166371000	1.588635000
1	4.987993000	0.062520000	5.191999000	8	-4.820106000	2.792938000	-0.197879000
1	-5.250058000	-0.693572000	1.875791000	1	-4.976700000	1.868124000	-0.469498000
1	-4.117453000	0.506372000	1.215025000	1	-4.227188000	3.193718000	-0.860342000
1	3.374854000	-1.067994000	-4.292677000	8	1.839198000	-3.007663000	1.643759000
1	4.948243000	-0.786119000	-3.504086000	1	2.034649000	-2.730637000	2.553950000
7	2.677604000	-2.848887000	-2.413704000	1	1.696089000	-2.150373000	1.167168000
19	-1.312248000	-2.091362000	-1.051371000	8	0.644895000	1.764317000	-3.797504000
8	-0.481989000	-1.989612000	-3.828489000	1	1.122972000	1.310784000	-3.084223000
8	0.325139000	-4.602410000	-1.180155000	1	-0.137123000	2.090288000	-3.319449000
8	-3.257821000	-1.732877000	-3.276317000				
8	-2.679701000	-4.556974000	-1.137603000				
6	1.644636000	-5.003247000	-1.520143000				
1	1.664516000	-5.451021000	-2.532402000				
6	2.648707000	-3.884546000	-1.367645000				
				³IM1 acetate, 6W, K+:			
				6	-2.747956000	5.648695000	1.136926000
				6	-1.348350000	5.516850000	1.232439000
				6	-0.579042000	6.688580000	1.372639000

6	-1.182665000	7.946474000	1.417183000	1	-5.116397000	-2.305680000	3.220920000
6	-2.573032000	8.063547000	1.318424000	1	0.505971000	6.602925000	1.455292000
6	-3.349795000	6.910227000	1.177459000	1	-0.563787000	8.839721000	1.531973000
6	-0.661812000	4.195295000	1.181227000	1	-3.046849000	9.047516000	1.349455000
6	-1.079489000	3.157331000	2.025075000	1	-4.436246000	6.988359000	1.089317000
7	-0.480195000	1.895312000	2.086249000	1	-3.367330000	4.761330000	1.006646000
6	-1.278160000	1.114680000	2.877755000	1	4.321124000	4.463936000	-2.464795000
6	-2.410342000	1.879998000	3.334327000	1	5.353645000	4.606203000	-4.724702000
6	-2.251071000	3.156803000	2.856672000	1	5.379704000	2.581660000	-6.196584000
26	1.282184000	1.391932000	1.380184000	1	4.373167000	0.465435000	-5.411060000
7	1.257720000	2.953545000	0.191866000	1	6.634246000	-4.190111000	2.353437000
6	1.994620000	3.094374000	-0.968401000	1	7.797542000	-3.666359000	4.498762000
6	1.520448000	4.235265000	-1.698941000	1	7.148565000	-1.636498000	5.795479000
6	0.554070000	4.837526000	-0.925448000	1	5.347614000	-0.138913000	4.947493000
6	0.368357000	4.025807000	0.238265000	1	-5.158501000	-0.260876000	2.134704000
6	3.119514000	2.308086000	-1.295030000	1	-3.974877000	0.831537000	1.381924000
6	3.744150000	2.404040000	-2.640720000	1	2.950082000	-1.288818000	-4.513439000
6	3.783257000	1.265373000	-3.485654000	1	4.597845000	-1.149819000	-3.849203000
6	4.366957000	1.336783000	-4.756147000	7	2.265830000	-3.036889000	-2.591650000
6	4.928168000	2.538367000	-5.202609000	19	-1.626011000	-1.952904000	-1.033611000
6	4.908129000	3.668593000	-4.385233000	8	-0.903318000	-1.979658000	-3.842972000
6	4.321095000	3.589194000	-3.118067000	8	-0.124473000	-4.589485000	-1.184971000
6	-0.956588000	-0.172403000	3.369896000	8	-3.610011000	-1.531568000	-3.109279000
6	-2.054497000	-0.953114000	3.992991000	8	-3.116993000	-4.337160000	-0.960964000
6	-2.039262000	-1.322712000	5.352561000	6	1.134337000	-5.097284000	-1.601105000
6	-3.088873000	-2.028250000	5.941823000	1	1.054842000	-5.559047000	-2.604103000
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6	-3.198671000	-1.316898000	3.239564000	1	3.190796000	-4.595749000	-1.552410000
8	-3.237068000	-1.021314000	1.891944000	1	2.175673000	-3.565738000	-0.555423000
6	-4.309402000	-0.213142000	1.431413000	6	-1.055150000	-5.640066000	-0.981029000
6	-4.889560000	-0.497223000	0.046972000	1	-1.361301000	-6.070285000	-1.951262000
7	-4.891743000	-1.744397000	-0.530276000	1	-0.575324000	-6.444920000	-0.392017000
8	3.196594000	0.128142000	-3.006688000	6	-2.264584000	-5.198331000	-0.192483000
6	3.527847000	-1.122476000	-3.592491000	1	-2.825731000	-6.110705000	0.072920000
6	3.335239000	-2.201580000	-2.520689000	1	-1.951347000	-4.682856000	0.728643000
8	4.178852000	-2.297135000	-1.631900000	6	-4.452552000	-4.247660000	-0.465346000
7	1.454621000	0.065899000	2.855275000	1	-5.134484000	-4.398611000	-1.313070000
6	0.404630000	-0.568459000	3.484847000	1	-4.637014000	-5.076740000	0.235513000
6	0.914090000	-1.626300000	4.311382000	6	-4.775692000	-2.963393000	0.288487000
6	2.293354000	-1.596549000	4.205684000	1	-5.739890000	-3.146706000	0.799760000
6	2.619617000	-0.575561000	3.260848000	1	-4.015214000	-2.801949000	1.057609000
6	3.885700000	-0.432374000	2.659003000	6	1.256649000	-2.985453000	-3.645396000
6	4.983320000	-1.307656000	3.169616000	6	0.481477000	-1.665940000	-3.720091000
6	5.351319000	-2.455768000	2.448272000	1	1.697739000	-3.239014000	-4.622684000
6	6.358731000	-3.299144000	2.923124000	1	0.517866000	-3.762565000	-3.430960000
6	7.009401000	-3.007094000	4.127069000	1	0.789392000	-1.052666000	-4.581894000
6	6.644701000	-1.869660000	4.854239000	1	0.653764000	-1.067216000	-2.812668000
6	5.635175000	-1.026407000	4.378999000	6	-1.689806000	-0.944566000	-4.417631000
7	3.179196000	1.112359000	0.863299000	1	-1.363595000	-0.757622000	-5.457731000
6	4.122204000	0.325710000	1.516576000	6	-3.134113000	-1.382751000	-4.432677000
6	5.334964000	0.293162000	0.733418000	1	-1.540330000	-0.009572000	-3.857409000
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8	-3.309223000	-0.803690000	1.873715000	1	1.944096000	-3.753131000	-0.420708000
6	-4.350523000	0.053204000	1.424051000	6	-1.433011000	-5.616844000	-0.825630000
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6	3.443202000	-1.501020000	-3.548229000	1	-3.249075000	-5.948691000	0.203965000
6	3.187723000	-2.527681000	-2.438263000	1	-2.282128000	-4.583024000	0.863099000
8	4.033365000	-2.655329000	-1.555115000	6	-4.737663000	-3.991534000	-0.388895000
7	1.459573000	0.066919000	2.819876000	1	-5.405148000	-4.118293000	-1.252114000
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6	6.467316000	-2.053993000	4.990932000	1	0.557819000	-1.228189000	-2.658135000
6	5.510175000	-1.180445000	4.465903000	6	-1.739959000	-0.950147000	-4.354836000
7	3.231634000	0.940181000	0.781557000	1	-1.379278000	-0.825686000	-5.392745000
6	4.141104000	0.148707000	1.467391000	6	-3.210863000	-1.285440000	-4.386670000
6	5.343939000	0.026290000	0.689420000	1	-1.534542000	-0.007328000	-3.826531000
6	5.116283000	0.665907000	-0.508288000	1	-3.745238000	-0.517240000	-4.978021000
6	3.804835000	1.235363000	-0.436702000	1	-3.343893000	-2.256759000	-4.894762000
8	-5.451395000	0.777312000	-0.493501000	6	-5.762279000	-1.550652000	-1.777564000
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1	0.181406000	-2.199987000	4.916443000	1	-6.138901000	-0.544201000	-1.982769000
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1	-3.061074000	1.808989000	3.943450000	1	-5.579748000	-1.831073000	-3.872728000
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1	0.316203000	5.690774000	-1.382477000	8	-2.541515000	-4.424635000	-3.601422000
