

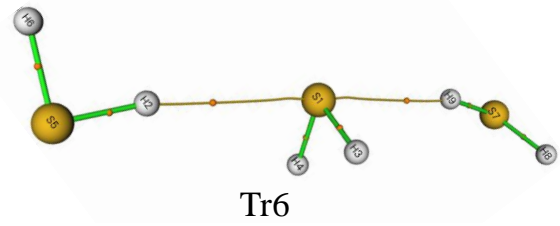
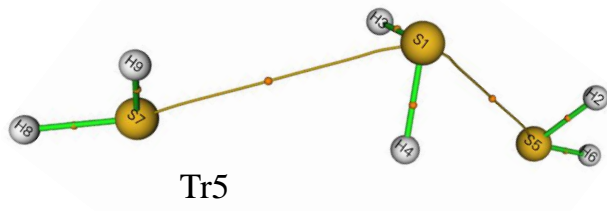
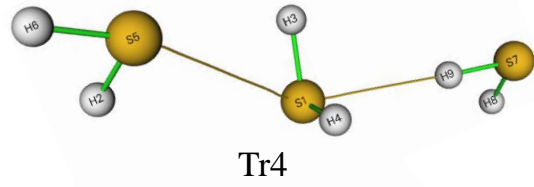
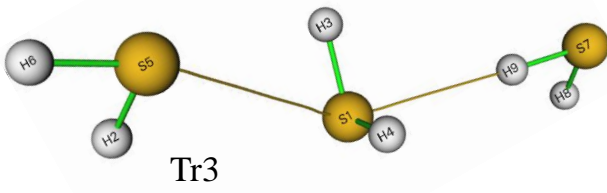
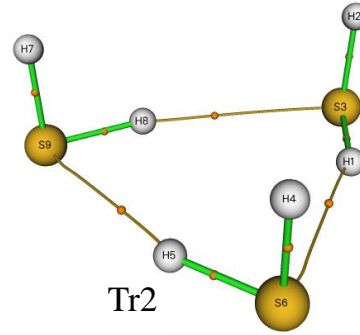
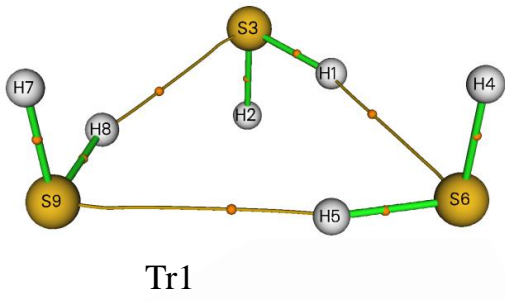
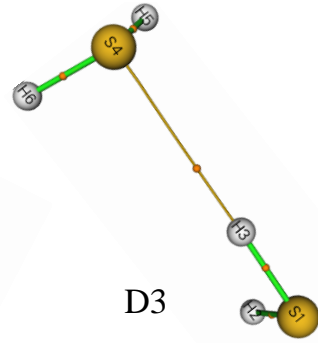
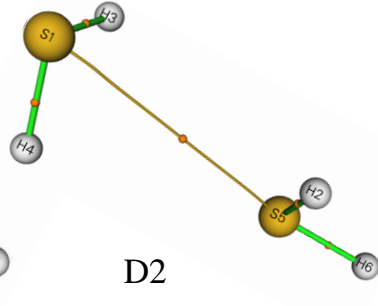
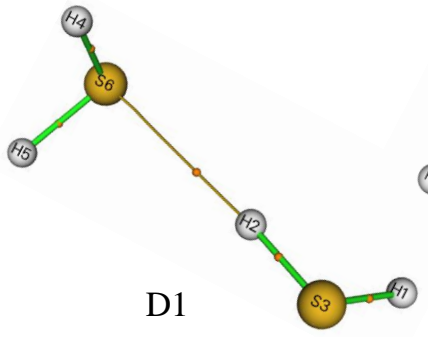
Supporting Information

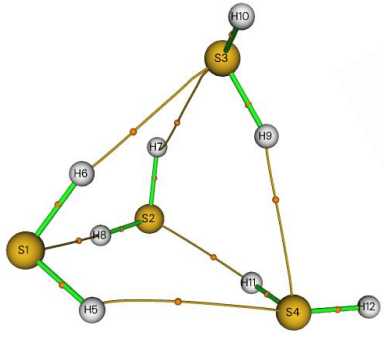
for

**A unified cost effective method for construction of reliable potential
energy surfaces for H₂S and H₂O clusters**

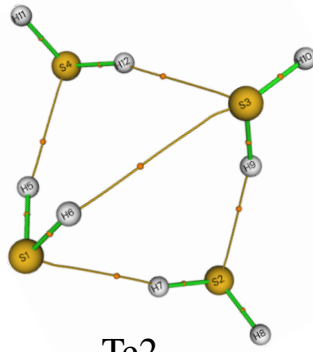
Monu, Binod Kumar Oram, Biman Bandyopadhyay*

Department of Chemistry, Malaviya National Institute of Technology Jaipur, JLN Marg, Jaipur–
302017, India

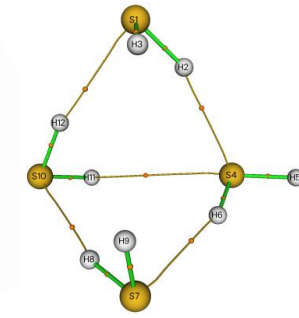




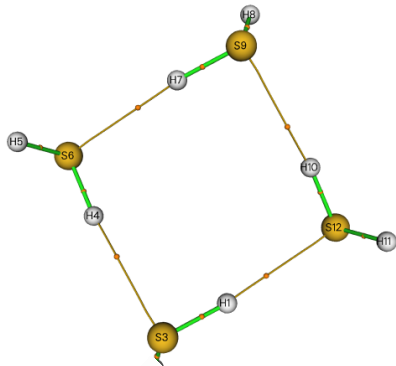
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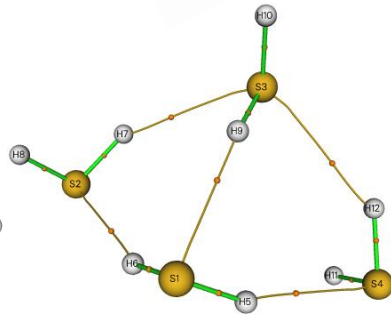
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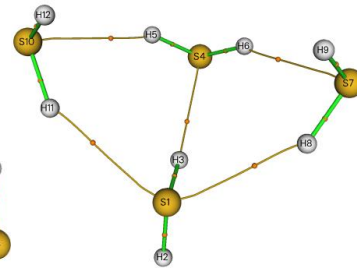
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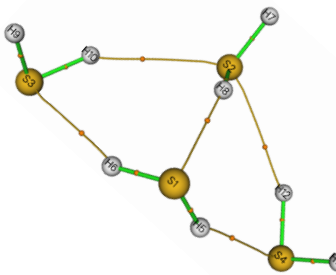
Te4



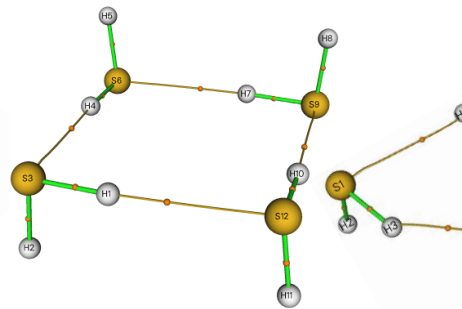
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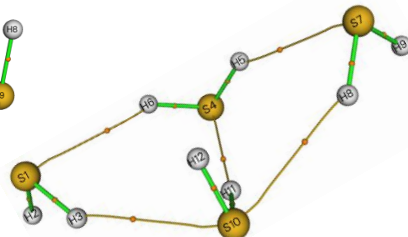
Te6



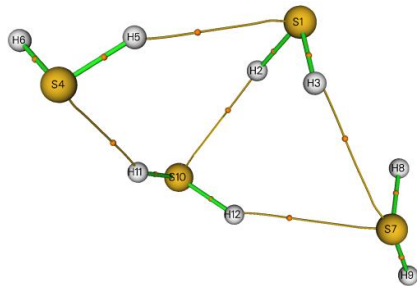
Te7



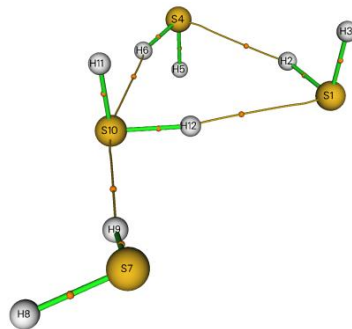
Te8



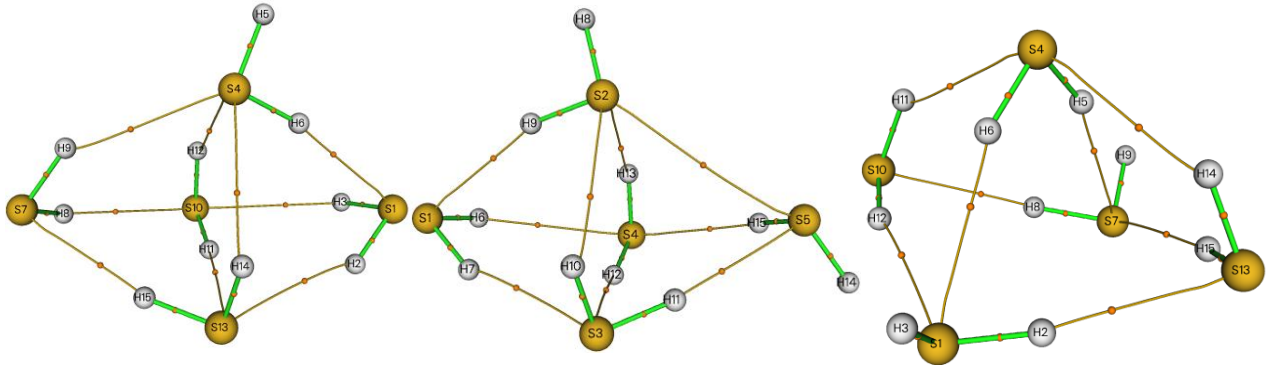
Te9



Te10



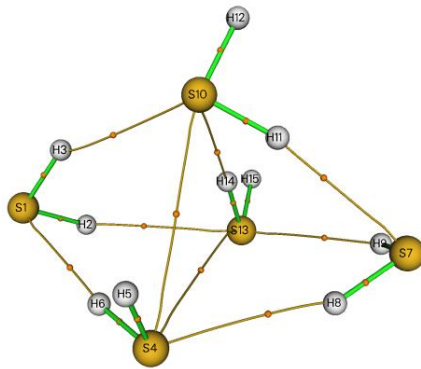
Te11



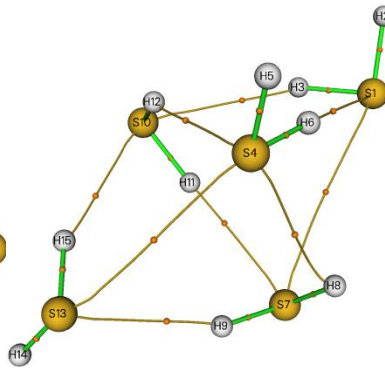
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P2

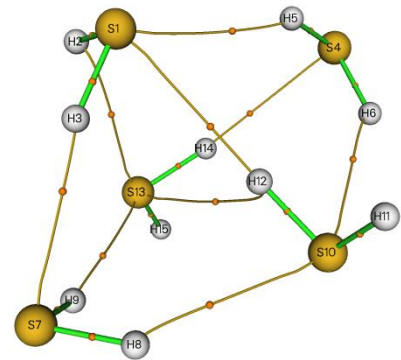
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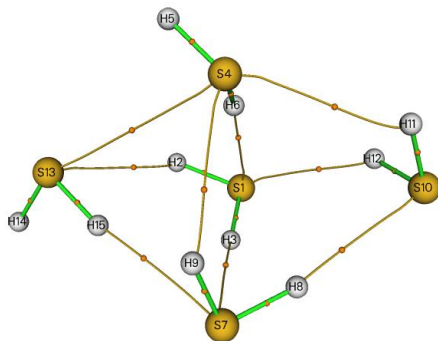
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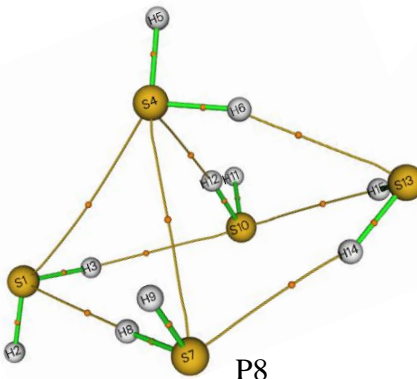
P5



