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Electronic Supplementary Information

Molecular structures of 1-Hydroxyethane-1,1-Diphosphonic acid for removing calcium sulfate scale under different pH conditions

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1. The Cartesian coordinates of CaH_4L, in angstroms
Charge: 2 Spin: Singlet

Ca	-0.39724400	0.45345500	1.05688300
O	-0.06080800	2.33833600	-0.36806300
O	-2.31594500	0.10433800	-0.28637200
P	-0.68394500	2.81554000	-1.62780800
P	-2.80160300	0.56725200	-1.61072800
C	-1.49891800	1.45640200	-2.59297400
O	-0.44397600	0.50413600	-2.79222600
O	0.30327200	3.52977400	-2.63517200
O	-3.32515400	-0.58235200	-2.56574100
H	-0.63334200	-0.00114500	-3.59747000
O	-1.76288100	3.92141000	-1.32295400
H	-2.14136800	4.38608900	-2.08685000
O	-4.06340900	1.49619400	-1.43401600
H	-4.53760000	1.75497700	-2.24150400
C	-2.05565700	1.97598500	-3.91874600
H	-1.25312700	2.42366500	-4.50392100
H	-2.83465200	2.72252900	-3.75967200
H	-2.48251000	1.14765800	-4.48584000
H	1.03310000	2.98317300	-2.97015000
H	-2.67172500	-1.26290600	-2.79479600

2. The Cartesian coordinates of CaH_3L, in angstroms
Charge: 1 Spin: Singlet

Ca	-0.17652800	0.19006000	0.63348400
O	-0.11212000	2.36916000	-0.36063900
O	-2.32473300	0.20387500	-0.32016900
P	-0.73245000	2.83945100	-1.62845600
P	-2.80241000	0.51431700	-1.71802300
C	-1.47724400	1.48353700	-2.62839000
O	-0.36499100	0.58465000	-2.82415000
O	0.26422000	3.63006800	-2.57965900
O	-3.18456100	-0.61913100	-2.61854200
H	-0.67405200	-0.14444300	-3.38261900
O	-1.84461600	3.91470200	-1.31737700
H	-2.29033200	4.31579200	-2.08038400
O	-4.02594700	1.55392500	-1.53236900
H	-4.56145000	1.65700500	-2.33292900
C	-1.99112900	2.00917600	-3.97074800
H	-1.17287800	2.45221700	-4.53864800
H	-2.77261600	2.75946800	-3.84093000
H	-2.40528800	1.18120200	-4.54750000
H	1.04695700	3.13253000	-2.86635300

3. The Cartesian coordinates of CaH_2L, in angstroms
Charge: 0 Spin: Singlet

Ca	-0.32148500	0.44568200	0.89618300
O	0.03844700	2.30167300	-0.45188100
O	-2.20633900	0.11293900	-0.40693800
P	-0.70213400	2.89436000	-1.63270500
P	-2.68235200	0.47731000	-1.79476800
C	-1.40956500	1.52405500	-2.67219900
O	-0.29195400	0.64731100	-2.95613200
O	0.39657600	3.57689400	-2.61509500
O	-3.04537100	-0.64390100	-2.72434700
H	-0.61365400	-0.05386300	-3.54180700
O	-1.75175400	3.92979400	-1.38257900
O	-3.95260800	1.45576900	-1.55193500
H	-4.48154800	1.59258200	-2.35137100
C	-1.98499100	2.08230700	-3.97703200
H	-1.21273500	2.61894200	-4.52914900
H	-2.81286500	2.76574200	-3.78777700
H	-2.34968700	1.26499000	-4.60254900
H	1.20530500	3.05065200	-2.69425200

4. The Cartesian coordinates of CaHL, in angstroms

Charge: -1 Spin: Singlet

Ca	-0.03375800	0.11497800	-0.02374200
O	-0.17538300	2.37176600	-0.42013500
O	-2.36866000	0.13617000	-0.37337700
P	-0.78947800	2.96792500	-1.71005400
P	-2.88667000	0.55585500	-1.73546700
C	-1.51736900	1.46699100	-2.60465500
O	-0.41525000	0.49320100	-2.60316000
O	0.28247400	3.51815100	-2.64343300
O	-3.39274200	-0.53047600	-2.64430000
H	-0.67791000	-0.26306300	-3.14888000
O	-1.93836700	3.92713800	-1.43908200
O	-4.07290700	1.62044400	-1.43874000
H	-4.62356100	1.78798700	-2.21714800
C	-1.91260900	1.81670900	-4.03422500
H	-1.07202700	2.26671700	-4.56334300
H	-2.73835900	2.53116500	-4.03785200
H	-2.23330300	0.92694700	-4.58052400

5. The Cartesian coordinates of CaL, in angstroms
Charge: -2 Spin: Singlet

Ca	-0.07833600	0.08931500	-0.08963600
O	-0.06629800	2.35292800	-0.44423800
O	-2.36716600	0.24448700	-0.33935200
P	-0.70652100	2.96253100	-1.71815500
P	-2.93557500	0.65150700	-1.72412400
C	-1.50810600	1.50541300	-2.59866300
O	-0.44876900	0.47371300	-2.64825300
O	0.36252900	3.50632400	-2.66559800
O	-3.20121200	-0.58815300	-2.58698000
H	-0.87303900	-0.32230700	-3.00758300
O	-1.81628200	3.95883600	-1.40302300
O	-4.11587800	1.60787400	-1.62873700
C	-1.90113500	1.89331000	-4.02187400
H	-1.03670700	2.26164200	-4.57702700
H	-2.65508300	2.68234900	-4.00797500
H	-2.31874900	1.03949000	-4.56046100

Table S1 The data of descaling rate (X = 3.00 g)

pH	3	4	5	6	7	8	9	10	11
Y_1 (g)	2.84	2.51	1.97	0.64	0.38	0.23	0.35	0.83	1.09
Y_2 (g)	2.85	2.52	2.00	0.66	0.41	0.29	0.38	0.86	1.12
Y_3 (g)	2.84	2.47	1.97	0.65	0.43	0.26	0.39	0.92	1.16
Descaling rate $_1$ (%)	4.9	16.1	33.5	77.9	86.4	90.5	87.3	71.3	62.8
Descaling rate $_2$ (%)	5.2	17.6	34.5	78.3	85.8	91.4	86.9	69.2	61.2
Descaling rate $_3$ (%)	5.1	16.7	34.1	78.3	86.6	91.4	87.6	71.0	62.6
Mean value (%)	5.3	16.5	34.3	78.8	87.5	92.3	88.5	72.5	63.7
Error value (%)	0.2	0.8	0.5	0.5	0.9	0.9	0.8	1.7	1.3