1	2.089861000	4.317506000	-2.889657000	1	-1.972142000	-3.637748000	-3.685420000
1	5.793877000	0.767113000	-1.352900000	1	-2.914252000	-4.344326000	-2.704952000
1	6.239590000	-0.504699000	1.000495000	6	0.912252000	0.028565000	-0.016909000
1	-1.218342000	-0.759782000	5.924382000	8	1.209618000	-1.157964000	0.121479000
1	-3.123000000	-1.895773000	7.025155000	8	0.292475000	0.438311000	-1.070321000
1	-5.149519000	-2.506595000	5.682050000	6	-3.390501000	1.896155000	-2.737150000
1	-5.227899000	-1.960061000	3.262558000	1	-3.494653000	2.986900000	-2.777686000
1	1.036061000	6.609764000	1.136643000	1	-4.348431000	1.410110000	-2.531712000
1	0.181652000	8.932600000	1.186026000	1	-3.022947000	1.574347000	-3.722959000
1	-2.281000000	9.366768000	1.177118000	6	-2.369864000	1.492300000	-1.695820000
1	-3.864608000	7.435522000	1.109346000	8	-2.572880000	0.582172000	-0.897779000
1	-3.013902000	5.121593000	1.049805000	8	-1.230238000	2.141502000	-1.731795000
1	4.497824000	4.096976000	-2.707634000	1	-0.388704000	1.401100000	-1.214079000
1	5.534893000	4.069828000	-4.969841000	8	-2.412571000	4.647596000	-1.684936000
1	5.463319000	1.970811000	-6.331441000	1	-2.113239000	5.315376000	-1.051677000
1	4.364490000	-0.051839000	-5.436384000	1	-1.734096000	3.940515000	-1.645658000
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1	6.924795000	-1.839217000	5.959907000	1	-0.136700000	-3.151469000	1.632061000
1	5.216281000	-0.288706000	5.024511000	8	-4.432657000	3.420804000	0.017442000
1	-5.192312000	0.042754000	2.137298000	1	-4.720661000	2.527360000	-0.250003000
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8	-3.724531000	-1.343641000	-3.070675000				
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6	-2.236893000	5.927762000	1.198351000	1	-1.081467000	-0.861501000	5.946676000
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6	4.278967000	0.897121000	-4.924577000	7	1.936569000	-3.251441000	-2.577681000
6	4.916657000	2.041506000	-5.415156000	19	-1.803014000	-1.868932000	-0.908895000
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8	3.941605000	-2.649596000	-1.711754000	6	-4.795131000	-3.932526000	-0.289581000
7	1.547567000	0.022354000	2.809559000	1	-5.493432000	-4.054704000	-1.128553000
6	0.464767000	-0.551372000	3.467391000	1	-5.027959000	-4.732439000	0.430526000
6	0.923222000	-1.617657000	4.292571000	6	-5.024719000	-2.613351000	0.438423000
6	2.309397000	-1.660724000	4.168871000	1	-5.997551000	-2.717275000	0.955871000
6	2.671551000	-0.668739000	3.211085000	1	-4.251424000	-2.493882000	1.201582000
6	3.952663000	-0.592931000	2.588798000	6	0.890942000	-3.135737000	-3.590200000
6	5.003511000	-1.509587000	3.111401000	6	0.215829000	-1.761474000	-3.655376000
6	5.334378000	-2.675398000	2.398198000	1	1.268376000	-3.436184000	-4.580762000
6	6.292379000	-3.563348000	2.892977000	1	0.104284000	-3.849787000	-3.331764000
6	6.932871000	-3.300262000	4.109039000	1	0.552248000	-1.172894000	-4.523267000
6	6.604976000	-2.147215000	4.829419000	1	0.449692000	-1.176984000	-2.752314000
6	5.643520000	-1.260334000	4.335465000	6	-1.915883000	-0.912977000	-4.356766000
7	3.293974000	0.917828000	0.744796000	1	-1.583509000	-0.777936000	-5.402665000
6	4.204643000	0.101433000	1.394966000	6	-3.381457000	-1.271902000	-4.349095000
6	5.381884000	-0.036267000	0.582591000	1	-1.716590000	0.029706000	-3.825379000
6	5.132144000	0.620387000	-0.603195000	1	-3.944565000	-0.505348000	-4.914794000
6	3.834920000	1.210601000	-0.487960000	1	-3.520259000	-2.242832000	-4.856167000
8	-5.424950000	0.848623000	-0.370829000	6	-5.831606000	-1.472993000	-1.644893000
1	4.818195000	-2.883986000	1.458886000	1	-6.727742000	-2.097660000	-1.486860000
1	0.301893000	-2.265797000	4.902148000	1	-6.174655000	-0.453593000	-1.846015000
1	2.998467000	-2.337867000	4.667134000	6	-5.092155000	-1.991817000	-2.874493000
1	-2.939749000	1.776751000	4.039508000	1	-5.741618000	-1.781013000	-3.744148000
1	-2.509595000	4.250356000	3.039473000	1	-4.932310000	-3.082139000	-2.854902000
1	0.323515000	5.664464000	-1.343789000	8	-2.686421000	-4.386974000	-3.568767000
1	2.070663000	4.298800000	-2.890684000	1	-2.119489000	-3.600922000	-3.672450000
1	5.785501000	0.715368000	-1.467355000	1	-3.038255000	-4.299282000	-2.664535000
1	6.274987000	-0.588489000	0.862402000	6	0.969355000	-0.001685000	0.035592000

1	-5.495563000	-4.013813000	0.370008000
1	-4.598032000	-4.356628000	1.843620000
6	-4.694474000	-2.282935000	1.432044000
1	-5.500233000	-2.266530000	2.189771000
1	-3.755191000	-2.023565000	1.923628000
6	0.183240000	-3.425942000	-4.372252000
6	-0.986616000	-2.630690000	-4.920755000
1	0.931153000	-3.500813000	-5.182586000
1	-0.172470000	-4.448011000	-4.198884000
1	-1.311664000	-3.142345000	-5.845693000
1	-0.701559000	-1.610420000	-5.215085000
6	-3.126317000	-1.751672000	-4.516178000
1	-3.230346000	-1.914333000	-5.602972000
6	-4.439449000	-2.116297000	-3.878196000
1	-2.879797000	-0.688384000	-4.355501000
1	-5.247687000	-1.573636000	-4.403794000
1	-4.610416000	-3.198227000	-4.007701000
6	-5.991062000	-1.614816000	-0.616932000
1	-6.802407000	-2.183396000	-0.131070000
1	-6.413425000	-0.667696000	-0.965475000
6	-5.532994000	-2.409912000	-1.827145000
1	-6.409473000	-2.468943000	-2.497462000
1	-5.249944000	-3.444361000	-1.583568000
8	-3.246822000	-4.865209000	-2.657566000
1	-2.760430000	-4.147634000	-3.100573000
1	-3.378115000	-4.553869000	-1.744062000
6	1.208876000	-0.313309000	0.094693000
8	1.441601000	-1.461960000	0.413103000
8	0.465593000	-0.104684000	-0.990305000
6	-3.350751000	1.578762000	-2.586991000
1	-4.026664000	2.431947000	-2.728549000
1	-3.904792000	0.634400000	-2.609002000
1	-2.598239000	1.593126000	-3.391556000
6	-2.612767000	1.690099000	-1.288995000
8	-2.288369000	0.761181000	-0.581641000
8	-2.299316000	2.957021000	-0.974976000
1	0.345287000	0.832642000	-1.298103000
8	-4.156508000	4.857901000	-1.728915000
1	-3.914091000	5.730899000	-2.066495000
1	-3.322736000	4.357597000	-1.672894000
8	-1.405669000	-1.845421000	1.421204000
1	-1.716987000	-1.038442000	1.860260000
1	-0.633029000	-2.184961000	1.917011000
8	-5.063319000	3.620680000	0.647055000
1	-5.193069000	2.720279000	0.291644000
1	-4.789458000	4.143524000	-0.129035000
8	0.872592000	-3.101367000	2.444018000
1	1.099790000	-2.655491000	3.277929000
1	1.272975000	-2.520455000	1.759389000
8	0.014478000	1.911758000	-2.602081000
1	0.843186000	1.684158000	-3.070638000
1	0.148523000	2.835662000	-2.333103000
1	-1.840277000	3.000755000	-0.102139000

UB3LYP data:

³CAT_{H3O+,K+}:

6	2.618393000	5.223118000	-1.170136000	1	-3.075149000	4.704348000	0.525830000
6	1.440087000	4.953331000	-1.895669000	1	-5.959695000	0.403783000	-0.666304000
6	0.906197000	5.995542000	-2.679838000	1	-5.433585000	-2.002072000	-1.796818000