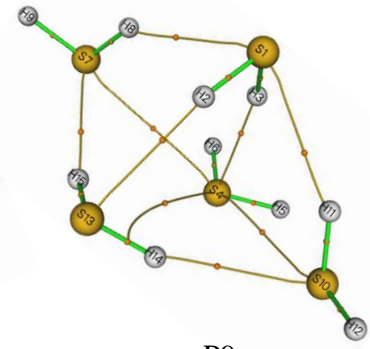
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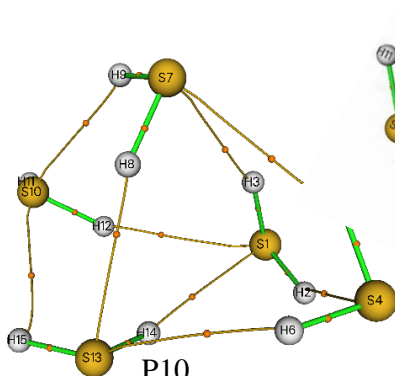
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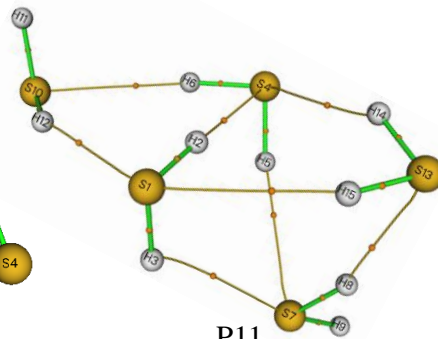
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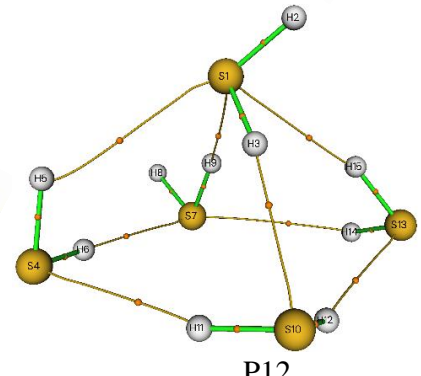
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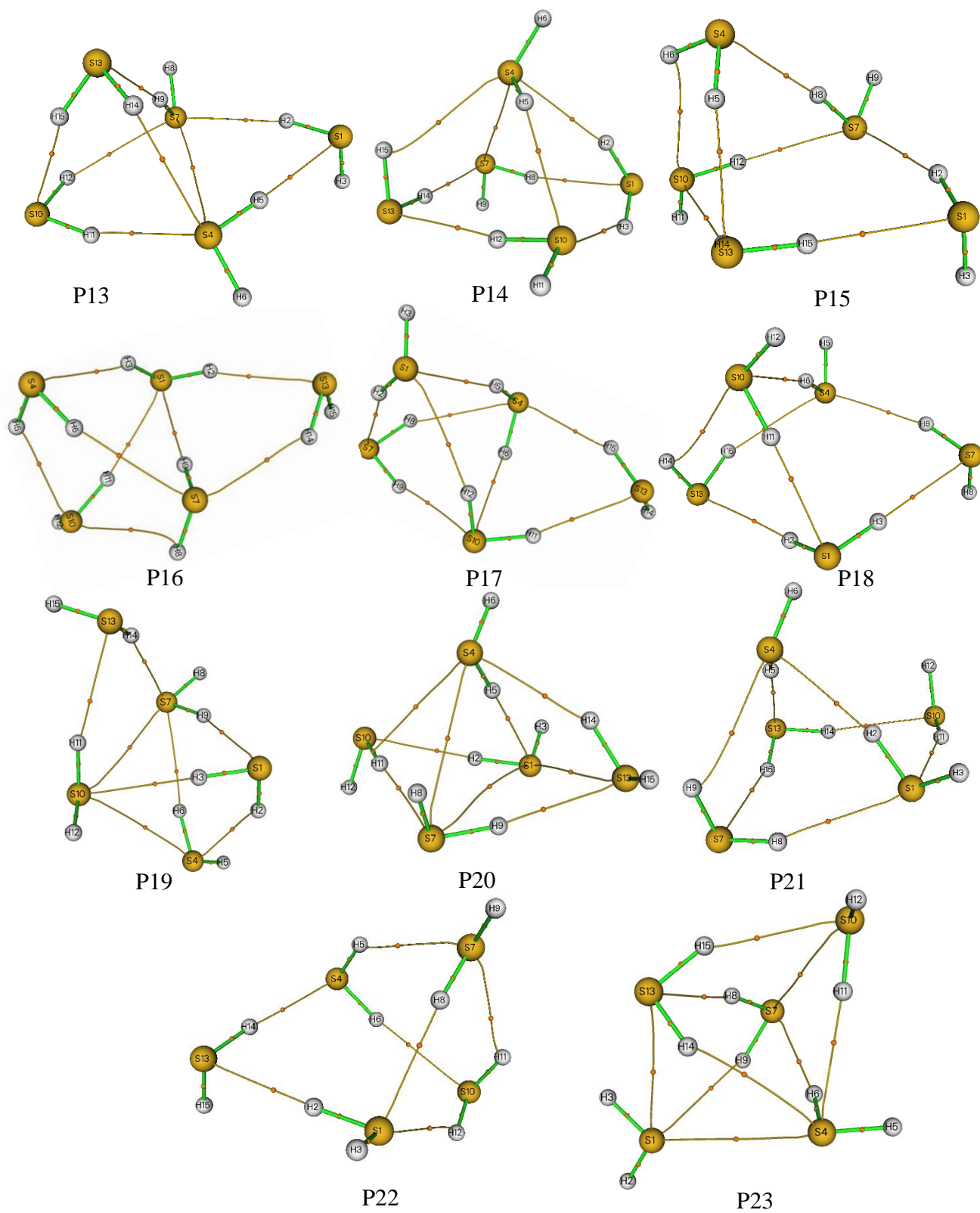
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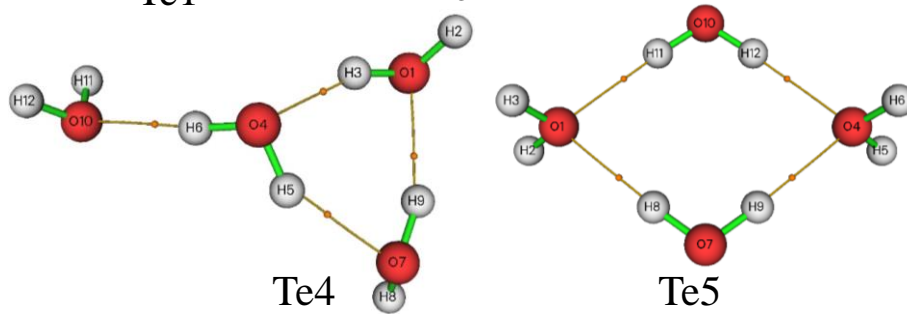
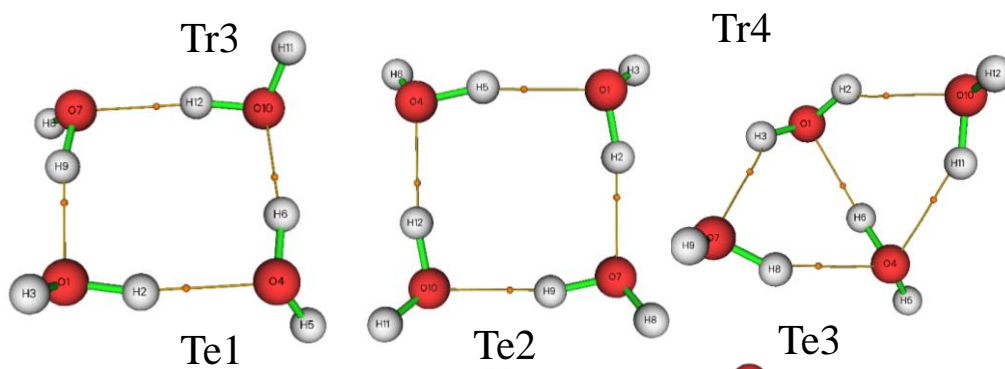
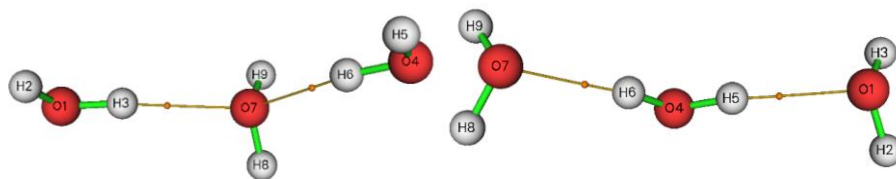
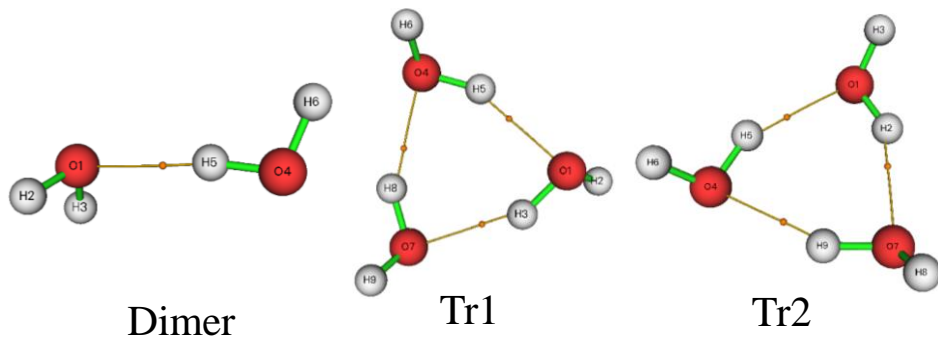
P11



P12



FigureS1: Molecular geometries of $(\text{H}_2\text{S})_n$, $n = 2-5$ cluster optimized at $\omega\text{B97XD/aug-cc-pV(D+d)Z}$ level of theory.



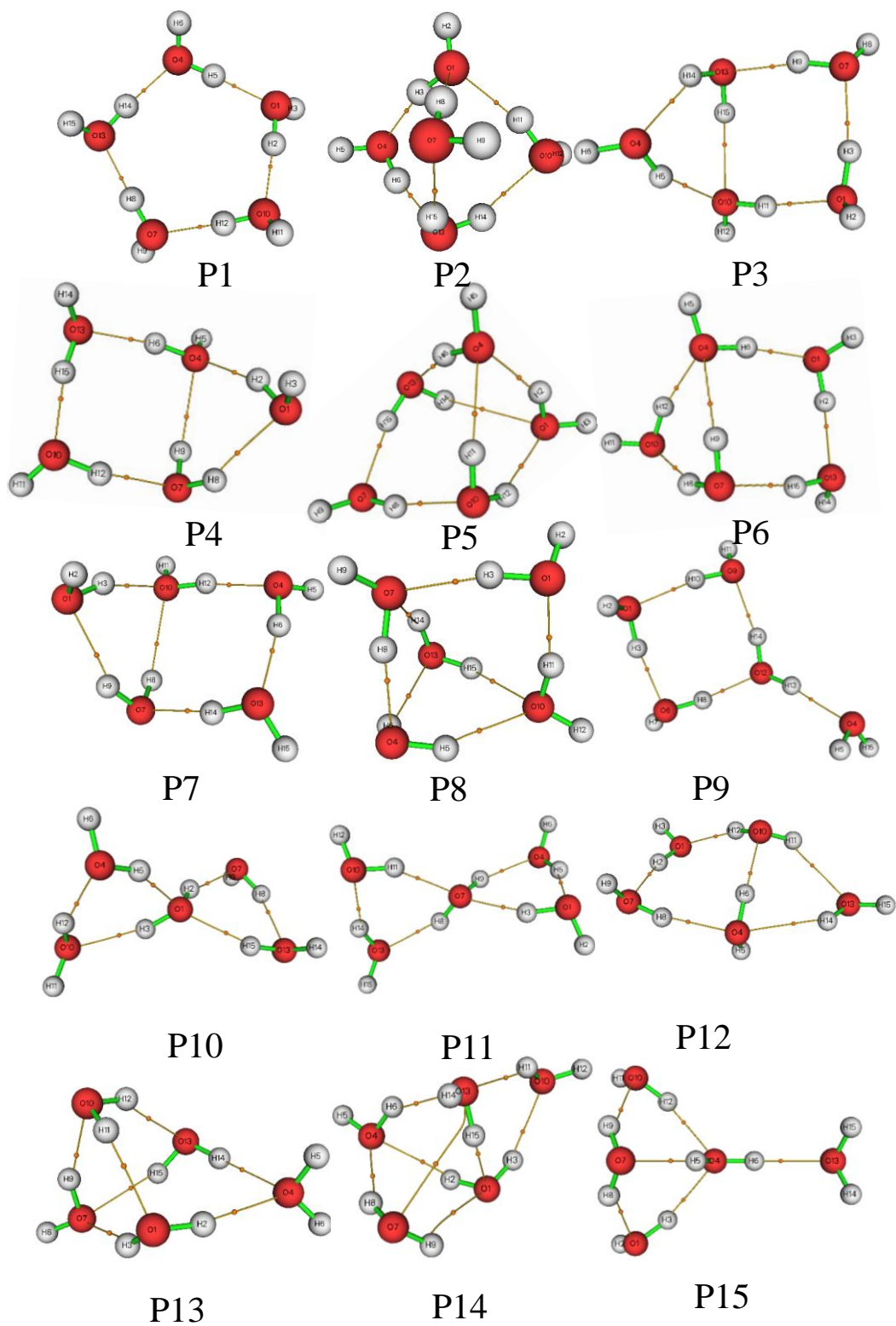


Figure S2: Molecular geometries of $(\text{H}_2\text{O})_n$, $n = 2-5$ cluster optimized at $\omega\text{B97XD/aug-cc-pVDZ}$ level of theory.

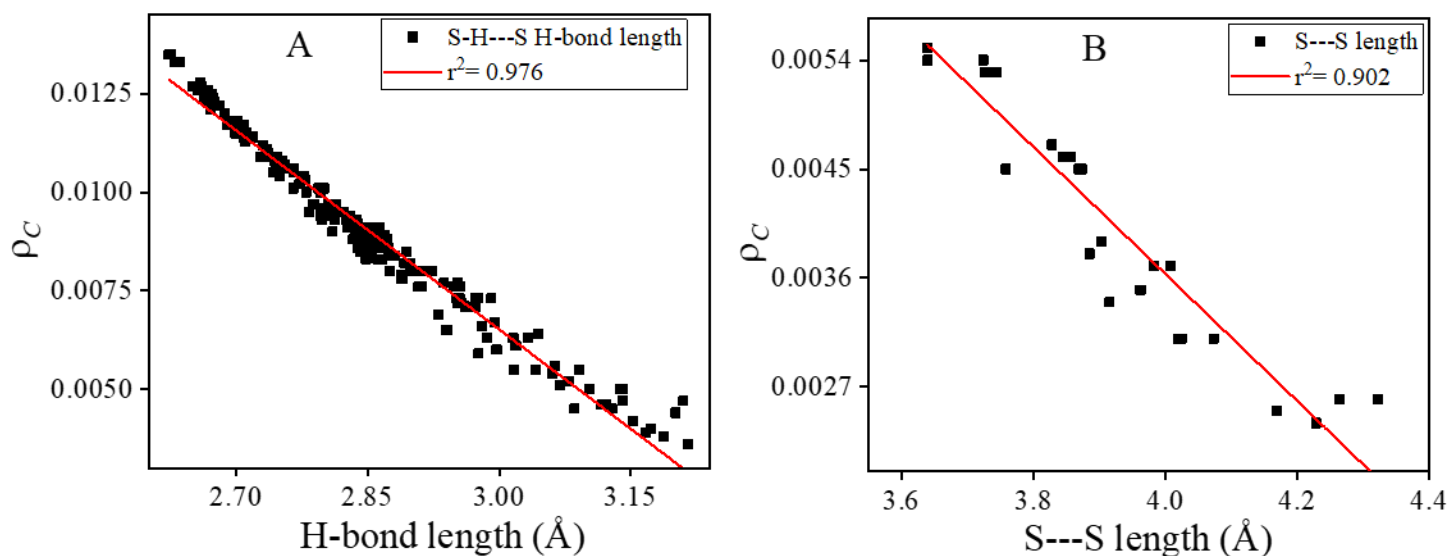


Figure S3: (A) H-bond length vs. charge density ρ_c (B) S---S bond length vs charge density ρ_c in $(\text{H}_2\text{S})_n$ $n = 2-5$ cluster respectively.