6	1.520347000	7.250970000	-2.738519000	1	3.272277000	-1.441814000	-5.016063000
6	2.690564000	7.497714000	-2.012154000	1	5.448827000	-2.535164000	-5.541229000
6	3.236666000	6.476196000	-1.226283000	1	6.822828000	-3.491159000	-3.674358000
6	0.769105000	3.619105000	-1.828416000	1	6.017309000	-3.361504000	-1.354631000
6	1.472804000	2.480891000	-2.289825000	1	-0.005235000	5.811720000	-3.254506000
7	1.022935000	1.158314000	-2.192913000	1	1.084956000	8.039009000	-3.359487000
6	2.084182000	0.363518000	-2.631128000	1	3.172604000	8.477921000	-2.057089000
6	3.175360000	1.188208000	-3.030162000	1	4.146604000	6.658044000	-0.647352000
6	2.786770000	2.503865000	-2.842055000	1	3.048738000	4.434937000	-0.547211000
26	-0.851116000	0.544590000	-1.765819000	1	-5.380086000	4.052207000	-0.793271000
7	-1.326374000	2.415542000	-1.196623000	1	-7.261956000	4.827099000	0.640327000
6	-2.469862000	2.799603000	-0.498739000	1	-7.703858000	3.687673000	2.825060000
6	-2.338045000	4.158450000	-0.059187000	1	-6.244800000	1.822580000	3.566657000
6	-1.136797000	4.628097000	-0.541577000	1	-5.377991000	-5.964897000	-0.843503000
6	-0.509374000	3.545702000	-1.243148000	1	-5.319145000	-7.034273000	-3.102068000
6	-3.613469000	2.004450000	-0.310934000	1	-4.004252000	-5.957636000	-4.935770000
6	-4.730466000	2.502568000	0.545979000	1	-2.771070000	-3.847436000	-4.512002000
6	-4.998424000	1.880488000	1.795207000	1	3.914542000	-2.899362000	1.306513000
6	-6.061283000	2.303117000	2.603744000	1	5.433375000	-2.819920000	0.403504000
6	-6.877180000	3.362963000	2.187733000	1	-4.391577000	0.111666000	4.099701000
6	-6.627784000	4.000822000	0.971382000	1	-5.630613000	-0.374040000	2.907097000
6	-5.565024000	3.566533000	0.168274000	7	-2.447271000	-1.402634000	2.643083000
6	2.096101000	-1.055278000	-2.618417000	19	1.818295000	-0.106328000	0.420122000
6	3.394830000	-1.749713000	-2.895442000	8	0.245680000	1.002326000	2.584381000
6	3.879508000	-1.860112000	-4.209112000	8	0.386032000	-2.918952000	3.156738000
6	5.101710000	-2.471924000	-4.507013000	8	3.014887000	1.612951000	2.529038000
6	5.867048000	-3.002737000	-3.467664000	8	3.017340000	-2.124029000	4.141561000
6	5.410675000	-2.923410000	-2.147992000	6	-0.938295000	-3.405691000	2.998496000
6	4.188326000	-2.300563000	-1.858642000	1	-1.458213000	-3.459920000	3.974605000
8	3.664930000	-2.248609000	-0.585949000	6	-1.730512000	-2.524885000	2.035346000
6	4.472933000	-2.309484000	0.568827000	1	-0.899631000	-4.435537000	2.592144000
6	4.727967000	-0.877768000	1.081732000	1	-2.486224000	-3.144437000	1.540919000
7	5.036173000	-0.689315000	2.393597000	1	-1.046072000	-2.148386000	1.256143000
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6	-4.561977000	-0.152779000	3.040009000	1	0.853565000	-3.320594000	5.142514000
6	-3.814046000	-1.429727000	2.633633000	1	0.915738000	-4.724157000	4.039105000
8	-4.460633000	-2.409600000	2.269752000	6	2.619179000	-3.468537000	3.906190000
7	-0.351643000	-1.342056000	-2.235495000	1	3.144513000	-4.144282000	4.605092000
6	0.936945000	-1.833818000	-2.443135000	1	2.875882000	-3.780208000	2.877067000
6	0.898298000	-3.259318000	-2.581410000	6	4.371477000	-1.912218000	4.505254000
6	-0.424091000	-3.639183000	-2.517297000	1	4.388758000	-0.995056000	5.111763000
6	-1.199535000	-2.450186000	-2.314821000	1	4.731670000	-2.734321000	5.150180000
6	-2.602842000	-2.425149000	-2.191857000	6	5.336856000	-1.780175000	3.322850000
6	-3.360626000	-3.689360000	-2.438180000	1	6.346650000	-1.620821000	3.739855000
6	-4.112403000	-4.312330000	-1.419750000	1	5.388493000	-2.727125000	2.773010000
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6	-4.774715000	-6.104280000	-2.917898000	6	-1.124970000	0.730916000	2.260693000
6	-4.035700000	-5.501894000	-3.942020000	1	-2.213210000	0.138268000	4.051301000
6	-3.340730000	-4.311916000	-3.703144000	1	-0.774970000	-0.808617000	3.715146000
7	-2.728871000	-0.060178000	-1.404921000	1	-1.714833000	1.655210000	2.334316000
6	-3.314140000	-1.272042000	-1.776189000	1	-1.209706000	0.383217000	1.216878000
6	-4.723767000	-1.212085000	-1.563468000	6	0.711449000	2.320885000	2.317784000
6	-4.992408000	0.015621000	-0.981099000	1	-0.005271000	3.067286000	2.705383000
6	-3.755439000	0.712643000	-0.880573000	6	2.037969000	2.521975000	3.020220000
8	4.595849000	0.060210000	0.298083000	1	0.800689000	2.498558000	1.228921000
1	-4.148558000	-3.854194000	-0.428448000	1	2.370045000	3.567100000	2.868035000
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1	-0.827230000	-4.646213000	-2.596439000	6	5.270147000	0.691461000	2.836548000
1	4.127985000	0.828315000	-3.412615000	1	6.068612000	0.674279000	3.594683000
1	3.368794000	3.398749000	-3.049223000	1	5.636904000	1.260982000	1.925090000
1	-0.712657000	5.620863000	-0.408675000	6	4.082312000	1.430168000	3.449481000
				1	4.465702000	2.413684000	3.783708000
				1	3.694025000	0.908627000	4.341726000
				8	1.293494000	-0.095115000	5.074581000

1	0.946809000	0.290091000	4.250098000	1	-1.840707000	2.616379000	-4.772449000
1	1.838320000	-0.839812000	4.755117000	1	-3.738471000	3.281557000	-2.935129000
³RC1H3O+,K+:							
6	1.223132000	1.393537000	-5.534236000	1	-5.883077000	0.835548000	1.217575000
6	-0.024817000	0.750993000	-5.433097000	1	-5.647999000	-1.642404000	2.241561000
6	-0.830642000	0.684885000	-6.585632000	1	1.008321000	-6.154703000	-2.049407000
6	-0.400465000	1.231085000	-7.798511000	1	2.930283000	-7.725667000	-1.821551000
6	0.845933000	1.862171000	-7.883793000	1	5.058283000	-6.914107000	-0.777166000
6	1.655971000	1.941810000	-6.746464000	1	5.260076000	-4.583830000	-0.020072000
6	-0.494510000	0.162847000	-4.138883000	1	-1.804176000	0.191314000	-6.527913000
6	0.162852000	-0.942703000	-3.615880000	1	-1.040266000	1.160205000	-8.682268000
7	-0.142190000	-1.597093000	-2.432449000	1	1.183012000	2.290052000	-8.831488000
6	0.797882000	-2.600223000	-2.300049000	1	2.629301000	2.436940000	-6.800263000
6	1.711980000	-2.581129000	-3.428324000	1	1.858830000	1.465826000	-4.648115000
6	1.305601000	-1.582764000	-4.252167000	1	-6.472782000	2.005159000	-1.596740000
26	-1.609431000	-1.145906000	-1.113474000	1	-7.784940000	4.043467000	-1.034032000
7	-2.183745000	0.387744000	-2.302370000	1	-6.757195000	5.825292000	0.391960000
6	-3.103671000	1.360652000	-1.967132000	1	-4.427814000	5.556558000	1.218139000
6	-3.081445000	2.414207000	-2.928646000	1	-4.819125000	-3.882597000	5.621216000
6	-2.126462000	2.605722000	-3.885127000	1	-5.942078000	-6.005678000	4.935185000
6	-1.576668000	0.815832000	-3.475506000	1	-5.846136000	-6.734974000	2.547643000
6	-3.937368000	1.352645000	-0.812253000	1	-4.641258000	-5.355949000	0.870504000
6	-4.719035000	2.591539000	-0.499762000	1	4.515903000	-2.263158000	1.317515000
6	-4.166535000	3.615537000	0.300136000	1	5.387475000	-2.593502000	-0.195953000