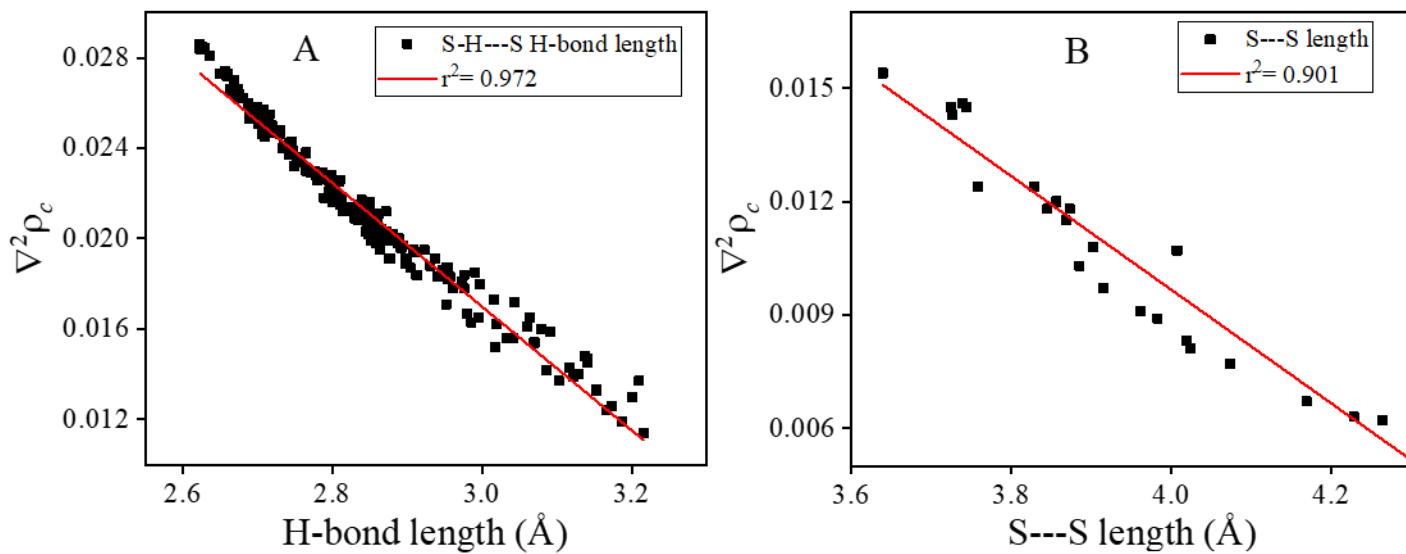


Figure S4: (A) H-bond length vs. Laplacian of charge density ($\nabla^2\rho_c$) (B) S---S bond length vs Laplacian of charge density ($\nabla^2\rho_c$) in $(\text{H}_2\text{S})_n$ $n = 2-5$ cluster respectively.

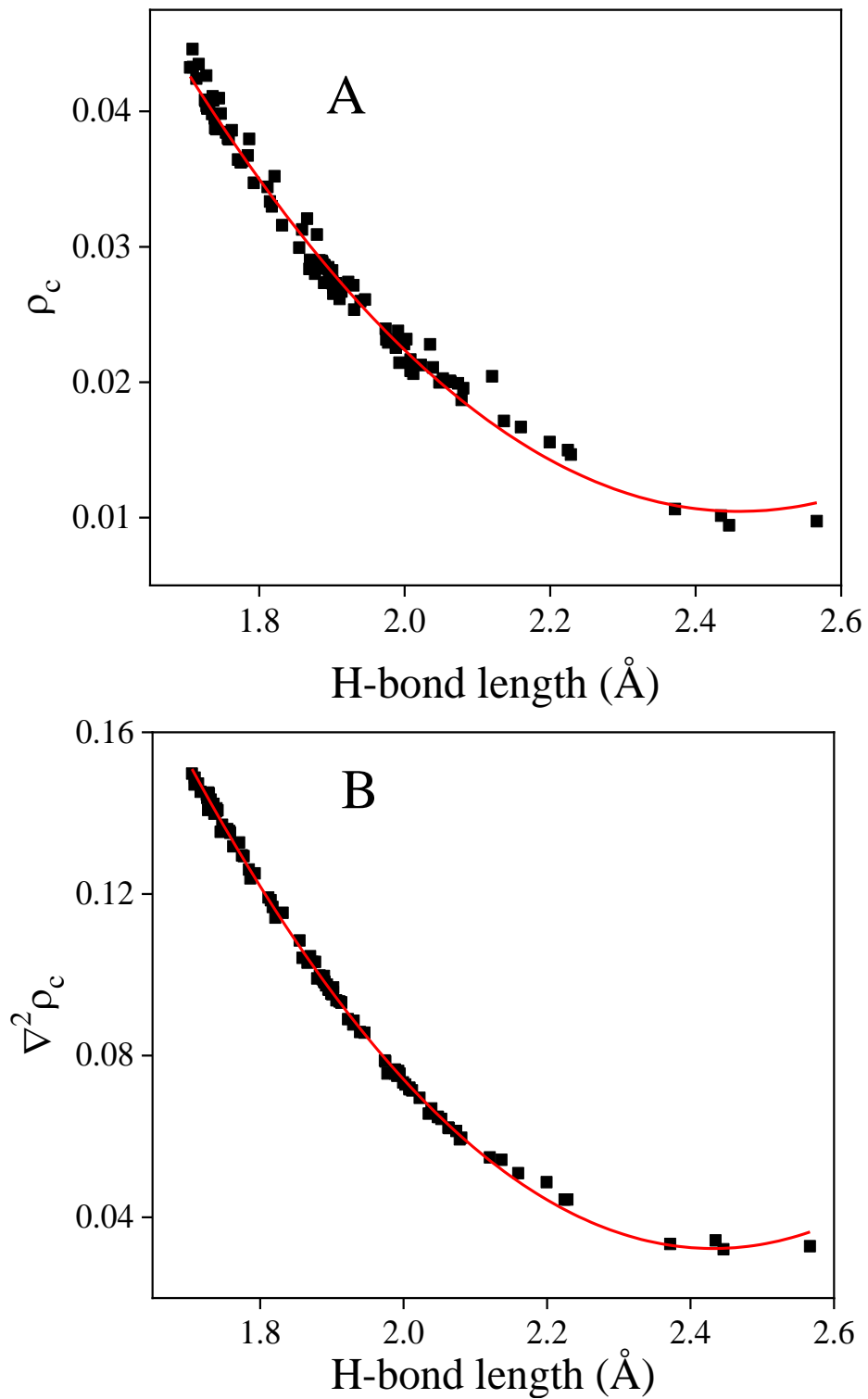


Figure S5: (A) H-bond length vs. charge density (ρ_c) (B) H-bond length vs. Laplacian of charge density ($\nabla^2 \rho_c$) in $(\text{H}_2\text{O})_n$ $n = 2-5$ cluster respectively.

TableS1: H-bond length (Å), S---S distance (Å) and their corresponding value of ρ and $\nabla^2\rho$ in dimers, trimers and tetramers calculated at ω B97X-D/aug-cc-pV(D+d)Z level of theory

Species	ω B97XD/aug-cc-pV(D+d)Z				
	S-H---S	S-H---S(Å)	S---S(Å)	ρ_c	$\nabla^2\rho_c$
D1	S3-H2---S6	2.772		0.0102	0.0229
D2	S1---S5		3.739	0.0053	0.0146
D3	S1-H3---S4	2.772		0.0102	0.0230
Tr1	S3-H1---S6	2.745		0.0108	0.0238
	S5-H6---S9	2.757		0.0106	0.0234
	S9-H8---S3	2.746		0.0109	0.0238
Tr2	S3-H1---S6	2.752		0.0107	0.0236
	S5-H6---S9	2.754		0.0107	0.0235
	S9-H8---S3	2.754		0.0107	0.0235
Tr3	S7-H9---S1	2.780		0.0100	0.0226
	S1---S5		3.724	0.0054	0.0145
Tr4	S4-H6---S7	2.811		0.0094	0.0215
	S1-H2---S7	2.811		0.0094	0.0215
Tr5	S1---S5		3.743	0.0053	0.0145
	S1---S7		3.743	0.0053	0.0145
Tr6	S9-H7---S1	2.830		0.0091	0.0209
	S5-H2---S1	2.812		0.0093	0.0215
Te1	S1-H6---S3	2.743		0.0108	0.0239
	S2-H8---S1	2.747		0.0108	0.0239
	S3-H9---S4	2.711		0.0114	0.0255
	S4-H11---S2	2.696		0.0118	0.0258
	S1-H5---S4	3.167		0.0039	0.0124
	S2-H7---S3	3.187		0.0038	0.0119
Te2	S2-H7---S1	2.717		0.0114	0.0248
	S1-H5---S4	2.705		0.0116	0.0251
	S4-H12---S3	2.719		0.0114	0.0250
	S3-H9---S2	2.673		0.0123	0.0266
	S1-H6---S3	3.216		0.0036	0.0114
Te3	S4-H6---S7	2.697		0.0117	0.0257
	S7-H8---S10	2.709		0.0117	0.0252
	S10-H12---S1	2.734		0.0110	0.0240
	S10-H11---S4	3.173		0.0040	0.0126
	S1-H2---S4	2.715		0.0114	0.0254
Te4	S3-H1---S12	2.687		0.0120	0.0260
	S12-H10---S9	2.680		0.0122	0.0262
	S9-H7---S6	2.687		0.0120	0.0259
	S6-H4---S3	2.681		0.0122	0.0262
Te5	S2-H7---S3	2.833		0.0088	0.0211
	S3-H9---S1	2.672		0.0124	0.0265
	S4-H12---S3	2.888		0.0079	0.0198

	S1-H5---S4	2.813		0.0097	0.0218
	S1-H6---S2	2.827		0.0094	0.0212
Te6	S4-H5---S10	2.834		0.0093	0.0211
	S1-H3---S4	2.669		0.0124	0.0266
	S10-H11---S1	2.846		0.0086	0.0208
	S7-H8---S1	2.847		0.0086	0.0208
	S4-H6---S7	2.837		0.0093	0.0211
Te7	S3-H10---S2	2.855		0.0084	0.0205
	S2-H8---S1	2.668		0.0124	0.0267
	S4-H12---S2	2.854		0.0084	0.0205
	S1-H5---S4	2.829		0.0094	0.0212
	S1-H6---S3	2.830		0.0094	0.0212
Te8	S3-H1---S12	2.675		0.0123	0.0264
	S12-H10---S9	2.675		0.0123	0.0264
	S9-H7---S6	2.675		0.0123	0.0264
	S6-H4---S3	2.675		0.0123	0.0264
Te9	S4-H6---S1	2.869		0.0089	0.0203
	S1-H3---S10	2.898		0.0080	0.0191
	S10-H11---S4	2.667		0.0124	0.0265
	S4-H5---S7	2.869		0.0089	0.0203
	S7-H8---S10	2.899		0.0080	0.0191
Te10	S10-H11---S4	2.822		0.0095	0.0214
	S10-H12---S7	2.861		0.0089	0.0207
	S1-H3---S7	3.201		0.0044	0.0130
	S1-H2---S10	2.690		0.0118	0.0254
	S4-H5---S1	2.834		0.0091	0.0208
Te11	S4-H6---S10	2.805		0.0096	0.0217
	S10-H12-S1	2.699		0.0118	0.0255
	S1-H2---S4	2.758		0.0106	0.0235
	S7-H9---S10	2.796		0.0096	0.0219

TableS2: H-bond length (Å), S---S distance (Å) and their corresponding value of ρ and $\nabla^2\rho$ in pentamers calculated at ω B97X-D/aug-cc-pV(D+d)Z level of theory

Level of theory	ω B97XD/aug-cc-pV(D+d)Z				
Species	S-H---S	S-H---S(Å)	S---S(Å)	ρ_c	$\nabla^2\rho_c$
P1	S13-H15---S7	2.701		0.0118	0.0251
	S7-H8---S10	2.852		0.0090	0.0210
	S10-H11---S13	2.877		0.0084	0.0191
	S4-H6---S1	2.668		0.0124	0.0264
	S1-H3---S10	2.923		0.0080	0.0195
	S1-H2---S13	2.995		0.0067	0.0165
	S10-H12---S4	2.909		0.0080	0.0194
	S7-H9---S4	3.042		0.0055	0.0156
	S13-H14---S4	3.060		0.0054	0.0161
P2	S2-H9---S1	2.713		0.0114	0.0249
	S1-H7---S3	2.904		0.0080	0.0187
	S1-H6---S4	2.973		0.0073	0.0181
	S4-H13---S2	2.809		0.0096	0.0225
	S4-H12---S3	2.952		0.0072	0.0171
	S3-H11---S5	2.679		0.0122	0.0262
	S5-H15---S4	2.806		0.0094	0.0218
	S3-H10---S2	3.138		0.0050	0.0148
	S2---S5		3.962	0.0035	0.0091
P3	S10-H12---S1	2.861		0.0083	0.0200
	S10-H11---S4	2.953		0.0077	0.0187
	S7-H8---S10	2.674		0.0124	0.0262
	S4-H5---S7	2.854		0.0089	0.0199
	S4-H6---S1	2.858		0.0088	0.0198
	S13-H15---S7	2.861		0.0083	0.0200
	S13-H14---S10	2.955		0.0076	0.0187
	S1-H2---S13	2.674		0.0123	0.0262
P4	S7-H8---4	2.846		0.0089	0.0207
	S10-H11---S7	2.663		0.0124	0.0266
	S4-H6---S1	2.707		0.0115	0.0246
	S1-H2---S13	2.850		0.0090	0.0216
	S13-H14---S10	2.742		0.0105	0.0237
	S7-H9---S13	2.937		0.0077	0.0191
	S1-H3---S10	3.019		0.0061	0.0162
	S4---S10		3.868	0.0045	0.0115
	S13---S4		4.228	0.0024	0.0063
P5	S7-H9---S13	2.742		0.0109	0.0242
	S13-H15---S10	2.853		0.0085	0.0201
	S10-H11---S7	2.733		0.0110	0.0240