6	-4.888008000	4.771663000	0.614821000	1	-1.898561000	4.713669000	2.093745000
6	-6.194486000	4.922702000	0.142078000	1	-3.403038000	3.966208000	2.674876000
6	-6.766006000	3.929144000	-0.656828000	7	-0.559566000	2.600921000	3.219984000
6	-6.027521000	2.785074000	-0.974157000	19	2.300921000	1.123201000	1.163203000
6	0.847282000	-3.555098000	-1.292448000	8	1.931762000	3.908156000	1.657873000
6	2.030684000	-4.468738000	-1.201663000	8	2.226346000	1.062341000	3.983927000
6	1.948860000	-5.805277000	-1.616029000	8	4.182030000	2.920255000	0.072899000
6	3.024687000	-6.690764000	-1.484614000	8	5.041341000	1.021695000	3.060501000
6	4.210627000	-6.236483000	-0.907835000	6	1.057879000	1.289233000	4.760564000
6	4.328512000	-4.907917000	-0.483664000	1	1.177426000	2.187281000	5.395030000
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8	3.303767000	-2.699648000	-0.289554000	1	0.924144000	0.438547000	5.454733000
6	4.479695000	-2.127626000	0.224535000	1	-1.038488000	1.083988000	4.578135000
6	4.528837000	-0.647865000	-0.193036000	1	-0.158239000	0.529695000	3.167099000
7	5.539855000	0.132006000	0.306807000	6	3.369492000	0.839118000	4.799865000
8	-2.850240000	3.471867000	0.732313000	1	3.731640000	1.797395000	5.212978000
6	-2.491239000	3.792323000	2.086421000	1	3.097893000	0.180627000	5.645878000
6	-1.823018000	2.547621000	2.694458000	6	4.478424000	0.148498000	4.036193000
8	-2.481605000	1.514989000	2.709721000	1	5.255353000	-0.145984000	4.764440000
7	-1.344653000	-2.964375000	-0.267289000	1	4.089136000	-0.772708000	3.564721000
6	-0.204651000	-3.741220000	-0.355524000	6	6.353107000	0.704512000	2.613600000
6	-0.251648000	-4.801669000	0.597476000	1	6.829693000	1.658403000	2.350333000
6	-1.452792000	-4.680067000	1.269232000	1	6.945341000	0.266286000	3.436282000
6	-2.108485000	-3.531203000	0.737596000	6	6.399243000	-0.263673000	1.421533000
6	-3.324157000	-3.007033000	1.258625000	1	7.449645000	-0.326925000	1.085501000
6	-4.049209000	-3.827568000	2.281067000	1	6.122364000	-1.267507000	1.759789000
6	-4.110459000	-3.432847000	3.630162000	6	0.193639000	3.851764000	3.388086000
6	-4.786482000	-4.208616000	4.578128000	6	0.736709000	4.522313000	2.127570000
6	-5.413581000	-5.398769000	4.195451000	1	-0.422906000	4.594959000	3.918864000
6	-5.357391000	-5.807543000	2.858120000	1	1.046517000	3.653396000	4.047766000
6	-4.679972000	-5.030880000	1.913332000	1	0.950439000	5.577580000	2.380852000
7	-3.270755000	-0.884522000	-0.016643000	1	-0.006465000	4.531588000	1.314163000
6	-3.823450000	-1.759811000	0.911263000	6	2.391715000	4.501357000	0.437557000
6	-5.003958000	-1.159893000	1.510641000	1	2.210046000	5.590211000	0.461765000
6	-5.122745000	0.090020000	0.996617000	6	3.875947000	4.293490000	0.258552000
6	-4.059941000	0.247487000	0.018956000	1	1.825258000	4.083825000	-0.414756000
8	3.724447000	-0.211124000	-1.008808000	1	4.199315000	4.877671000	-0.624684000
1	-3.616613000	-2.507884000	3.938285000	1	4.411041000	4.683770000	1.142424000
1	0.516068000	-5.557354000	0.742047000	6	5.932959000	1.306973000	-0.485768000
1	-1.833237000	-5.310545000	2.069080000	1	7.030451000	1.277117000	-0.593586000
1	2.534047000	-3.278698000	-3.574332000	1	5.492414000	1.182918000	-1.483214000
1	1.730025000	-1.294944000	-5.210707000	6	5.580672000	2.701441000	0.017942000
				1	6.041133000	3.409853000	-0.697910000
				1	6.027432000	2.915729000	1.003731000

6	-2.190948000	-3.478144000	3.693237000	6	-4.997227000	1.848634000	1.827536000
1	-1.261401000	-5.338171000	3.350953000	6	-6.058341000	2.265386000	2.641448000
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1	-2.766558000	-3.518945000	2.762158000	6	-6.628732000	3.974251000	1.022136000
6	0.504871000	-4.917755000	1.727042000	6	-5.567952000	3.545823000	0.213559000
1	0.948901000	-5.631167000	2.443786000	6	2.103951000	-1.036208000	-2.610233000
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6	1.598282000	-4.384542000	0.829075000	6	3.878963000	-1.838815000	-4.211341000
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1	1.196379000	-3.636282000	0.121010000	6	5.869010000	-2.985258000	-3.482850000
6	3.963723000	-3.899196000	1.094640000	6	5.420517000	-2.906521000	-2.160440000
1	4.636064000	-4.107377000	1.938372000	6	4.201406000	-2.280929000	-1.863043000
1	4.037808000	-4.762972000	0.413031000	8	3.687049000	-2.228013000	-0.586727000
6	4.422351000	-2.664063000	0.321658000	6	4.503525000	-2.288057000	0.562324000
1	5.415692000	-2.905163000	-0.100561000	6	4.742967000	-0.856958000	1.084381000
1	3.754220000	-2.502524000	-0.531122000	7	5.047554000	-0.672873000	2.397798000
6	-1.611347000	-1.735753000	5.407118000	8	-4.136979000	0.852713000	2.197448000
6	-0.414202000	-0.804567000	5.589359000	6	-4.556732000	-0.193813000	3.056484000
1	-2.441936000	-1.292164000	5.982647000	6	-3.803579000	-1.465012000	2.641866000
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1	-0.553820000	0.148281000	5.050721000	6	0.942422000	-1.824746000	-2.455316000
6	1.916900000	-0.531910000	5.629111000	6	0.908146000	-3.244149000	-2.606498000
1	1.839195000	-0.368659000	6.719370000	6	-0.419518000	-3.625663000	-2.552108000
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1	1.843296000	0.457286000	5.138546000	6	-2.604686000	-2.418030000	-2.213878000
1	4.028072000	-0.546781000	5.876098000	6	-3.358568000	-3.679065000	-2.476670000
1	3.304495000	-2.174775000	5.756207000	6	-4.127784000	-4.308631000	-1.473941000
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1	1.674074000	-3.369604000	4.832185000	6	-4.991678000	-0.004397000	-0.942769000
1	2.355528000	-4.061629000	3.635005000	6	-3.755305000	0.700111000	-0.849793000
6	0.672233000	1.515662000	-0.112864000	8	4.603085000	0.083990000	0.305639000
8	1.331571000	2.233348000	0.469251000	1	-4.176213000	-3.858535000	-0.479460000
8	-0.574426000	0.450547000	2.042089000	1	1.776839000	-3.879698000	-2.768222000
8	-1.301312000	2.995145000	2.725635000	1	-0.820590000	-4.632864000	-4.638983000
1	-2.210601000	2.646664000	2.786789000	1	4.133858000	0.851281000	-3.390350000
1	-1.376183000	0.207536000	1.552938000	1	3.359967000	3.415026000	-3.040400000
1	-0.713284000	1.402204000	2.266603000	1	-0.732157000	5.619969000	-0.391625000
1	-1.348733000	3.644739000	2.006793000	1	-3.087008000	4.690688000	0.558561000
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				1	-0.097451000	5.818702000	-3.215584000
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⁵CAT_{H3O+,K+}:							
6	2.607330000	5.254455000	-1.231047000				
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7	1.024865000	1.169902000	-2.175189000				
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				1	-2.196992000	-1.287247000	-6.446501000
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				1	1.952579000	1.305129000	-7.356983000
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				1	-8.306133000	2.840806000	-0.971813000
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				1	5.466307000	-2.118712000	0.163488000
5RC1 H3O+,K+:							
6	0.725570000	0.355787000	-5.853101000				
6	-0.440608000	-0.379998000	-5.568441000				
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8	4.410387000	1.582528000	2.630505000	6	-4.283448000	-0.562448000	0.456030000
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1	0.960040000	2.697380000	5.403616000	6	-6.946094000	-3.962652000	0.250188000
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1	3.369605000	2.305839000	4.934974000	6	2.405358000	4.457336000	0.332277000
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1	4.634384000	0.300199000	4.264310000	6	4.928788000	5.708084000	0.344511000
1	3.357711000	-0.157070000	3.105204000	6	4.796745000	4.413231000	-0.168759000
6	5.806180000	1.499996000	2.367412000	6	3.540931000	3.790395000	-0.192925000
1	6.113283000	2.516295000	2.088916000	8	3.307073000	2.564189000	-0.748052000
1	6.358580000	1.231603000	3.284810000	6	4.333251000	1.653003000	-1.046670000
6	6.183899000	0.501228000	1.256423000	6	4.589603000	0.718407000	0.156584000
1	7.236582000	0.686347000	0.982514000	7	5.453302000	-0.343020000	-0.008024000
6	6.151569000	-0.519428000	1.653345000	8	-3.331891000	-3.202062000	0.301287000
6	-0.252890000	5.038528000	2.318960000	6	-2.673341000	-4.163457000	-0.520827000
6	0.507907000	5.359477000	1.036671000	6	-1.849330000	-3.405733000	-1.576974000
1	-1.115820000	5.724873000	2.362942000	8	-2.408536000	-2.493830000	-2.177371000
1	0.381839000	5.317241000	3.170393000	7	-0.891541000	3.003079000	-0.907385000
1	0.600391000	6.460571000	0.987371000	6	0.293308000	3.678644000	-0.763304000
1	-0.052297000	5.045912000	0.139377000	6	0.611594000	4.359831000	-2.001176000
6	2.496758000	5.207193000	-0.196891000	6	-0.398921000	4.081390000	-2.879341000
1	2.442496000	6.308467000	-0.269975000	6	-1.332026000	3.209928000	-2.188646000
6	3.955654000	4.820161000	-0.184825000	6	-2.469634000	2.611519000	-2.792999000
1	1.999536000	4.785728000	-1.090637000	6	-2.804861000	3.033707000	-4.192358000
1	4.439838000	5.359141000	-1.020989000	6	-2.672288000	2.143022000	-5.273506000
1	4.433864000	5.148524000	0.755254000	6	-2.985248000	2.543182000	-6.576356000
6	5.665879000	1.617278000	-0.942288000	6	-3.439489000	3.843009000	-6.823659000
1	6.728601000	1.492714000	-1.215928000	6	-3.575999000	4.739680000	-5.758579000
1	5.059371000	1.389387000	-1.827065000	6	-3.260089000	4.338707000	-4.456798000
6	5.483056000	3.085608000	-0.591370000	7	-3.112102000	1.112233000	-0.935262000
1	5.861752000	3.661682000	-1.458102000	6	-3.286892000	1.626731000	-2.191248000
1	6.105331000	3.383367000	0.271505000	6	-4.429564000	0.976642000	-2.820323000
8	3.818067000	4.447516000	3.103248000	6	-4.892697000	0.046171000	-1.937468000
1	3.085710000	4.645083000	2.493220000	6	-4.073774000	0.157371000	-0.740082000
1	3.996386000	3.502143000	2.951566000	8	4.014236000	0.935514000	1.214079000
6	-0.175570000	-0.099550000	-0.080396000	1	-2.311639000	1.128085000	-5.089392000
8	0.368188000	-0.450163000	0.963455000	1	1.488084000	4.981099000	-2.173007000
8	0.007288000	0.950006000	-0.756555000	1	-0.493261000	4.424278000	-3.906851000
8	-1.350251000	2.578121000	-2.001102000	1	2.301338000	4.088545000	3.038129000
1	-2.071509000	2.817362000	-1.324602000	1	0.916545000	2.837368000	4.966578000
1	-0.826280000	1.862041000	-1.585069000	1	-3.336269000	-0.484099000	5.008755000
1	-1.842334000	2.195820000	-2.787043000	1	-4.883264000	-1.584850000	3.101192000
				1	-5.732547000	-0.631680000	-2.069833000
				1	-4.824049000	1.201500000	-3.808321000
				1	1.692618000	6.275815000	1.227665000
				1	3.915132000	7.405131000	1.230831000
				1	5.914673000	6.179876000	0.351908000
				1	5.681641000	3.904022000	-0.551081000
				1	-2.999249000	2.337596000	5.834489000
				1	-2.803114000	2.091589000	8.297754000
				1	-0.908422000	0.795423000	9.281581000
				1	0.784847000	-0.251315000	7.773257000
				1	0.583379000	-0.003095000	5.310478000
				1	-7.018153000	-0.571566000	0.554687000
				1	-8.556809000	-2.523901000	0.413199000
5IM1 H3O+,K+:							
6	-0.158487000	0.460719000	5.965355000				
6	-1.220942000	1.186534000	5.396666000				
6	-2.169254000	1.766859000	6.258542000				
6	-2.057790000	1.628616000	7.645704000				
6	-0.995721000	0.904429000	8.197552000				
6	-0.046491000	0.320210000	7.352214000				
6	-1.345340000	1.335231000	3.908929000				
6	-0.391645000	2.140879000	3.247466000				
7	-0.347579000	2.388731000	1.899634000				
6	0.725528000	3.205351000	1.664539000				
6	1.414983000	3.470423000	2.919204000				

1	-7.607686000	-4.830710000	0.196115000	6	-0.656167000	7.904188000	-1.651212000
1	-5.153048000	-5.161160000	0.145445000	6	0.491166000	8.289580000	-0.949862000
1	-2.870013000	1.836246000	-7.402197000	6	1.329984000	7.310382000	-0.406930000
1	-3.685254000	4.155886000	-7.841672000	6	-0.460835000	4.103905000	-1.438318000
1	-3.933270000	5.756739000	-5.940270000	6	0.450497000	3.295026000	-2.157909000
1	-3.373419000	5.043334000	-3.629142000	7	0.347978000	1.930839000	-2.313028000
1	3.984304000	1.080190000	-1.918859000	6	1.473505000	1.495492000	-2.961744000
1	5.269927000	2.146168000	-1.349414000	6	2.322446000	2.634841000	-3.257932000
1	-2.102815000	-4.835774000	0.129661000	6	1.682580000	3.745750000	-2.781971000
1	-3.401494000	-4.774185000	-1.076325000	26	-1.178276000	0.651415000	-1.614223000
7	-0.567730000	-3.781503000	-1.867494000	7	-2.179556000	2.374530000	-0.930561000
19	2.572455000	-1.727137000	-0.685811000	6	-3.277828000	2.290809000	-0.118154000
8	1.828335000	-4.199306000	0.424971000	6	-3.462189000	3.564624000	0.558734000
8	2.419023000	-3.145577000	-3.041353000	6	-2.461214000	4.398487000	0.108571000
8	4.062163000	-2.565191000	1.482622000	6	-1.655772000	3.635779000	-0.819089000
8	5.102139000	-2.585979000	-2.041297000	6	-4.116324000	1.157160000	0.040927000
6	1.239766000	-3.595594000	-3.695390000	6	-5.195832000	1.222144000	1.084182000
1	1.226759000	-4.698958000	-3.772632000	6	-4.967501000	0.784247000	2.405406000
6	-0.005745000	-3.049566000	-3.026243000	6	-5.972300000	0.822756000	3.375084000
1	1.239829000	-3.208420000	-4.731045000	6	-7.247352000	1.277796000	3.031052000
1	-0.797740000	-3.015745000	-3.788476000	6	-7.503886000	1.717064000	1.729883000
1	0.172980000	-1.999854000	-2.738228000	6	-6.483463000	1.692974000	0.776097000
6	3.614368000	-3.494011000	-3.726266000	6	1.755594000	0.155383000	-3.327769000
1	3.921672000	-4.519299000	-3.454841000	6	3.133568000	-0.157409000	-3.832540000
1	3.447735000	-3.460952000	-4.818461000	6	3.362801000	-0.345558000	-5.207954000
6	4.722093000	-2.509588000	-3.417336000	6	4.623454000	-0.681898000	-5.703879000
1	5.588299000	-2.760212000	-4.055200000	6	5.689425000	-0.855498000	-4.815872000
1	4.394456000	-1.485243000	-3.671817000	6	5.488655000	-0.677883000	-3.446425000