	S10-H12---S4	2.839		0.0092	0.0217
	S4-H6---S1	2.711		0.0115	0.0252
	S1-H3---S10	2.841		0.0088	0.0209
	S7-H8---S4	3.141		0.0047	0.0147
	S13---S4		3.885	0.0038	0.0103
	S1---S7		3.983	0.0037	0.0089
P6	S7-H9---S13	2.875		0.0080	0.0200
	S7-H8---S10	2.976		0.0073	0.0184
	S1-H3---S7	2.707		0.0117	0.0262
	S1-H2---S13	3.079		0.0052	0.0199
	S13-H14---S4	2.690		0.0118	0.0198
	S4-H6---S10	2.872		0.0088	0.0200
	S10-H12---S1	2.827		0.0091	0.0187
	S4-H5---S1	3.033		0.0063	0.0262
P7	S7-H8---S10	2.752		0.0108	0.0207
	S10-H12---S1	2.961		0.0071	0.0266
	S1-H3---S7	2.898		0.0082	0.0246
	S4-H6---S1	2.801		0.0095	0.0216
	S1-H2---S13	2.864		0.0091	0.0237
	S13-H15---S7	2.875		0.0080	0.0191
	S7-H9---S4	3.044		0.0064	0.0162
	S10-H11---S4	3.064		0.0056	0.0115
	S13---S4		3.845	0.0046	0.0118
P8	S1-H3---S10	2.787		0.0097	0.0229
	S7-H8---S1	2.691		0.0118	0.0256
	S10-H12---S4	2.671		0.0121	0.0266
	S13-H15---S10	2.955		0.0073	0.0182
	S4-H6---S13	2.708		0.0115	0.0252
	S13-H14---S7	2.809		0.0096	0.0218
	S1---S4		4.073	0.0031	0.0077
	S7---S4		3.828	0.0047	0.0124
P9	S13-H14---S10	2.873		0.0085	0.0200
	S1-H3---S4	2.794		0.0101	0.0226
	S10-H11---S1	2.856		0.0086	0.0207
	S1-H2---S13	2.709		0.0116	0.0251
	S7-H8---S1	2.857		0.0086	0.0207
	S13-H15---S7	2.874		0.0085	0.0199
	S7---S4		3.639	0.0055	0.0154
	S13---S4		4.322	0.0026	0.0074
	S4---S10		3.639	0.0054	0.0154
P10	S4-H5---S7	2.986		0.0063	0.0163
	S4-H6---S13	3.070		0.0051	0.0154
	S1-H2---S4	2.862		0.0091	0.0211

	S1-H3---S7	2.845		0.0091	0.0203
	S13-H14---S1	2.862		0.0086	0.0199
	S10-H12---S1	2.796		0.0094	0.0221
	S13-H15---S10	3.091		0.0055	0.0159
	S7-H8---S13	2.779		0.0103	0.0228
	S7-H9---S10	2.957		0.0072	0.0183
P11	S7-H8---S13	2.712		0.0115	0.0250
	S4-H5---S7	2.796		0.0100	0.0226
	S13-H15---S1	2.948		0.0076	0.0186
	S1-H2---S4	2.710		0.0113	0.0245
	S13-H14---S4	2.980		0.0066	0.0167
	S10-H12---S1	2.830		0.0092	0.0212
	S4-H6---S10	2.755		0.0107	0.0235
	S1-H3---S7	3.086		0.0045	0.0142
P12	S10-H12---S13	2.873		0.0086	0.0203
	S10-H11---S4	2.777		0.0104	0.0230
	S4-H6---S7	2.745		0.0106	0.0239
	S4-H5---S1	3.122		0.0046	0.0139
	S1-H3---S10	2.623		0.0135	0.0284
	S7-H9---S1	2.783		0.0095	0.0229
	S13-H15---S1	2.913		0.0080	0.0184
	S13-H14---S7	3.016		0.0063	0.0173
P13	S7-H9---S13	2.665		0.0124	0.0265
	S1-H2---S7	2.716		0.0114	0.0255
	S10-H12---S7	2.973		0.0071	0.0180
	S13-H15---S10	2.765		0.0105	0.0231
	S13-H14---S4	2.997		0.0060	0.0180
	S10-H11---S4	2.866		0.0083	0.0204
	S4-H5---S1	2.692		0.0118	0.0253
	S7---S4		4.169	0.0025	0.0067
P14	S13-H14---S7	2.660		0.0127	0.0273
	S10-H12---S13	2.668		0.0126	0.0270
	S7-H8---S1	2.699		0.0115	0.0253
	S1-H3---S10	2.940		0.0065	0.0183
	S1-H2---S4	2.826		0.0093	0.0212
	S4-H5---S10	2.810		0.0090	0.0226
	S13-H15---S4	3.141		0.0050	0.0145
	S7---S4		4.024	0.0031	0.0081
P15	S1-H2---S7	2.746		0.0105	0.0243
	S13-H15---S1	2.736		0.0110	0.0240
	S13-H14---S10	2.881		0.0084	0.0202
	S10-H12---S7	2.798		0.0093	0.0228
	S7-H8---S4	2.636		0.0133	0.0281

	S4-H5---S13	2.672		0.0125	0.0265
	S4-H6---S10	3.117		0.0046	0.0143
P16	S13-H14---S7	2.908		0.0076	0.0195
	S1-H2---S13	2.774		0.0104	0.0229
	S7-H9---S1	2.789		0.0097	0.0218
	S1-H3---S4	2.800		0.0101	0.0222
	S4-H6---S7	2.892		0.0082	0.0196
	S4-H5---S10	2.951		0.0073	0.0183
	S10-H11---S1	2.765		0.0101	0.0230
	S7-H8---S10	3.210		0.0047	0.0137
P17	S7-H9---S10	2.912		0.0076	0.0184
	S1-H2---S7	2.718		0.0114	0.0247
	S7-H8---S4	2.954		0.0076	0.0185
	S4-H5---S1	2.814		0.0096	0.0212
	S4-H6---S10	2.894		0.0085	0.0197
	S10-H11---S13	2.735		0.0111	0.0241
	S13-H15---S4	2.805		0.0097	0.0220
	S10-H12---S1	3.017		0.0055	0.0152
P18	S7-H9---S4	2.730		0.0109	0.0248
	S1-H3---S7	2.735		0.0110	0.0240
	S1-H2---S13	2.869		0.0088	0.0202
	S10-H11---S1	2.629		0.0133	0.0284
	S13-H14---S10	3.153		0.0042	0.0133
	S4-H6---S10	2.656		0.0126	0.0274
P19	S13-H15---S4	2.838		0.0086	0.0214
	S4-H6---S7	2.848		0.0083	0.0202
	S1-H2---S4	2.850		0.0091	0.0213
	S7-H9---S1	2.650		0.0127	0.0273
	S1-H3---S10	2.860		0.0088	0.0200
	S10-H11---S13	2.730		0.0112	0.0246
	S13-H14---S7	2.780		0.0100	0.0229
	S4---S10		3.902	0.0039	0.0108
S7---S10		3.758	0.0045	0.0124	
P20	S1-H2-S10	2.699		0.0118	0.0258
	S10-H11---S7	2.747		0.0107	0.0238
	S7-H9---S13	2.701		0.0116	0.0252
	S13-H14---S4	2.836		0.0089	0.0215
	S4-H5---S1	2.690		0.0117	0.0256
	S1---S7		4.264	0.0026	0.0062
	S7---S4		3.856	0.0046	0.0120
	S4---S10		4.007	0.0037	0.0107
	S1---S13		3.873	0.0045	0.0118
P21	S13-H15---S7	2.864		0.0089	0.0203

	S13-H14---S10	2.754		0.0106	0.0234
	S4-H5---S13	2.625		0.0135	0.0285
	S7-H9---S4	3.129		0.0045	0.0140
	S7-H8---S1	2.841		0.0085	0.0213
	S1-H2---S4	2.668		0.0123	0.0270
	S10-H11---S1	2.728		0.0109	0.0248
P22	S13-H14---S4	2.659		0.0128	0.0272
	S1-H2---S13	2.623		0.0135	0.0286
	S4-H6---S10	2.754		0.0106	0.0234
	S10-H12---S1	2.976		0.0059	0.0178
	S7-H8---S1	2.708		0.0114	0.0257
	S10-H11---S7	2.931		0.0069	0.0188
	S4-H5---S7	2.889		0.0078	0.0200
P23	S10-H11---S4	2.749		0.0104	0.0232
	S13-H15---S10	2.765		0.0106	0.0238
	S7-H8---S13	2.852		0.0088	0.0199
	S4-H6---S7	2.702		0.0116	0.0252
	S7-H9---S1	2.991		0.0073	0.0185
	S13-H14---S4	3.103		0.0050	0.0137
	S7---S10		4.019	0.0031	0.0083
	S1---S13		3.726	0.0053	0.0143
	S1---S4		3.915	0.0034	0.0097

Table S3: H-bond length (\AA) and their corresponding value of ρ and $\nabla^2\rho$ in dimers, trimers and tetramers calculated at $\omega\text{B97X-D/aug-cc-pVDZ}$ level of theory

Species	$\omega\text{B97XD/aug-cc-pVDZ}$			
	O-H---O	O-H-- -O(\AA)	ρ_c	$\nabla^2\rho_c$
Dimer	O4-H5---O1	1.93	0.0254	0.0886
Tr1	O7-H8---O4	1.91	0.0273	0.0937
	O4-H5---O1	1.89	0.0290	0.0993
	O1-H3---O7	1.89	0.0288	0.0994
Tr2	O7-H9---O4	1.90	0.0273	0.0952
	O1-H2---O7	1.90	0.0274	0.0956
	O4-H5---O1	1.90	0.0273	0.0953
Tr3	O4-H6---O7	1.97	0.0232	0.0785
	O1-H3---O7	1.97	0.0232	0.0785
Tr4	O4-H6---O7	1.98	0.0229	0.0756
	O4-H5---O1	1.99	0.0229	0.0755
Te1	O4-H6---O10	1.76	0.0379	0.1351
	O10-H12---O7	1.76	0.0379	0.1351
	O7-H9---O1	1.76	0.0379	0.1351
	O1-H2---O4	1.76	0.0379	0.1351
Te2	O4-H5---O1	1.77	0.0362	0.1295
	O1-H2---O7	1.76	0.0380	0.1355
	O7-H9---O10	1.77	0.0362	0.1295
	O10-H12---O4	1.76	0.0380	0.1355
Te3	O1-H2---O10	2.05	0.0203	0.0643
	O1-H3---O7	2.05	0.0203	0.0643
	O7-H8---O4	1.99	0.0226	0.0765
	O4-H6---O1	1.79	0.0380	0.1239
	O10-H11---O4	1.99	0.0226	0.0765
Te4	O7-H9---O1	1.90	0.0285	0.0964
	O1-H3---O4	1.81	0.0344	0.1191
	O4-H5---O7	2.00	0.0228	0.0734
	O4-H6---O10	1.90	0.0265	0.0957
Te5	O10-H12---O4	2.01	0.0206	0.0713
	O10-H11---O1	2.01	0.0206	0.0713
	O7-H9---O4	2.01	0.0206	0.0713
	O7-H8---O1	2.01	0.0206	0.0713

Table S4: H-bond length (\AA) and their corresponding value of ρ and $\nabla^2\rho$ in pentamers calculated at $\omega\text{B97X-D/aug-cc-pVDZ}$ level of theory

$\omega\text{B97XD/aug-cc-pVDZ}$				
Species	O-H---O	O-H--- O(\AA)	ρ_c	$\nabla^2\rho_c$
P1	O4-H5---O1	1.73	0.0403	0.1445
	O1-H2---O10	1.73	0.0402	0.1449
	O10-H12---O7	1.73	0.0404	0.1451
	O7-H8---O13	1.73	0.0403	0.1448
	O13-H14---O4	1.74	0.0388	0.1412
P2	O7-H8---O1	1.89	0.0273	0.0976
	O10-H11---O1	1.87	0.0285	0.1032
	O13-H15---O7	1.92	0.0274	0.0890
	O4-H6---O13	1.73	0.0426	0.1408
	O1-H3---O4	1.70	0.0432	0.1498
	O13-H14---O10	1.94	0.0260	0.0858
P3	O1-H3---O7	1.74	0.0398	0.1423
	O7-H9---O13	1.75	0.0398	0.1371
	O13-H15---O10	2.04	0.0211	0.0669
	O10-H11---O1	1.71	0.0424	0.1473
	O13-H14---O4	2.00	0.0232	0.0728
	O4-H5---O10	1.89	0.0273	0.0997
P4	O13-H15---O10	1.73	0.0402	0.1433
	O10-H12---O7	1.74	0.0408	0.1401
	O7-H9---O4	2.07	0.0199	0.0613
	O4-H6---O13	1.73	0.0409	0.1446
	O7-H8---O1	1.99	0.0238	0.0750
	O1-H2---O4	1.88	0.0280	0.1032
P5	O10-H11---O4	2.02	0.0213	0.0695
	O4-H6---O13	1.72	0.0435	0.1453
	O13-H15---O7	1.79	0.0347	0.1251
	O7-H8---O10	1.78	0.0367	0.1260
	O1-H2---O4	1.90	0.0270	0.0968
	O13-H14---O1	2.45	0.0094	0.0321
	O10-H12---O1	2.08	0.0196	0.0597
P6	O13-H15---O7	1.76	0.0386	0.1318
	O7-H9---O4	2.23	0.0147	0.0443
	O4-H6---O1	1.73	0.0408	0.1438

	O1-H2---O13	1.73	0.0406	0.1431
	O7-H8---O10	1.90	0.0282	0.0954
	O10-H12---O4	1.86	0.0299	0.1085
P7	O13-H14---O7	1.74	0.0411	0.1399
	O7-H8---O10	2.16	0.0167	0.0509
	O10-H12---O4	1.74	0.0395	0.1404
	O4-H6---O13	1.74	0.0387	0.1407
	O1-H3---O10	1.87	0.0290	0.1046
	O7-H9---O1	1.93	0.0272	0.0877
P8	O4-H5---O10	1.99	0.0229	0.0755
	O10-H11---O1	1.75	0.0384	0.1360
	O1-H3---O7	1.77	0.0364	0.1327
	O7-H8---O4	1.74	0.0410	0.1354
	O4-H6---O13	2.12	0.0204	0.0548
	O13-H14---O7	2.37	0.0106	0.0334
	O13-H15---O10	2.01	0.0217	0.0716
P9	O1-H3---O6	1.76	0.0385	0.1355
	O6-H8---O12	1.71	0.0433	0.1488
	O12-H14---O9	1.81	0.0333	0.1184
	O9-H10---O1	1.78	0.0363	0.1294
	O12-H13---O4	1.91	0.0262	0.0934
P10	O1-H3---O10	1.88	0.0290	0.0998
	O10-H12---O4	1.89	0.0286	0.0981
	O4-H5---O1	1.90	0.0283	0.0964
	O1-H2---O7	1.89	0.0284	0.0974
	O7-H8---O13	1.89	0.0287	0.0984
	O13-H15---O1	1.89	0.0288	0.0989
P11	O7-H8---O13	1.89	0.0285	0.0982
	O13-H14---O10	1.89	0.0288	0.0993
	O10-H11---O7	1.90	0.0281	0.0963
	O7-H9---O4	1.89	0.0285	0.0982
	O4-H5---O1	1.89	0.0288	0.0993
	O1-H3---O7	1.90	0.0281	0.0963
P12	O7-H8---O4	1.86	0.0313	0.1042
	O4-H6---O10	1.71	0.0446	0.1470
	O10-H12---O1	1.83	0.0316	0.1153
	O1-H2---O7	1.82	0.0330	0.1167
	O10-H11---O13	2.20	0.0156	0.0487
	O13-H14---O4	2.22	0.0150	0.0444
P13	O13-H14---O4	2.01	0.0208	0.0720