6	6.351401000	-1.978704000	-1.717730000	6	4.225303000	-0.320401000	-2.953756000
1	6.828904000	-2.612479000	-0.958292000	8	4.036625000	-0.163279000	-1.588065000
1	7.015395000	-1.986153000	-2.598550000	6	4.811948000	0.886840000	-1.013874000
6	6.247761000	-0.531993000	-1.227539000	6	4.703692000	1.046958000	0.511830000
1	7.280796000	-0.174740000	-1.058305000	7	5.197647000	0.072393000	1.357820000
1	5.831439000	0.082605000	-2.033182000	8	-3.663453000	0.397772000	2.759510000
6	0.117693000	-4.900003000	-1.206088000	6	-3.418423000	-0.751726000	3.611091000
6	0.508641000	-4.722866000	0.266368000	6	-2.778389000	-1.862902000	2.762409000
1	-0.507121000	-5.803706000	-1.279484000	8	-3.401203000	-2.230223000	1.771110000
1	1.029444000	-5.131679000	-1.769712000	7	-0.476456000	-0.843965000	-2.900554000
1	0.471595000	-5.718001000	0.747980000	6	0.827237000	-0.913125000	-3.322533000
1	-0.198282000	-4.068144000	0.798512000	6	1.089622000	-2.246801000	-3.837760000
6	2.148483000	-4.013380000	1.807799000	6	-0.081517000	-2.943809000	-2.748624000
1	1.853383000	-4.913034000	2.378142000	6	-1.061709000	-2.055812000	-3.147576000
6	3.632671000	-3.813498000	2.010601000	6	-2.390309000	-2.422925000	-2.808066000
1	1.574652000	-3.158481000	2.208305000	6	-2.864264000	-3.774149000	-3.248480000
1	3.837786000	-3.853348000	3.097545000	6	-3.165038000	-4.778447000	-2.309344000
1	4.185512000	-4.637972000	1.527052000	6	-3.600775000	-6.040465000	-2.723999000
6	5.920354000	-1.004857000	1.221639000	6	-3.747004000	-6.322087000	-4.086556000
1	7.023731000	-0.999529000	1.220448000	6	-3.451700000	-5.333364000	-5.031027000
1	5.580930000	-0.383797000	2.059174000	6	-3.012390000	-4.072647000	-4.615685000
6	5.474472000	-2.442335000	1.477744000	7	-2.976322000	-0.409560000	-1.496273000
1	5.883837000	-2.723104000	2.467346000	6	-3.276396000	-1.629715000	-2.041025000
1	5.900134000	-3.151940000	0.747379000	6	-4.618615000	-2.016244000	-1.631180000
8	4.241900000	-5.175037000	-0.953468000	6	-5.068065000	-1.052392000	-0.778363000
1	3.378221000	-4.927358000	-0.578029000	6	-4.030868000	-0.037534000	-0.706704000
1	4.611078000	-4.332117000	-1.272071000	8	4.303022000	2.123903000	0.937239000
6	-0.115884000	-0.083818000	-0.232395000	1	-3.046494000	-4.566874000	-1.243928000
8	0.592766000	0.056073000	-1.238502000	1	2.038184000	-2.601470000	-4.232590000
8	0.182855000	-1.243464000	0.466678000	1	-0.257778000	-3.974683000	-4.045941000
8	-1.424397000	-2.468665000	2.275946000	1	3.267353000	2.596399000	-3.795804000
1	-2.184569000	-2.666595000	1.692302000	1	2.017094000	4.777703000	-2.853605000
1	-0.449402000	-1.429720000	1.199231000	1	-2.298275000	5.435206000	0.393223000
1	-1.832439000	-2.026310000	3.037170000	1	-4.292473000	3.829912000	1.211912000
				1	-6.024822000	-1.016840000	-0.263121000
				1	-5.142653000	-2.916489000	-1.942227000
				1	2.523919000	-0.219812000	-5.896676000
				1	4.770803000	-0.814294000	-6.778178000
				1	6.679028000	-1.134629000	-5.185638000
⁵RC2 H3O+,K+:							
6	1.025423000	5.955486000	-0.566957000				
6	-0.125899000	5.553211000	-1.270070000				
6	-0.963014000	6.549231000	-1.807199000				

1	3.711677000	1.970695000	-3.755308000	1	5.513901000	-0.138199000	5.000413000
1	2.666869000	4.364829000	-3.133951000	1	4.910231000	-1.684585000	4.376070000
1	-1.723047000	5.854771000	-0.309798000	8	2.586065000	-3.130238000	5.059882000
1	-3.857698000	4.543286000	0.666252000	1	1.952153000	-2.397849000	4.971621000
1	-6.083744000	-0.185365000	-0.418959000	1	3.032600000	-3.175893000	4.196644000
1	-5.369729000	-2.337105000	-1.862376000	6	-0.282593000	0.582154000	0.296175000
1	2.728931000	-0.728641000	-5.712458000	8	-0.349270000	-0.291403000	1.126228000
1	4.909169000	-1.658724000	-6.462374000	8	0.261192000	1.851586000	0.946235000
1	6.657831000	-2.239973000	-4.765572000	8	-1.536152000	2.782207000	2.370703000
1	6.209291000	-1.851120000	-2.350462000	1	-2.297306000	2.114701000	2.446603000
1	-1.049825000	6.265042000	-3.172176000	1	0.450879000	2.498480000	0.242882000
1	-0.272326000	8.622413000	-3.147623000	1	-0.709135000	2.366101000	1.791683000
1	1.739403000	9.265526000	-1.814651000	1	-1.888145000	3.538285000	1.846460000
1	2.960125000	7.524533000	-0.504760000				
1	2.178850000	5.169226000	-0.530005000				
1	-6.372702000	2.945414000	-0.536973000	5IM2 H3O+,K+:			
1	-8.145037000	3.332202000	1.167093000	6	0.149903000	6.778454000	-0.571967000
1	-7.751263000	2.638935000	3.540374000	6	-0.146609000	6.118700000	-1.778290000
1	-5.597473000	1.595792000	4.183719000	6	-0.260543000	6.885957000	-2.951721000
1	-4.537782000	-6.339075000	-1.395367000	6	-0.088262000	8.273144000	-2.919402000
1	-4.734725000	-7.076207000	-3.773578000	6	0.205567000	8.917387000	-1.713032000
1	-3.912824000	-5.584383000	-5.600020000	6	0.325561000	8.165239000	-0.539656000
1	-2.905432000	-3.382656000	-5.053044000	6	-0.330410000	4.630607000	-1.824986000
1	5.846340000	0.075899000	-1.031077000	6	0.678364000	3.881288000	-2.483759000
1	4.435197000	1.165463000	-1.141136000	7	0.686529000	2.520635000	-2.690396000
1	-2.831748000	0.306678000	4.290177000	6	1.924732000	2.179555000	-3.188788000
1	-4.462462000	-0.239612000	3.857882000	6	2.721079000	3.379620000	-3.327745000
7	-1.940772000	-1.993681000	3.115479000	6	1.945310000	4.429469000	-2.917988000
19	1.996733000	-1.046652000	2.053461000	26	-0.597128000	1.150120000	-1.750415000
8	0.901164000	-0.703207000	4.754040000	7	-1.786425000	2.760244000	-1.095928000
8	0.773310000	-3.615313000	2.277805000	6	-2.928345000	2.645918000	-0.347008000
8	3.635018000	-0.081855000	4.114280000	6	-3.346546000	3.965834000	0.090190000
8	3.734358000	-3.266392000	2.309099000	6	-2.455302000	4.859631000	-0.434837000
6	-0.530222000	-0.099808000	2.590771000	6	-1.462119000	4.090096000	-1.167591000
1	-0.582694000	-4.418980000	3.648681000	6	-3.639357000	1.449098000	-0.105225000
6	-1.630206000	-3.126161000	2.215430000	6	-4.845907000	1.498144000	0.790783000
1	-0.719218000	-5.005670000	1.986446000	6	-4.737218000	1.239221000	2.176280000
1	-2.551780000	-3.717963000	2.097394000	6	-5.876369000	1.227406000	2.990002000
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6	1.739390000	-4.659814000	2.262704000	6	-7.263431000	1.739412000	1.070930000
1	1.965229000	-4.986809000	3.293474000	6	-6.121598000	1.754972000	0.264959000
1	1.334999000	-5.529314000	1.711371000	6	2.366279000	0.864446000	-3.490328000
6	3.009333000	-4.241143000	1.552297000	6	3.793297000	0.672481000	-3.909803000
1	3.631294000	-5.142254000	1.414909000	6	4.240022000	1.197880000	-5.138698000
1	2.766983000	-3.847893000	0.547641000	6	5.542752000	1.010280000	-5.600181000
6	5.133252000	-3.167933000	2.026407000	6	6.446801000	0.278443000	-4.822982000
1	5.649120000	-3.074780000	2.992537000	6	6.038611000	-0.246638000	-3.598635000
1	5.489714000	-4.103948000	1.566033000	6	4.726983000	-0.060914000	-3.133308000