	O13-H15---O7	2.05	0.0200	0.0648
	O1-H3---O7	2.05	0.0200	0.0648
	O1-H2---O4	2.01	0.0209	0.0720
	O10-H11---O1	2.03	0.0228	0.0656
	O10-H12---O13	2.04	0.0228	0.0656
	O7-H9---O10	1.82	0.0352	0.1141
P14	O1-H3---O10	1.97	0.0239	0.0788
	O1-H2---O4	2.14	0.0171	0.0542
	O10-H11---O13	1.99	0.0214	0.0762
	O13-H15---O1	1.88	0.0309	0.0991
	O4-H6---O13	1.95	0.0261	0.0857
	O7-H8---O4	2.08	0.0187	0.0593
	O7-H9---O1	2.43	0.0102	0.0342
	O13-H15---O7	2.57	0.0097	0.0328
P15	O7-H9---O10	2.06	0.0201	0.0622
	O7-H8---O1	2.06	0.0200	0.0620
	O1-H3---O4	1.91	0.0267	0.0931
	O4-H5---O7	1.87	0.0321	0.1030
	O10-H12---O4	1.91	0.0267	0.0931
	O4-H6---O13	1.87	0.0284	0.1039

Table S5: Geometry and frequencies of $(\text{H}_2\text{S})_n$ $n = 2-5$ clusters optimized at $\omega\text{B97X-D/aug-cc-pV(D+d)Z}$ level of theory

Species	Geometry	Frequency
Monomer	H0.000000000.97376600-0.82750000 H0.000000000-0.97376600-0.82750000 S0.000000000.000000000.10343800	1197.82222747.27052763.3579
Dimer	H2.327465001.23946600-0.01282900 H0.747542000.08978300-0.02271700 S2.08791200-0.086348000.00127300 H-2.02738800-0.767974001.02095800 H-2.06553700-0.87714700-0.92599400 S-2.024292000.10609000-0.00498700	46.616463.583987.5946 109.3311183.7616296.9873 1200.76241203.33272679.8299 2735.94832754.23912754.3388
Dimer2	S-0.00963300-1.923768000.00000000 H1.213879001.252077000.00000000 H-0.69290500-1.289909000.97399500 H-0.69290500-1.28990900-0.97399500 S-0.009633001.814861000.00000000 H0.480202003.070253000.00000000	70.9427115.5163126.8843 153.9528192.6187246.6297 1194.39071201.98802731.9153 2736.78122747.93852756.4494
Dimer3	S0.087901002.104440000.00000000 H-1.259148002.138032000.00000000 H0.117688000.752620000.00000000 S0.08790100-2.018734000.00000000 H-0.83567900-2.130973000.97499000 H-0.83567900-2.13097300-0.97499000	64.908073.839997.2351 109.9509176.7771303.8155 1198.97831205.05882680.4524 2730.13992745.53942746.8328
Trimer2	H1.261510001.04614400-0.08653200 H0.696205002.336445001.26991800 S0.642655002.25019500-0.07397700 H1.68326700-1.770915001.26930000 H0.27613900-1.61518900-0.08005000 S1.62828600-1.68123000-0.07428700 H-2.37633800-0.567942001.26938300 H-1.539130000.57002100-0.08283600 S-2.27104400-0.56887600-0.07418400	66.910768.142485.0257 88.223289.7938113.6768 183.8040188.1253196.8591 244.7958255.3741407.6221 1204.04541204.63251205.5839 2658.99812668.30262670.7886 2745.50432747.83072748.5394
Trimer1	H1.132100001.17311400-0.00407900 H0.413611002.50319800-1.24605100 S0.386961002.299930000.08595500 H1.89858400-1.565950001.26325900 H0.45747500-1.57998100-0.05984200 S1.80779000-1.48630300-0.07907200 H-2.37012900-0.869358001.25355800 H-1.584698000.39174700-0.01817900 S-2.19143400-0.81692500-0.08117400	67.956072.179683.8325 89.9615105.8416122.7169 189.7815192.8916204.6958 251.0979264.6766413.1805 1204.77331205.23291205.7166 2657.20512667.30512668.1537 2743.34152748.30012748.5809
Trimer3	S0.000000000.860792000.00000000 H-3.482392001.266034000.00000000 H-0.427272000.033492000.97518500 H-0.427272000.03349200-0.97518500 S-3.60490600-0.075200000.00000000 H-4.95170100-0.029837000.00000000 S3.75038600-0.869791000.00000000	12.268250.428457.9427 74.540278.157796.0785 98.4548125.5975127.5475 199.6802200.4087307.8980 1196.10301202.28601204.5591 2684.93412732.45022737.6468 2748.83432755.54662757.1845

	H4.416020000.301773000.00000000 H2.54493900-0.257766000.00000000	
Trimer4	S-4.152344000.025250000.00983200 H-2.80807200-0.10970700-0.01482400 H-4.35123000-1.30714500-0.01578700 S4.152395000.025243000.00977400 H4.35096000-1.30721700-0.01493200 H2.80809100-0.10941100-0.01476300 S-0.000007000.00942500-0.02045900 H-0.000259000.877046001.01107200 H-0.000185000.99772900-0.93711700	4.096215.281946.2679 50.036368.283968.7736 85.4656111.1947116.9505 221.9073248.0373317.3918 1199.57651201.61261202.7658 2692.72162695.32032733.0584 2750.58982750.68392752.5513
Trimer5	S0.000000000.000000001.50333700 H-0.062263003.256789000.56409600 H-0.97473500-0.005986000.57147700 H0.974735000.005986000.57147700 S0.000000002.98547600-0.75365100 H-0.057639004.28559100-1.10385700 S0.00000000-2.98547600-0.75365100 H0.05763900-4.28559100-1.10385700 H0.06226300-3.256789000.56409600	12.276358.041263.0146 68.1992105.9132114.2198 114.8737136.7460144.2434 183.4741200.2084255.4760 1194.08611196.54131201.9100 2737.54372737.75212738.0080 2753.45442757.38562757.6253
Trimer6	S0.00012200-0.15910500-0.15082000 H-2.80591500-0.154688000.03688700 H-0.088117000.98082100-0.86468800 H0.143517000.506395001.01276800 S-4.128744000.112930000.10215200 H-4.46062700-1.06250400-0.46671000 S4.13818500-0.024761000.11841000 H4.228175001.06738500-0.66575800 H2.82995700-0.20243500-0.16838000	12.554618.416446.6402 57.757673.615180.5060 99.5188109.4784150.7958 198.7109271.0220310.8336 1199.17741203.69041204.7343 2697.25702701.12882729.6591 2746.21182746.51072749.7248
Tetramer1	S0.48821300-2.121409001.27345200 S2.037684000.46323100-1.41606900 S-2.04534300-0.33870300-1.33970900 S-0.320815001.911316001.46632800 H0.16615100-1.143815002.14438900 H-0.49847500-1.770042000.41639100 H1.002939000.05993300-2.18062000 H1.83062300-0.52235900-0.51162500 H-1.804326000.55944400-0.35652700 H-3.22708100-0.71556200-0.81383300 H0.561347001.721097000.45663400 H-0.587005003.180336001.10115600	24.287932.682060.8499 70.959081.644183.0447 97.4076102.1999131.1230 134.0872150.7250161.1638 178.2428202.1503311.5123 330.9482354.2125382.0626 1198.84921200.06251204.4997 1206.39712656.16582668.2362 2672.18322678.80092738.1738 2744.33272750.35192751.7917
Tetramer2	S-0.08586500-2.134911001.16872200 S2.40600700-0.08530400-1.25803300 S0.107765002.008038001.23425900 S-2.424548000.08355600-1.24695900 H-0.97719700-1.594210000.30439200 H-0.19022000-1.096110002.02188300 H1.73207600-0.96015900-0.47409900 H3.46563100-0.05553800-0.42572600 H0.985466001.545849000.31184400	8.322728.902567.9983 80.405987.640893.6559 107.2338124.2140129.8063 139.7343144.6453160.1849 169.4022184.2954314.9664 337.8759348.1125396.0470 1200.11191202.02571205.0646 1206.09802651.05552656.7385 2667.61752674.58832741.2732

	H0.119933003.259209000.73503700 H-3.456768000.01959800-0.38258200 H-1.732645000.93929700-0.45857000	2743.08272746.58342746.7934
Tetramer3	S2.546755000.008258001.15194600 H1.85552200-0.905107000.43058300 H1.69705100-0.078608002.19429200 S0.00185300-1.95217500-1.25477900 H-0.09911400-3.25888700-0.94386700 H-0.94570700-1.58197800-0.36167900 S-2.51477000-0.027838001.18549800 H-1.850057000.856742000.40392700 H-1.629916000.103590002.19337200 S-0.036956002.10642600-1.17343200 H0.080061001.11147800-2.07577900 H0.942036001.59804800-0.38858600	17.683138.060567.2744 79.338984.995993.6544 100.0353113.2571125.4852 146.3277155.5336169.8396 174.9257216.8319310.9506 328.7951357.9407382.8100 1199.48441202.26771207.1131 1208.01372648.88872657.8384 2661.05182667.09722735.7315 2745.98042746.59852750.7601
Tetramer4	H-1.73652100-1.110323000.24470200 H-3.41239300-0.28891000-0.34549700 S-2.63083300-0.226947000.75069900 H-1.110030001.73609000-0.24405300 H-0.289137003.412590000.34512300 S-0.227013002.63043200-0.75063600 H1.736226001.109758000.24408100 H3.412721000.28907400-0.34539200 S2.630864000.226996000.75058600 H1.10994900-1.73587500-0.24447400 H0.28996200-3.412679000.34504700 S0.22693300-2.63046300-0.75062000	-4.066122.188675.0155 81.724582.892083.2099 103.1594108.7919110.0209 116.6334197.6984200.0522 204.3407213.2779231.6347 325.8345336.4471433.9344 1202.05981203.58821204.9680 1207.66512631.38152640.0004 2649.38402651.60132743.8297 2744.48422746.09692747.3402
Tetramer5	S0.029085001.989216001.06009300 S2.92199300-0.00257000-1.06913000 S-0.05124200-1.959582000.89868800 S-2.983861000.08088100-0.96643200 H-0.997831001.664863000.24191900 H0.960611001.630393000.14770600 H2.27846200-0.96440000-0.37108400 H3.748577000.27968700-0.04277900 H-0.02584600-0.669687001.31384100 H0.12468200-2.448848002.14140900 H-2.22752400-0.30048000-2.01485700 H-2.51672600-0.91863600-0.18767000	12.486642.847560.1525 64.432869.051875.7001 92.532998.7158107.8188 140.8105150.3466162.1997 215.6414233.1090251.9784 261.2896334.7233419.5337 1197.16351201.55561203.4086 1207.58082645.24542671.3529 2689.01952691.87412702.0845 2741.94782745.42222748.9049
Tetramer6	S0.00237700-1.93518200-0.88629200 H-0.00231900-2.40918700-2.14725900 H0.00283400-0.63974300-1.28510200 S-0.002139002.01357400-0.99723600 H-0.985955001.65938600-0.13976900 H0.978465001.66092300-0.13552900 S3.050471000.033873000.91563000 H2.43429500-0.936677000.20571000 H2.45539200-0.342697002.06461400 S-3.050865000.030508000.91571400 H-2.42792800-0.936847000.20728300	15.710949.756859.6437 66.077570.859793.3726 95.0313112.9387122.8030 146.7360156.3509181.2451 218.9896229.5221256.0944 267.1346329.8234422.7132 1197.47511202.18881203.9145 1208.82252645.32472679.7858 2692.86722701.57292704.2182 2744.41972745.36042746.4499

	H-2.45229800-0.339514002.06500600	
Tetramer7	S0.000346001.957402000.94148800 S-0.00022500-1.988119000.72925000 S3.108933000.05075400-0.92962000 S-3.108751000.05108700-0.92963600 H-0.982837001.624884000.07438600 H0.981331001.625549000.07167900 H-0.00033300-2.488273001.98007200 H0.00010900-0.701952001.15682600 H3.807884000.354966000.18195600 H2.44687100-0.95418400-0.31513200 H-3.811255000.353887000.18009200 H-2.44661700-0.95286700-0.31358400	12.991958.662964.1336 66.309780.475591.6668 94.0033103.7843114.1874 145.2877153.1024163.7124 219.4701236.5410258.5476 268.3621332.9421423.9606 1198.34761202.67381203.6811 1208.41482645.67232676.7699 2689.75132703.20822705.2730 2746.31802747.15912747.3934
Tetramer8	H-1.74687300-1.303092000.04661600 H-2.95134300-0.49850000-1.27202800 S-2.82653900-0.484904000.06978200 H-1.298423001.716939000.01268900 H-0.549881003.035022001.25133200 S-0.486307002.79816700-0.07371600 H1.746567001.30310700-0.05397800 H2.967977000.501166001.25062100 S2.825523000.48442000-0.08939700 H1.29786900-1.71643700-0.00691600 H0.55273700-3.05273900-1.22802300 S0.48615900-2.796775000.09331100	-4.066122.188675.0155 81.724582.892083.2099 103.1594108.7919110.0209 116.6334197.6984200.0522 204.3407213.2779231.6347 325.8345336.4471433.9344 1202.05981203.58821204.9680 1207.66512631.38152640.0004 2649.38402651.60132743.8297 2744.48422746.09692747.3402
Tetramer9	S-3.28490900-0.00194700-0.72043500 H-3.83396700-0.525864000.39324800 H-2.594420000.92580100-0.02174400 S-0.00043400-1.990688000.69150800 H0.98367100-1.62145900-0.15844700 H-0.98486200-1.62132400-0.15801000 S3.28447300-0.00244800-0.72055200 H2.596273000.92477500-0.01893000 H3.83646300-0.527961000.39092500 S0.000619001.994199000.70245300 H0.000253000.662720000.95696500 H0.000597001.79746400-0.63157200	20.663251.894361.0840 64.048979.544484.4789 91.6613119.8521128.3499 143.9650175.5134196.9317 216.1451236.3239253.1551 273.9113313.6740423.6914 1201.94281202.83631204.1345 1207.10232641.13432689.4651 2690.34822693.11592705.2177 2739.20862743.26212743.5720
Tetramer10	S0.00179000-1.99485100-0.70350100 H0.00013900-0.66297100-0.95602800 H-0.00103000-1.800003000.63080600 S3.282354000.004003000.72228700 H2.59093800-0.922968000.02340500 H3.836725000.52369000-0.39074000 S-3.283339000.002264000.72185500 H-2.59382800-0.923635000.01977100 H-3.834425000.52871600-0.38961200 S-0.000964001.98920400-0.69392500 H0.986229001.624595000.15448400 H-0.982210001.622662000.16045400	20.682252.005661.5483 64.301679.855684.2191 92.0155120.7335128.2779 144.3414176.1867196.8299 216.4897236.2826253.4397 274.2287314.0206424.3544 1201.92941202.83281204.1666 1207.07012640.86482689.0863 2690.26632693.04642704.7883 2738.90462743.54712743.9681
Tetramer11	S-1.253508002.31274300-0.12964600	7.839012.548349.4444