6	5.515839000	-2.016549000	1.092829000	8	4.447750000	-0.688884000	-1.943933000
1	6.609417000	-2.083892000	0.936671000	6	3.633538000	-0.080145000	-0.947840000
1	5.029048000	-2.159805000	0.121952000	6	4.254834000	-0.202043000	0.452504000
6	-1.251849000	-1.783320000	4.391672000	7	4.497713000	-1.445164000	0.993075000
6	-0.486720000	-0.454148000	4.539188000	8	-3.465175000	1.104466000	2.694871000
1	-1.960129000	-1.903508000	5.226459000	6	-3.161525000	0.222343000	3.764597000
1	-0.517382000	-2.587354000	4.509485000	6	-2.771229000	-1.162682000	3.220534000
1	-0.878005000	0.120903000	5.396706000	8	-3.163424000	-1.476464000	2.104247000
1	-0.602301000	0.156950000	3.629750000	7	0.309530000	-0.365305000	-2.872660000
6	1.591937000	0.449406000	5.233357000	6	1.564102000	-0.296751000	-3.416585000
1	1.177328000	0.756249000	6.211104000	6	1.939231000	-1.601288000	-3.929534000
6	3.059052000	0.136769000	5.392607000	6	0.885498000	-2.436703000	-3.695382000
1	1.458919000	1.292101000	4.529145000	6	-0.138462000	-1.651646000	-3.025523000
1	3.552022000	0.989888000	5.895964000	6	-1.382504000	-2.152960000	-2.575293000
1	3.184640000	-0.756628000	6.029501000	6	-1.704289000	-3.584576000	-2.882252000
6	5.723524000	-0.271559000	2.895627000	6	-1.819063000	-4.532585000	-1.848659000
1	6.724856000	-0.726145000	2.986641000	6	-2.113706000	-5.869557000	-2.132058000
1	5.848631000	0.817022000	2.850238000	6	-2.303522000	-6.282697000	-3.455072000
6	4.952110000	-0.601980000	4.168303000	6	-2.196257000	-5.349695000	-4.491792000
				6	-1.897935000	-4.013437000	-4.207886000

7	-2.204831000	-0.119437000	-1.395630000	1	1.862736000	-0.231687000	6.565704000
6	-2.342226000	-1.413136000	-1.843287000	6	3.274812000	-1.063468000	5.210477000
6	-3.638933000	-1.917451000	-1.439913000	1	1.842915000	0.530366000	4.953828000
6	-4.245814000	-0.932995000	-0.714887000	1	4.040873000	-0.436439000	5.704933000
6	-3.346947000	0.199257000	-0.700856000	1	3.320805000	-2.069441000	5.662350000
8	4.486639000	0.834352000	1.066254000	6	5.344609000	-1.470048000	2.194150000
1	-1.671389000	-4.215822000	-0.813395000	1	6.195574000	-2.149247000	2.012739000
1	2.875823000	-1.840566000	-4.427537000	1	5.742505000	-0.455419000	2.312107000
1	0.809099000	-3.489958000	-3.952491000	6	4.704241000	-1.889916000	3.516759000
1	3.745486000	3.423704000	-3.687790000	1	5.471748000	-1.720113000	4.294185000
1	2.226040000	5.478965000	-2.882876000	1	4.455323000	-2.962960000	3.547762000
1	-2.477481000	5.942472000	-0.343278000	8	2.212576000	-4.072346000	4.569266000
1	-4.227889000	4.183323000	0.689740000	1	1.681988000	-3.290433000	4.793350000
1	-5.224118000	-0.964884000	-0.243733000	1	2.357488000	-4.009155000	3.608862000
1	-4.036872000	-2.900235000	-1.678158000	6	0.757554000	1.539050000	-0.104242000
1	3.524688000	1.750601000	-5.752200000	8	1.451979000	2.140393000	0.562632000
1	5.846708000	1.425877000	-6.563494000	8	-0.663867000	0.409040000	1.844065000
1	7.472217000	0.119905000	-5.165810000	8	-1.351378000	2.935663000	2.628986000
1	6.726844000	-0.814056000	-2.968792000	1	-2.270595000	2.616026000	2.700698000
1	-0.492728000	6.388847000	-3.896859000	1	-1.495773000	0.130837000	1.428672000
1	-0.186068000	8.852439000	-3.841143000	1	-0.822407000	1.349057000	2.105304000
1	0.342075000	10.001440000	-1.687561000	1	-1.394096000	3.622658000	1.945769000
1	0.561144000	8.658984000	0.406630000				
1	0.253757000	6.196277000	0.346937000				
1	-6.213215000	1.956499000	-0.805169000				
1	-8.244914000	1.936380000	0.634007000				
1	-8.017336000	1.455875000	3.081139000				
1	-5.786577000	1.047284000	4.062347000				
1	-2.193195000	-6.591055000	-1.314806000				
1	-2.535250000	-7.327404000	-3.677177000				
1	-2.348783000	-5.661614000	-5.528221000				
1	-1.821685000	-3.289275000	-5.022614000				
1	3.549088000	0.998098000	-1.120368000				
1	2.622175000	-0.519086000	-0.966113000				
1	-2.363058000	0.700423000	4.340880000				
1	-4.015806000	0.086278000	4.447634000				
7	-2.065993000	-2.024827000	4.024789000				
19	1.209754000	-1.413804000	2.264747000				
8	0.845560000	-1.296669000	5.099514000				
8	-0.172072000	-3.872597000	2.411444000				
8	3.536264000	-1.135083000	3.814835000				
8	2.609906000	-3.819435000	1.566798000				
6	-0.940662000	-4.278571000	3.542090000				
1	-0.301728000	-4.261298000	4.441503000				
6	-2.204867000	-3.457117000	3.709965000				
1	-1.275948000	-5.322422000	3.410352000				
1	-2.789313000	-3.932472000	4.518565000				
1	-2.793002000	-3.520746000	2.788136000				
6	0.496587000	-4.958399000	1.780323000				
1	0.968911000	-5.609267000	2.537197000				
1	-0.226347000	-5.570984000	1.209185000				
6	1.562482000	-4.460120000	0.830866000				
1	1.964121000	-5.331554000	0.286857000				
1	1.132987000	-3.769219000	0.082310000				
6	3.921384000	-3.909751000	1.007447000				
1	4.613032000	-4.115440000	1.836420000				
1	3.977589000	-4.777202000	0.329449000				
6	4.369454000	-2.683497000	0.214824000				
1	5.344959000	-2.941657000	-0.238105000				
1	3.675348000	-2.517092000	-0.616564000				
6	-1.595385000	-1.675376000	5.373439000				
6	-0.401949000	-0.730735000	5.502867000				
1	-2.413848000	-1.226739000	5.961986000				
1	-1.344716000	-2.615085000	5.884826000				
1	-0.339936000	-0.457414000	6.572221000				
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UPBE0 data:

³CAT_{H3O+,K+}:

6	3.471829000	3.882265000	-2.302857000	1	-2.140902000	5.048131000	-0.396249000
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6	1.792630000	4.753224000	-3.788069000	1	-5.922951000	-1.312463000	-1.365701000
6	2.649106000	5.792643000	-4.150731000	1	1.820162000	-4.266194000	-3.593493000
6	3.924601000	5.880769000	-3.591316000	1	3.625717000	-5.837258000	-2.191250000
6	4.330945000	4.919226000	-2.663818000	1	5.778880000	-5.837258000	-2.191250000
6	1.260922000	2.679399000	-2.463442000	1	5.700460000	-4.034964000	-0.522197000
6	1.684958000	1.338330000	-2.625018000	1	0.797859000	4.688008000	-4.236559000
7	1.015948000	0.227588000	-2.121343000	1	2.319487000	6.536091000	-4.881814000
6	1.859692000	-0.850520000	-2.337365000	1	4.597712000	6.693887000	-3.875179000
6	3.023347000	-0.430026000	-3.025031000	1	5.324143000	4.981944000	-2.210431000
6	2.905123000	0.934269000	-3.227145000	1	3.795285000	3.140318000	-1.568061000
26	-0.919427000	0.133126000	-1.638503000	1	-4.611493000	4.679791000	-1.437483000
7	-0.988368000	2.129884000	-1.564727000	1	-6.249602000	6.012486000	-0.120046000
6	-1.987317000	2.888376000	-0.975478000	1	-6.806451000	5.326976000	2.215871000
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6	-0.315641000	4.331700000	-1.426984000	1	-6.725378000	-4.805434000	0.558770000
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6	-4.208134000	3.268638000	0.126910000	1	-3.661747000	-4.330334000	-3.321989000
6	-4.526653000	2.914315000	1.462583000	1	5.110385000	-2.592026000	1.341044000