	H-2.263418001.424759000.02560800 H-1.132724002.508105001.19836600 S-3.55860100-1.003683000.19763900 H-3.85146000-1.07307200-1.11603100 H-2.29512800-1.447350000.00681900 S4.350023000.082456000.12381700 H5.02114800-1.04057000-0.19830300 H3.15906000-0.44940600-0.23020100 S0.49650000-1.30266800-0.22865300 H0.66539000-1.350345001.10798000 H0.146509000.00630900-0.20475200	70.926376.788389.9111 102.3829110.3884116.1831 123.8201133.8281174.1878 195.8269218.5099263.4398 292.8324303.8542434.9071 1202.55141203.71621204.7735 1206.13662645.67492666.4444 2677.60302697.82532738.8054 2743.40432744.63242748.0297
Pentamer1	S-3.331588000.068578000.20015200 H-2.44299200-0.508585001.03699700 H-2.729082001.271964000.31253100 S-0.19777000-0.71816800-2.15850800 H-0.72414000-0.51240000-3.38131200 H-1.37250900-0.48682300-1.52411900 S3.355747000.13505200-0.04169100 H2.639852001.224436000.31415700 H2.59205500-0.07080200-1.13451800 S0.002769002.283058000.55345200 H-0.070700001.041177001.08303700 H0.033486001.79059800-0.70417700 S0.21298100-1.775681001.59642000 H0.00016200-2.375016000.40693000 H1.39963900-1.259976001.19328700	30.901740.862245.6309 61.060565.055977.0632 79.071189.984893.9262 108.8898124.9986141.1555 142.7720167.8026174.8009 207.8773221.5584246.1328 257.1933269.4638295.4211 305.3517393.1931400.9080 1195.10941199.37811201.3439 1203.72191206.99922646.2016 2647.98562694.34482701.2468 2704.35402706.68642718.1165 2731.26142733.93162748.0498
Pentamer2	S3.33582200-0.000644000.11889000 S0.06668100-0.39782100-2.17483000 S-0.14221700-1.968533001.36705800 S0.043173002.238066000.82802300 S-3.268244000.09380100-0.09325200 H2.794098001.211093000.36547800 H2.37919700-0.629187000.83663500 H0.45316600-0.01088900-3.40627800 H1.32057200-0.31228100-1.67056300 H0.10369000-2.502024000.15312300 H-1.28893900-1.384173000.94257300 H0.149517000.967535001.27549100 H0.029877001.82656400-0.45973900 H-4.039272000.263525000.99923000 H-2.465333001.131931000.22981700	25.348629.552044.7442 60.888368.294971.7820 75.286387.404992.1602 100.2468120.0854151.4996 160.8217175.1813190.3494 205.3815212.6175224.9875 245.1543284.2563301.7677 313.1371386.7647404.2776 1196.79031198.86171203.4304 1207.15731216.35242644.6425 2660.66132692.00402697.3302 2700.54722704.90002716.7436 2729.37572739.35712744.5599
Pentamer3	S0.303994002.350227001.09842500 H1.387592001.566349000.87810800 H0.750264003.322802000.27941300 S-0.000359000.00017700-2.31916800 H0.04081400-0.96477800-1.37308400 H-0.041210000.97426700-1.38254400 S-0.30441500-2.350659001.09813200 H-1.38806200-1.566279000.87969100 H-0.74804500-3.318818000.27245400 S-3.184302000.262487000.11922000	17.075943.899753.5279 58.095072.791477.0910 81.545892.358895.3372 101.7466134.6219140.1989 147.5646163.0279166.0669 172.8025228.9562240.7388 274.6996290.0640302.3439 315.9318396.5959404.7313 1199.32661199.97921201.3258 1208.54671209.78182632.3917

	H-2.700997000.07355000-1.12730900 H-2.193199001.128121000.42515000 S3.18487700-0.262870000.11901500 H2.70293100-0.07781000-1.12861300 H2.19319500-1.127214000.42676400	2633.92812692.01612699.5721 2701.16222704.47112713.8799 2714.98292745.77232746.2026
Pentamer4	S3.34378900-0.05888200-0.00724300 H2.67016900-1.12420600-0.49324600 H2.535303000.021772001.07001700 S0.111907001.87873400-1.48931900 H0.132981002.69303700-0.41525800 H1.258147001.25855200-1.12170800 S-3.30366400-0.08719300-0.22116100 H-2.348755000.56798700-0.91803000 H-2.69494800-1.27669900-0.41444500 S-0.202849000.662567002.16930900 H-1.389489000.469108001.54435100 H-0.622417000.087434003.31338700 S0.06206000-2.26365700-0.64575000 H0.06196700-1.437245000.42574300 H0.21714900-3.364841000.11581000	16.323340.642743.1865 58.217066.580573.9593 78.559992.083894.0526 116.4133126.3852141.1791 149.9245158.3350166.9400 196.8175211.4954222.1059 254.2476275.1154294.8143 312.6916343.5178409.5509 1197.70181201.82021203.0654 1204.57231207.01732640.4368 2647.73702661.49282688.8826 2709.36352719.78322734.7485 2738.01452741.99742747.5093
Pentamer5	S3.28355900-0.09251600-0.09141600 H4.090405000.616148000.72300000 H2.545947000.99140300-0.41878600 S-0.03644000-0.612748002.13113500 H0.41507700-0.391392003.38121000 H1.20099900-0.529124001.58760300 S-0.03945700-1.64091200-1.64912600 H0.44788300-2.21083900-0.52862700 H-1.24873900-1.40885600-1.08615200 S0.027120002.29032700-0.61852300 H0.065462001.04288500-1.14375800 H-0.015681001.804346000.64188900 S-3.29453500-0.020191000.09886700 H-4.056791000.25891700-0.97704000 H-2.488524001.04315300-0.11432900	13.678930.314844.0496 55.919268.313075.7434 79.379890.5657100.2729 118.5954120.6513131.4140 146.8364157.7138174.1027 203.4420213.6728226.8180 250.4171261.4236292.4812 323.8817386.1129424.2568 1196.19381200.02921201.9561 1204.35931205.60312657.1927 2662.35452664.95942694.0117 2698.88092703.57882736.9163 2741.69592742.81272744.6085
Pentamer6	S-0.225301001.175573002.05446200 H-0.091030002.202690001.19100200 H-1.416378000.803461001.52580100 S3.34779000-0.077358000.07635900 H2.474254000.211172001.06447100 H2.71694900-1.23716600-0.20852600 S-3.32887900-0.14729100-0.13695800 H-2.75454900-1.36574000-0.05064000 H-2.406554000.27347500-1.02932500 S0.05933400-2.32598800-0.17955600 H0.19472300-2.976264000.99361200 H0.04799900-1.113758000.41930700 S0.113506001.43345400-1.78370400 H1.282974000.93134400-1.32167700 H0.488419001.33655100-3.07367600	24.989541.999044.5173 60.015863.633073.2605 75.894890.782891.3691 98.4011115.5252122.2054 142.9419151.7417159.0971 180.8891207.9664218.9812 240.6285262.8244276.3861 301.1079356.2200397.5792 1194.40931197.55641200.3082 1202.24571206.80862648.2961 2650.19332683.45252705.9289 2711.56882722.47322727.7918 2737.04222740.20032751.8960

Pentamer7	S-0.138221002.36409100-0.48164900 H-1.362073002.105484000.02865200 H-0.165222001.24433500-1.23827100 S0.06541500-0.902121002.03244800 H-0.92339900-0.557051002.88033700 H0.030512000.286611001.38897700 S0.13760000-1.56166100-1.89762600 H1.27373000-1.06399800-1.35370500 H-0.22674700-2.13899800-0.73360500 S3.273145000.152294000.09411100 H2.99881900-0.488897001.24855300 H2.424721001.161456000.38493700 S-3.20629200-0.080504000.18204000 H-3.954574000.37108000-0.84418800 H-2.20212900-0.47359700-0.63086900	34.079937.441948.5986 58.961565.469469.7289 70.901188.674994.3648 100.6988115.9409135.2994 149.3628160.4383172.4179 179.0470199.1629218.4324 244.6391252.6181261.6721 303.3291334.1801381.0474 1194.55281195.92801201.3954 1203.29321207.20862659.0136 2686.38222694.10032703.0994 2710.20342713.06062725.8521 2739.92752740.97232746.4880
Pentamer8	S3.26712900-0.025417000.00897500 H3.96847100-0.01274400-1.14196500 H2.51239900-1.07565800-0.38347000 S-0.159494000.349701002.17827300 H-0.54349400-0.304196003.29237000 H-1.399355000.306785001.63537800 S0.079211002.15512300-1.18891100 H1.169904001.43780400-0.82823800 H0.030891002.79350100-0.00246500 S0.04673300-2.30321500-0.81119700 H0.16526900-3.46390300-0.13686200 H0.00543900-1.566564000.32491500 S-3.29189300-0.02726700-0.27210700 H-2.294306000.69629700-0.82909200 H-2.68219700-1.19412000-0.57110300	18.066925.645645.0632 58.260467.368370.4007 79.337985.130896.3598 102.2247126.4635130.7876 146.9404167.3178181.6895 193.6988221.4176222.8911 238.8608276.0297304.9702 311.5841374.1424411.0759 1198.07501200.21331203.5611 1205.54731213.50112648.0573 2654.78472658.19842689.2388 2697.63642712.23942739.0345 2739.25742740.36862750.9539
Pentamer9	S-0.00102500-0.725600002.27353000 H-0.00055400-1.513997001.17185800 H-0.001415000.399818001.52285700 S-0.000341002.15503600-0.65159900 H0.978644002.95417800-0.18258200 H-0.977991002.95513800-0.18144000 S-3.085209000.30172200-0.11396400 H-2.49896200-0.242583000.97461100 H-4.11980800-0.56028500-0.08712600 S3.085786000.30277200-0.11252600 H2.49606100-0.239897000.97500400 H4.11481100-0.56594600-0.08720400 S0.00134000-2.08784200-1.47539300 H0.98251600-1.16074700-1.41245600 H-0.98212200-1.16307300-1.41429000	23.951245.741455.6387 58.393667.604168.2498 71.871886.0502102.4782 109.4142126.0501145.9006 163.4403164.0929171.9306 194.2759214.6980232.1965 240.3550255.3026273.0395 326.1119383.9479425.0870 1198.62941201.82611203.4497 1205.15621211.56912647.0322 2677.29052694.59052695.0785 2698.18202709.01482729.0510 2746.15092746.58092748.0358
Pentamer10	S0.094209002.21371500-0.88611000 H1.261173001.61398800-1.20888500 H0.134316001.717737000.37154500 S3.30615600-0.04105600-0.08117100 H2.535833000.255664000.98688900 H2.77737100-1.27608400-0.19489600	24.036935.453950.2945 51.196561.623363.4336 70.246088.987092.1296 95.4578113.4025126.6733 141.3514147.9749165.4081 172.4168217.1158220.9413

	S-0.03910200-0.261913002.40737600 H-0.06325200-1.080313001.32988200 H-1.306437000.150143002.19100100 S-3.18895100-0.02758100-0.08270200 H-4.205584000.81585100-0.34812200 H-2.281254000.74875400-0.71515400 S-0.00851500-1.89969500-1.32483100 H-0.13609700-0.56857900-1.51688000 H-1.33681200-2.11268600-1.41636700	222.4050235.7441250.4651 302.5690342.5962380.0647 1194.13591196.13841201.8268 1203.67681206.70302658.8907 2679.37472693.39582698.0742 2703.39522715.52052718.3718 2734.64092743.26412746.3196
Pentamer11	S-0.38282800-1.78075000-1.08392800 H-0.32740900-0.974163000.00292600 H-0.15549000-0.75656200-1.93142000 S-0.435825001.011462001.84352200 H0.024225001.604277000.71848200 H-1.690204000.884427001.35091200 S1.637465001.72737800-1.56223800 H2.412492000.95159000-0.76815000 H2.295625002.85779500-1.24037600 S-3.883650000.07592800-0.10678700 H-4.27056500-0.847001000.79592100 H-2.99309200-0.76471100-0.67958700 S3.08757600-1.064724000.91586600 H1.99382600-0.698416001.61752700 H2.34679100-1.765923000.03080500	16.169131.411843.7515 49.609665.121474.4298 80.243883.208591.9974 99.0158113.8774129.0040 135.0573156.6239163.7037 200.7909210.3365218.2918 253.2139284.6096287.6952 304.1326377.7814423.2097 1198.89321202.71671203.6995 1204.86481207.33912649.7873 2653.05322667.75732682.8207 2689.98062707.04342719.5277 2730.01172741.25952748.1537
Pentamer12	S0.164324000.215620002.25708700 H-0.676902000.801404003.13123100 H0.110032001.248296001.37913500 S3.06269300-0.17474000-0.52919700 H2.91149900-0.110373000.80946100 H2.14459000-1.16028100-0.65235500 S-0.19920700-2.58828000-0.63851000 H0.16037900-3.712008000.01268800 H-0.34725400-1.887501000.50733300 S0.095322002.60906600-0.86338700 H1.107863001.72928400-1.04142800 H-0.850424001.70723700-1.20802500 S-3.089407000.09937600-0.39840000 H-2.84484600-1.15341200-0.83425300 H-2.25455300-0.039315000.65474200	19.477936.391848.8932 54.753461.139372.9990 77.202683.859493.6969 109.3623122.1063139.2622 156.1721161.4479178.3602 190.3106202.6191218.5689 232.2136274.7182303.6249 332.6260357.0003421.9644 1195.82491199.61351206.3919 1207.68201209.01032620.5917 2670.16932674.63502690.8494 2694.16962710.60192731.5017 2732.41362740.84062742.7955
Pentamer13	S-3.74975800-0.033235000.02209100 H-2.79149900-0.98854000-0.00414400 H-3.99853000-0.16072400-1.29645500 S-0.346591002.04601900-0.64370600 H-1.521531001.41439300-0.41042000 H-0.868352002.81366000-1.61979400 S-0.33292500-2.10752600-0.28398300 H-0.36431500-3.160265000.55669300 H0.13158800-1.269651000.67519400 S3.05579200-0.17539500-1.34902100 H1.917272000.52886000-1.53011900 H2.37770800-1.33626200-1.22982200	6.826121.971849.9252 59.059061.497871.9090 79.948887.157295.5762 96.4846116.8736119.9529 131.7577150.9706172.6718 188.9885200.1623233.1358 242.7740273.3849282.2630 317.0004359.8124421.1613 1197.61941200.43191201.6623 1205.28341209.57782637.5363 2655.02292656.38902680.4188 2703.56812717.62712734.3464

	S1.490907000.295187002.35348900 H0.933476001.472639002.00479800 H2.305383000.285069001.27214300	2740.40982741.72212748.4243
Pentamer14	S0.91291200-2.76277300-0.49876000 H0.50089100-2.070179000.58700200 H-0.19240500-2.43983200-1.20184800 S-0.175193000.116882002.24455800 H-1.40223100-0.175420001.76047100 H-0.38244100-0.566775003.38730900 S2.772106000.80776300-0.40643900 H2.21708200-0.40381900-0.64416200 H3.243193000.91757000-1.66428400 S-2.61419900-0.85650600-0.68200200 H-3.83127000-0.41606300-1.05489700 H-2.036415000.35662400-0.85896100 S-0.757032002.69027700-0.67680100 H0.465580002.10567400-0.66867300 H-0.799479002.761939000.66916400	16.223421.281649.7401 52.094960.558076.2932 81.204886.039289.8357 99.3305119.7268124.1976 134.0496155.7224156.8478 176.9249204.4266216.7169 237.8932297.9807300.2680 306.7666361.7807404.0199 1195.57581200.34211204.5652 1207.76841210.61582633.9654 2643.45252658.57652683.4527 2701.92222727.22942739.7914 2743.97412747.75982750.3431
Pentamer15	S-3.54890800-0.03045200-0.11905200 H-2.67996800-1.06453200-0.05655800 H-3.69636300-0.15282100-1.45308800 S1.291129000.164488002.36431600 H0.751613001.134486001.58606500 H2.488971000.245553001.75044900 S-0.26928100-2.35790400-0.29512400 H0.21230200-1.572368000.70081500 H-0.16412800-3.481024000.44141500 S2.78650000-0.05071700-1.33769200 H3.16556100-0.26506400-2.61241900 H2.08457200-1.20243000-1.27037700 S-0.334568002.46989400-0.45692100 H0.434888001.60339400-1.15143800 H-1.395390001.62986400-0.42330000	10.647820.158339.4940 57.532869.490570.5183 79.199782.768889.4006 94.815299.9610100.9875 122.9060145.6094156.7530 163.2980190.6624225.9027 255.2991275.1796311.8404 359.7278375.0254418.6605 1193.75871198.03631203.3609 1204.36291208.31542606.9145 2640.80982662.17512684.3892 2701.89452711.64532732.3499 2744.68042745.21792751.2436
Pentamer16	S0.415194001.31569800-1.62982600 H1.599349001.15241000-0.99545900 H-0.203118001.81170700-0.53295700 S-2.138439001.689208001.48680900 H-2.868793001.018249000.57053700 H-1.500596000.563248001.87443700 S0.41687500-1.531513001.32795800 H-0.25702100-2.547997000.75317300 H0.40371500-0.794875000.19379400 S-2.59226000-1.38594100-1.11783700 H-1.51621500-0.65794800-1.49343400 H-3.11178500-1.39186900-2.36109500 S3.908398000.061720000.08767700 H3.16908200-0.952022000.58720500 H4.12909400-0.58764800-1.07272100	14.612639.554945.8110 56.343558.214970.6940 73.917775.558687.5410 92.6831115.9643117.8669 130.4898163.5530190.0406 201.6031211.9010223.6227 231.2453261.3310269.1764 333.2446337.2786408.6142 1198.04261200.50121201.4712 1203.06551217.01852658.9100 2678.32492679.35512690.5959 2698.95452702.84792714.6689 2743.18622745.34032750.2348
Pentamer17	S1.828692002.06001300-1.10531700 H2.508522001.01080800-0.58402000	12.710032.370139.6361 47.121163.984473.6668

	H2.267134002.90909600-0.15505300 S-0.366467000.470017001.98128100 H0.138346001.240998000.99072100 H-0.43120300-0.603633001.16365700 S2.98705000-1.364798000.64784500 H2.28506500-0.787314001.64639300 H1.85943700-1.754571000.01425900 S-0.52739900-1.40102600-1.61642800 H-1.77165300-1.08378400-1.18692500 H-0.17737300-0.10329400-1.73417000 S-3.887211000.19770400-0.01932500 H-4.29892200-0.806954000.77921700 H-2.934016000.588095000.85703100	76.477986.625891.2218 97.4393108.6487120.2815 122.6600143.0390161.9129 200.2670205.3587223.0934 252.4535266.2270282.7810 311.2757379.8341407.1425 1197.09501200.67971202.5009 1203.11041204.83592658.9294 2664.89352670.89512679.8169 2699.09532706.53942720.2142 2727.87942746.21352746.7215
Pentamer18	S-0.31549900-2.474669000.47307500 H0.47922900-1.586281001.11072100 H-1.37273300-1.630258000.43782900 S-0.291495002.390275000.23384000 H-0.308644003.49022700-0.54387700 H0.170667001.59919800-0.76496600 S-3.537302000.010562000.11868900 H-3.710861000.114798001.45109300 H-2.657836001.037610000.08756000 S1.42677800-0.21267700-2.24879500 H0.77802500-1.15485900-1.52086000 H0.65289800-0.40335900-3.33473600 S2.752224000.115895001.52197000 H3.28544000-0.008796000.28987200 H2.128504001.271533001.20689100	13.665422.700436.2451 58.652871.009676.1643 85.230686.240692.5643 100.9088118.9241132.4962 141.2639146.4103158.0627 176.5822193.6725214.8831 283.5612287.8095321.5180 346.4765389.9400420.5817 1195.55951201.13451203.3843 1206.22451207.62292622.1370 2634.78192662.74492680.2761 2695.91872706.98492740.9884 2743.67562743.97242747.7628
Pentamer19	S-0.422836002.10186900-1.24078900 H-1.689452001.72816800-0.95214900 H-0.057637000.82080500-1.46589900 S-3.31587200-0.388987000.04403000 H-4.243743000.182868000.83676400 H-2.38660100-0.405800001.02376700 S0.160160000.165232002.16351200 H0.209265001.120158003.11314900 H-0.014305001.062129001.16251500 S0.11303800-1.98157100-0.91997200 H1.36482100-1.46683100-0.93248200 H0.02721200-2.00081700-2.26482500 S3.470362000.08797200-0.15798000 H2.635189000.205631000.89925000 H4.07761100-0.998563000.35910700	13.138319.482842.8197 58.588768.230774.3275 77.162587.997698.4847 110.1601116.6271120.0803 129.3790146.9419158.3547 162.4259183.8953190.5985 242.6874255.6244300.4750 306.0089365.5300419.9361 1195.88221198.30401199.9817 1202.77441206.87242641.1082 2661.79212690.91452696.8160 2715.44992716.72902745.2712 2745.37372746.27362747.8727
Pentamer20	S-0.00552500-2.2222400-0.76732700 H1.26316800-1.76432300-0.64648200 H0.24590200-3.31832900-0.02458700 S-0.007377000.500334002.21197800 H0.03819300-0.492314001.29282600 H-0.00781600-0.359410003.24956800 S-0.019222002.00368600-1.33896100 H-0.206676002.71448700-0.20914200	18.860635.954738.3680 50.259063.644276.6381 79.348990.732694.0288 116.8626127.1536142.5951 154.3575160.3632176.9965 198.6274206.0400213.8371 232.0001262.4240304.9741 311.9132382.8892401.2004

	H-1.114922001.23940600-1.11718000 S3.26113700-0.05512300-0.03793800 H2.210205000.73516400-0.35623600 H3.74522000-0.02804800-1.29590400 S-3.20658400-0.19533900-0.19026300 H-2.48462200-0.037424000.94063900 H-4.047517000.809435000.12667800	1198.46231200.95321202.7730 1207.47541209.16192652.7275 2656.10802668.54962679.0255 2698.51522739.32202739.8795 2742.42502742.81732743.2283
Pentamer21	S0.264789002.400125000.32635100 H-0.111169001.63434500-0.72616200 H0.338277003.52048400-0.41833600 S-1.25296900-0.21250500-2.27588000 H-0.64572700-1.14558700-1.50160000 H-0.46185400-0.45879000-3.33778600 S-2.857271000.097390001.35654100 H-2.216214001.260491001.11138800 H-3.29568000-0.005538000.08563000 S3.518984000.028955000.27066500 H2.636998001.054192000.28594400 H3.40264600-0.13221100-1.06237100 S0.29910000-2.470452000.55838100 H1.35139800-1.625047000.65558700 H-0.56080500-1.598546001.13078300	11.405820.447540.6041 57.463768.275973.1160 83.880584.997487.2688 94.7552116.6518126.7031 129.1816145.9971155.2262 174.9474194.2169211.9523 274.7688284.4963322.4254 339.1209376.2701402.9978 1194.18091200.30791202.2431 1204.93891206.18712627.2912 2653.93522672.09162680.2433 2688.86482714.56122740.5263 2743.09242743.95692744.2839
Pentamer22	S0.20238800-0.71927300-2.15427700 H0.61210800-0.15053800-3.30514100 H1.38917700-0.50760900-1.53562800 S-0.11408500-1.821358001.53965500 H-0.13452500-2.690617000.50952700 H-1.26527500-1.227277001.14517700 S-0.061904002.265508000.60671800 H-0.065483001.39417000-0.42867700 H-0.224506003.33241500-0.20073600 S-3.347072000.05874100-0.00589000 H-2.682453001.132916000.47281900 H-2.52440600-0.03605000-1.07125600 S3.310711000.092915000.20851600 H2.36265200-0.553291000.92272500 H2.692111001.281334000.37563700	12.199419.091541.0182 57.717462.593178.7776 81.226284.027993.0028 103.7667109.3719115.6844 122.3711145.5438158.4330 170.3403197.7591207.3313 247.9209281.7329298.3228 321.1992370.2154414.5076 1194.53741199.80421203.2547 1206.24321207.51072618.4983 2639.69912672.88102674.5371 2713.31972717.96662743.7784 2744.40982746.22442754.0371
Pentamer23	S-3.07397800-0.06315400-0.17217200 H-4.379775000.24267600-0.03953900 H-3.19858300-1.224563000.49886600 S0.067296001.79927000-1.58419500 H1.032788002.73990900-1.59429100 H0.030420001.74857300-0.23168500 S-0.018206000.749296002.27854100 H-0.03450200-0.410895001.58495700 H-1.324407000.972224002.02202300 S3.20713000-0.196576000.07546000 H2.260883000.41633100-0.67211900 H3.79454000-0.75177200-1.00316700 S-0.12864700-2.31584700-0.53487800 H-0.17303300-1.28975600-1.40981200	16.791831.199544.9456 49.097758.467363.5072 74.981979.589193.0756 96.3176106.8642120.0276 135.4487138.8740159.3566 172.2573182.0703204.4950 223.8329255.8509308.1318 309.5951330.0564389.4819 1196.18471199.28351200.1096 1201.77251206.53202661.2651 2677.13782681.75872703.3353 2723.48772728.05442735.5988 2740.24132750.21972754.1304

H1.13414700-2.01055000-0.15931800

Table S6: Geometry and frequencies of (H₂O)_n n = 2-5 clusters optimized at ωB97X-D/aug-cc-pVDZ level of theory

Species	Geometry	Frequency
Monomer	O0.000000000.000000000.11722200 H0.000000000.76092200-0.46888900 H0.000000000-0.76092200-0.46888900	1630.17733883.81723995.5824
Dimer	H-0.547504000.002069000.04949900 O-1.50123800-0.00097300-0.12120100 H-1.908952000.006091000.74729500 O1.381932000.001014000.11461300 H1.70261900-0.76737700-0.36570400 H1.708291000.75889400-0.37839300	137.0066160.6412163.9911 196.4262377.3560649.4118 1627.88971651.02263757.4963 3872.97853962.47193980.8344
Tr1	O-0.159901001.594146000.11320000 H-0.095313002.19944000-0.62891100 H0.634059001.030421000.06266100 O-1.30833400-0.93346400-0.09739700 H-1.209520000.03383800-0.02270000 H-1.90694100-1.190407000.60701500 O1.46905500-0.65318700-0.08782600 H0.59224000-1.07757500-0.06020600 H1.97891800-1.055684000.61833000	174.6122184.5086193.6477 202.0201225.3307248.9552 354.2906364.8615459.6474 598.1812677.0467901.3304 1638.59891642.4953662.4231 3604.16683667.42033678.2363 3950.52143954.14003955.7648
Tr2	O0.29501000-1.58136100-0.07192100 H-0.54950600-1.09777100-0.02598600 H0.24684900-2.262583000.60157000 O1.222304001.04591000-0.07164900 H1.229914000.07271900-0.02741200 H1.836619001.346202000.60090100 O-1.517537000.53543700-0.07221500 H-2.084016000.913952000.60291500 H-0.678076001.02759200-0.02571200	140.9210144.9132192.5947 193.7559198.5356231.4871 366.1267366.4869522.6090 563.9170564.6172857.0893 1643.16431643.40131673.5572 3624.85123684.27843684.9187 3959.08123959.62533961.1910
Tr3	O-2.71321000-0.34880900-0.00001800 H-2.77037600-1.306670000.00003600 H-1.76697900-0.14951400-0.00000800 O2.71320800-0.348809000.00001700 H2.77037900-1.30667000-0.00004300 H1.76697600-0.149519000.00000800 O0.000002000.732287000.00000200 H-0.000003001.31750600-0.76389600 H0.000002001.317508000.76389900	21.520874.267382.5027 139.2119161.4080161.4592 172.6623202.9079318.8657 461.8268593.7136628.6118 1633.80321636.51231647.1605 3781.39733793.86373864.5622 3961.96583964.93053965.7135
Tr4	O2.62495600-0.45243300-0.00154800 H3.01167000-0.00276000-0.75823100 H3.02087700-0.029946000.76591600	34.846452.579564.9540 123.4917138.4643140.1011 141.9575190.4559288.4722