6	-5.458085000	3.644347000	2.203129000	1	5.937129000	-1.977766000	-0.109873000
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6	2.677771000	-4.215296000	-2.918029000	8	0.337909000	-2.191440000	2.717083000
6	3.689394000	-5.171849000	-3.010165000	8	3.219470000	2.106989000	2.170075000
6	4.776823000	-5.095266000	-2.145984000	8	3.070818000	-1.476724000	3.213612000
6	4.851396000	-3.065964000	-1.205666000	6	-1.017461000	-2.542373000	2.920182000
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6	5.037360000	-1.866126000	0.520722000	1	-1.149792000	-3.606410000	2.646297000
6	5.028522000	-0.398888000	0.943220000	1	-2.835611000	-2.318520000	1.831478000
7	5.342097000	-0.054226000	2.217031000	1	-1.468431000	-1.471429000	1.106901000
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6	-3.253993000	-2.400832000	-1.458597000	6	5.472108000	-0.999825000	3.310696000
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6	-5.256822000	-5.481542000	-2.434987000	1	-1.956711000	1.135554000	3.885285000
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6	-5.058401000	-0.658818000	-1.268378000	6	0.968523000	2.844320000	1.800532000
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6	-3.691860000	1.100824000	-0.945737000	6	2.283458000	3.112391000	2.481336000
8	4.779889000	0.435550000	0.083044000	1	1.089206000	2.778478000	0.702250000
1	-5.081772000	-2.950032000	0.497992000	1	2.658631000	4.103990000	2.162912000
1	0.692315000	-4.800481000	-1.159508000	1	2.116726000	3.156539000	3.574274000
1	-2.004957000	-1.940577000	-1.048783000	6	5.512025000	1.366781000	2.491473000
1	3.840975000	-1.081882000	-3.329973000	1	6.336310000	1.475788000	3.213264000
1	3.613544000	1.595024000	-3.722942000	1	5.815430000	1.842432000	1.549711000
1	0.313651000	5.214502000	-1.523430000	6	4.318151000	2.119840000	3.050208000
				1	4.661245000	3.158784000	3.217660000
				1	4.005840000	1.723723000	4.034097000
				8	1.506137000	0.455130000	4.636033000

1	1.122231000	1.006341000	3.932973000	1	-1.606261000	4.683694000	-2.950895000
1	1.867676000	-0.288872000	4.128270000	1	-3.749988000	4.253531000	-1.317036000
³RC1_{H3O+, K+}							
6	1.679553000	4.062450000	-3.779712000	1	-5.683705000	-2.667117000	0.248349000
6	0.461352000	3.472331000	-4.151844000	1	1.797538000	-4.317930000	-4.128426000
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6	0.268700000	5.118205000	-5.935475000	1	5.897085000	-5.158790000	-3.108029000
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6	-0.083911000	2.303413000	-3.409450000	1	-0.287912000	5.524771000	-6.783903000
6	0.629489000	1.116053000	-3.398954000	1	1.881006000	6.550765000	-6.102931000
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6	2.319693000	-0.319296000	-3.799915000	1	-6.392988000	2.483806000	-1.165463000
6	1.881776000	0.925949000	-4.104114000	1	-7.934323000	3.874316000	0.206131000
26	-1.357753000	-0.371961000	-1.641032000	1	-7.246544000	4.581488000	2.502241000
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6	-1.292713000	2.492325000	-2.681726000	1	-3.880122000	-5.197490000	-2.498300000
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6	-4.853043000	2.380406000	0.325565000	1	4.599522000	-0.215089000	-2.351572000
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6	-6.583294000	3.964889000	1.891127000	7	-1.372978000	0.189250000	3.833377000
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6	4.992424000	-4.556290000	-2.996760000	1	0.148718000	-1.439731000	5.458602000
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6	-5.186329000	-6.869184000	0.169024000	1	0.436167000	0.529020000	4.777464000
6	-4.833446000	-6.589415000	-1.152180000	1	-0.381173000	3.202983000	3.826947000
6	-4.153297000	-5.412486000	-1.461935000	1	-0.192690000	1.999042000	2.516083000
7	-3.132550000	-0.771796000	-0.835703000	6	1.994919000	3.550989000	3.199918000
6	-3.695004000	-2.011935000	-0.592818000	1	1.615068000	4.394555000	3.804346000
6	-5.006612000	-1.852922000	-0.000151000	6	3.492537000	3.503688000	3.290163000
6	-5.194064000	-0.526551000	0.195048000	1	1.680855000	3.716332000	2.152415000
6	-4.037468000	0.142666000	-0.359311000	1	3.904047000	4.500629000	3.044944000
8	4.421013000	1.609932000	-0.800339000	1	3.788193000	3.260476000	4.326861000
1	-3.903975000	-4.084464000	-1.657906000	6	5.965366000	1.557627000	1.439725000
1	1.124595000	-4.957123000	-1.628803000	1	7.008745000	1.312060000	1.701971000
1	-1.400839000	-5.529968000	-0.831306000	1	5.987706000	2.321625000	0.651752000
1	3.210165000	-0.825219000	-4.168682000	6	5.316084000	2.173278000	2.661894000
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1	1.214220000	-0.382360000	6.044962000	6	-0.507533000	-3.188195000	-3.174458000
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1	2.558692000	-2.935704000	4.194339000	6	-5.168386000	-0.238186000	-0.845587000
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³TS2 H3O+, K+							
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6	0.016083000	2.362073000	3.501970000	6	-5.859600000	1.489255000	3.211421000
1	1.236555000	2.184926000	5.216928000	6	-7.108354000	1.972636000	2.827091000
1	-0.784744000	2.151006000	4.225477000	6	-7.358468000	2.274558000	1.489983000
1	0.220250000	1.399097000	3.001976000	6	-6.357301000	2.084828000	0.539793000
6	3.594703000	2.706375000	4.322096000	6	1.729083000	-0.400482000	-3.303723000
1	3.917223000	3.760135000	4.249252000	6	3.087791000	-0.844635000	-3.731987000
1	3.408369000	2.477500000	5.386826000	6	3.325759000	-1.250986000	-5.053243000
6	4.694657000	1.786050000	3.859756000	6	4.575414000	-1.708365000	-5.462156000
1	5.552385000	1.908653000	4.544619000	6	5.617254000	-1.783310000	-4.537818000
1	4.353798000	0.736439000	3.925247000	6	5.404840000	-1.389351000	-3.220017000
6	6.322720000	1.534164000	2.128948000	6	4.153506000	-0.913097000	-2.817098000
1	6.835987000	2.280613000	1.506707000	8	3.952517000	-0.545283000	-1.504915000
1	6.968706000	1.360760000	3.006012000	6	4.707214000	0.584049000	-1.111230000
6	6.190183000	0.214448000	1.383289000	6	4.656601000	0.958873000	0.370595000
1	7.215063000	-0.146857000	1.177730000	7	5.125793000	0.095452000	1.331334000
1	5.727621000	-0.521931000	2.050887000	8	-3.599781000	0.866933000	2.623544000
6	0.148085000	4.520083000	2.097603000	6	-3.412528000	-0.162205000	3.609903000
6	0.545008000	4.622295000	0.628105000	6	-2.819508000	-1.390775000	2.918175000
1	-0.470086000	5.397913000	2.341979000	8	-3.456020000	-1.860872000	1.985822000
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1	0.512819000	5.690283000	0.341778000	6	0.750642000	-1.406620000	-3.162255000
1	-0.163421000	4.082895000	-0.020607000	6	0.950170000	-2.804682000	-3.484462000
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5RC2	H3O+, K+						
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