	O0.000154000.847053000.00000100 H0.770537000.263457000.00308500 H-0.770790000.26420200-0.00365600 O-2.62490600-0.452270000.00152600 H-3.02235000-0.03051700-0.76554900 H-3.01157400-0.003237000.75860800	511.6201623.3244637.2647 1630.07831630.77141653.3077 3766.32983850.52693872.5858 3875.90513980.09623980.3049
Te1	O-0.13156900-1.923167000.01257500 H0.68808600-1.38312800-0.01471400 H-0.04241200-2.490200000.78147000 O1.92316700-0.13157000-0.01257000 H2.49021100-0.04241900-0.78145900 H1.38312800.688086000.01470500 O-1.923168000.13156900-0.01255200 H-2.490223000.04241000-0.78143000 H-1.38312800-0.688086000.01472600 O0.131570001.923167000.01254700 H0.042419002.490219000.78142900 H-0.688087001.38312900-0.01472400	51.099181.9191214.3386 218.8856248.4110248.4705 261.1544261.1962268.3337 299.9716406.1426445.9224 459.7831459.8118760.2082 836.4244836.46411011.2645 1642.28111655.85331655.8863 1685.16093422.36373520.2472 3520.26313559.38783949.2938 3950.07163950.13683951.3631
Te2	O1.515000001.196906000.09698000 H1.524199000.216647000.04120100 H2.096123001.49997800-0.60360700 O-1.205103001.506162000.09415700 H-0.224855001.547616000.07964600 H-1.501461002.07310500-0.62086600 O1.20516900-1.50628300-0.09269100 H1.50081000-2.072259000.62339400 H0.22490900-1.54765900-0.07905900 O-1.51488800-1.19681400-0.09844300 H-2.09702300-1.500586000.60099600 H-1.52412700-0.21660900-0.04172500	31.649077.2692202.8300 214.2995217.2521249.3120 258.0015264.0591268.3008 279.6936390.2483414.7163 498.8739549.7425671.4286 767.6958845.8128975.3690 1651.66731656.49111674.8733 1686.32133429.90873519.1246 3531.07043562.19863950.3781 3951.29553952.25353953.2411
Te3	O-0.00000100-1.32058900-0.91072200 H-0.76512000-1.33421600-0.31592200 H0.76511900-1.33421700-0.31592200 O0.000000001.36651200-0.62908800 H0.000000001.98630100-1.36113900 H0.000000000.46249500-1.01911300 O2.04986900-0.097470000.70035300 H1.531958000.678057000.43453900 H2.259667000.027829001.62791800 O-2.04986900-0.097469000.70035400 H-1.531958000.678058000.43453900 H-2.259662000.027828001.62792000	45.149249.7960134.8571 148.3002150.9707168.7076 189.8638254.2335257.7104 325.4560368.6705393.7940 420.9259552.8231555.1696 609.4329785.7577968.3188 1627.07241633.62211654.6912 1667.53373450.89083731.6212 3742.92593756.94943822.8442 3952.64963962.09463964.2790
Te4	O1.644250001.40758000-0.31791800 H2.124656001.961477000.30135300 H0.818319001.152883000.14357500 O-0.403732000.036830000.88034100 H0.12988000-0.736786000.63771200	25.778243.575475.6015 147.9514174.7515190.0989 194.3088209.2379221.3250 260.8472266.5464374.5218 408.2527525.8890587.0598

	H-1.25853800-0.077052000.43793900 O1.86260100-1.38083600-0.12374200 H1.93123600-1.83955700-0.96367500 H2.04703900-0.44425200-0.32201800 O-2.97558600-0.13090400-0.37818500 H-3.125115000.60015400-0.98388700 H-3.68774100-0.078227000.26503100	654.6894748.4464953.0513 1626.09281645.39651651.3386 1667.70063541.65953650.9258 3711.03273785.13003874.8507 3948.73663955.79263983.5355
Te5	O2.250043000.00000000-0.00000100 H2.829468000.00000000-0.76628600 H2.82947000-0.000001000.76628200 O-2.250043000.000000000.00000000 H-2.829474000.00000100-0.76628100 H-2.82946400-0.000001000.76628800 O0.000000001.945997000.00000100 H0.762567001.354731000.00000100 H-0.762567001.35473100-0.00000100 O0.00000000-1.945997000.00000000 H0.76256700-1.35473100-0.00000100 H-0.76256700-1.35473100-0.00000200	41.466563.6846113.7502 123.8539126.1474130.6095 147.4069154.8533157.5160 158.3198168.8234271.1022 417.7207428.6107536.6862 549.4735556.5337610.0009 1626.00701627.34861644.7327 1692.99023794.86273804.8757 3869.78743873.37503879.6307 3901.28713988.70463988.8683
P1	O0.078708002.29570300-0.06042100 H0.872543001.726582000.05207100 H0.255507002.82458600-0.84123900 O-2.167176000.77674400-0.07625800 H-1.370134001.35272600-0.08223500 H-2.779073001.190916000.53506600 O1.29557700-1.89085400-0.15350200 H0.31627500-1.90168100-0.06584300 H1.48341600-2.34103900-0.97967500 O2.211847000.639213000.16400300 H2.733352000.634736000.96911100 H1.91840400-0.290347000.03426400 O-1.40597900-1.829457000.06334800 H-1.73966600-0.905639000.03341300 H-1.79444100-2.221629000.84771300	25.060443.082766.5852 69.6623194.9644200.5005 205.8610235.6674256.6450 258.5014271.4161304.5632 319.3159323.8761419.1494 434.8939461.8977475.1986 531.5038729.7247799.0854 876.1888892.9465996.7576 1644.67181655.47011666.3149 1685.22591694.18593394.1532 3480.09513486.04403535.3421 3538.62243949.09583950.4404 3952.97283954.13313959.1117
P2	O-0.133211000.196633001.66484000 H-0.338227000.299634002.59577200 H-0.994350000.137128001.18333700 O-2.170179000.08591500-0.05019700 H-2.80714300-0.62820500-0.11914400 H-1.53736300-0.04190600-0.79914200 O1.15031700-1.848712000.18831700 H0.81698700-1.230150000.86083000 H2.10461500-1.742176000.19794700 O1.279212001.72606500-0.22150100 H0.834343001.363477000.56452600 H1.086715002.66616900-0.21848600 O-0.11540900-0.21677200-1.76412800	29.769352.009793.7123 169.5415176.3392206.7754 218.4996228.7227253.3754 268.4300275.5559278.7734 293.3746351.3349399.3899 431.4412494.8060514.8182 650.1841667.1242728.1865 789.4058910.1296963.1921 1645.17511645.78191667.2039 1691.43371704.43263325.5749 3422.13483654.32163678.2725 3706.77323735.53463946.0079 3949.80663952.54503955.8517

	H0.397196000.56655300-1.50143600 H0.35138000-0.93556400-1.30286000	
P3	O1.537483001.54384300-0.35500000 H1.531437001.80268100-1.27936100 H1.851949000.61157800-0.35024500 O-2.27273400-0.27056800-0.98560300 H-1.983522000.44811300-0.39697400 H-3.23067800-0.28220700-0.93508400 O2.05811400-1.11080000-0.30639600 H2.73115400-1.540419000.22500000 H1.19324500-1.409149000.05630800 O-0.850231001.286461000.86093800 H0.008997001.482354000.41741000 H-1.007697002.006094001.47452900 O-0.40948500-1.561810000.73497800 H-1.07456800-1.513127000.02945800 H-0.52549800-0.702921001.16762600	37.901450.531276.5487 116.4297167.3310175.7816 214.6178228.9195256.0905 262.7004280.9655287.6603 313.2150356.1392407.4375 433.9718463.1110502.8944 556.2456657.2088737.4034 828.8108884.43351001.8086 1644.64831652.55831658.2166 1682.49801707.40663378.9957 3458.34363512.18603678.5704 3745.84073804.66233943.5137 3954.04253956.23123957.8862
P4	O2.43404100-0.222383000.84748200 H1.976938000.521397000.41722800 H2.36066500-0.062347001.79065300 O0.776254001.39284900-0.73244300 H0.941274002.13780900-1.31302900 H-0.123117001.52539000-0.35451300 O0.50999400-1.49739900-0.80675600 H1.20969400-1.44706900-0.13486200 H0.56173300-0.61526300-1.20234100 O-1.92787000-1.251552000.34823100 H-2.57893100-1.76313300-0.13613300 H-1.05674000-1.46930600-0.05710000 O-1.724703001.442377000.28185300 H-1.907909001.781710001.16037100 H-1.925322000.479667000.32279300	41.783546.778475.3128 107.9067172.6891191.3185 215.5409237.3896257.1920 269.5835282.4514294.9004 303.7239373.9610382.2767 430.6901452.8662492.9810 540.9565666.6385770.2076 845.0138869.6865985.9594 1631.55231648.56471663.1611 1682.30931716.21693392.4069 3465.92203507.32173672.0570 3739.85433813.33453951.1269 3953.62453955.52503958.9248
P5	O1.65566700-0.44138500-1.24792800 H1.89832700-0.14287000-0.35456900 H2.47211600-0.70670100-1.67608400 O1.278496000.462407001.33866100 H1.673561000.952285002.06160600 H0.666099001.078617000.86715200 O-2.39144100-0.06000000-0.24160900 H-1.78306400-0.776357000.03974400 H-3.15533100-0.110198000.33579400 O-0.33304100-1.740534000.42960800 H0.14806300-1.192574001.06763500 H0.21714700-1.65672200-0.36304400 O-0.340560001.76161200-0.34451800 H0.091810001.43645100-1.14235200 H-1.181697001.26126600-0.30958900	37.037762.757972.8095 112.8019165.8803192.1392 203.9083223.7137230.2049 247.3802272.3562285.8669 359.3945377.9749397.8451 441.1348488.6785508.8109 577.6909631.6278698.8181 745.7680877.82981003.7947 1631.07421651.98381659.4064 1685.65401698.88363367.9101 3505.01403582.96163686.1864 3763.23483820.22943882.5257 3957.68993958.45293959.8273

P6	O1.784417001.31817300-0.35949800 H1.873935000.33880500-0.40540500 H2.547493001.618966000.13840300 O-0.733079001.543520000.59572000 H-0.933933002.432874000.89241300 H0.192555001.569457000.25892500 O-0.62080200-1.403694001.00937200 H-1.26998100-1.281788000.29374600 H-0.60680600-0.526126001.41229800 O-2.17232400-0.22275100-1.00082400 H-3.12413200-0.10259200-0.99893900 H-1.801126000.56694500-0.56498100 O1.79725400-1.38484700-0.26434600 H1.73725900-1.90136100-1.07084600 H0.94101000-1.518391000.20100200	33.459840.835553.6752 75.4539193.3163196.3674 211.6710223.2656250.3946 259.5037273.1333287.9226 293.9433355.3913404.2971 421.2744456.8647560.9672 610.1955673.8956706.8735 811.9255840.6182953.4711 1652.02601657.16241678.3778 1694.42451704.91913394.0417 3470.20443508.47453631.9859 3694.09943856.57933948.7254 3949.92923954.71553956.4902
P7	O-2.26659000-0.132417000.95703800 H-1.95906600-0.135653001.86651100 H-1.804750000.612171000.53121300 O1.799761001.307754000.37099700 H2.587000001.63510700-0.06843400 H1.899133000.330221000.40346900 O-0.67159100-1.41195400-0.97899800 H-0.65153400-0.53126100-1.37679200 H-1.32539500-1.28926600-0.26754200 O-0.691383001.51028600-0.67316100 H-0.899804002.37600500-1.02871600 H0.227425001.56273700-0.32600200 O1.67769400-1.396116000.36907300 H0.84806700-1.52297400-0.14680600 H2.29579900-2.057513000.05350700	27.251536.086967.8024 93.3883184.9098212.7276 216.6332226.7076247.7087 255.4391266.2069279.5208 289.0571363.8477377.6507 427.1456486.9083516.8460 554.7837685.4340754.5317 810.9146823.5589952.7440 1642.36991660.53481664.3068 1685.28231715.03533405.5114 3473.21863520.60573650.3011 3696.69303842.70723947.3333 3952.50633956.85983958.8397
P8	O-2.28178500-0.037729000.04431200 H-2.74116200-0.044037000.88696700 H-1.696094000.747892000.06733500 O1.510740000.32316000-1.28078500 H0.95967900-0.47332300-1.34478400 H1.995703000.15834500-0.45729800 O-0.289114001.823173000.07495800 H0.368774001.41032400-0.53347400 H-0.333339002.75172100-0.16136600 O-0.23388600-1.75926700-0.39583300 H-1.07903900-1.27833600-0.25968600 H-0.46307000-2.65892000-0.63553200 O1.44688000-0.353016001.52579600 H0.886553000.428651001.59096000 H0.87931600-1.012880001.09929100	25.776646.844580.6774 119.2477148.8218215.1968 230.5999235.6191252.9245 265.2185276.5031281.4036 347.9985374.0326403.7575 413.6937460.3890514.4900 558.5788618.7604747.0135 816.3832863.2365962.9639 1638.41181655.49121669.4344 1682.97551702.09453397.4531 3489.12793558.93093742.0760 3751.17273801.00233889.3453 3946.78033951.95323958.0284
P9	O-2.61281900-0.155237000.60652600 H-2.80156600-0.312374001.53399800	19.698935.467339.5630 56.453878.9797166.2324

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P10	O0.00085200-0.06544100-0.01654300 H0.609634000.503575000.48810400 H-0.619935000.52088300-0.48580900 O-2.44909800-1.049008000.87947200 H-1.48810100-0.901366000.80671300 H-2.65558400-0.970016001.81331600 O2.358265000.944615001.05981700 H2.706409000.333997000.38402400 H2.767784001.793510000.87949400 O-2.366194001.08661600-0.90649800 H-2.763211000.92552700-1.76519400 H-2.710748000.38829600-0.31972700 O2.45701200-0.90820400-1.01709500 H2.65264500-1.84121400-0.90679200 H1.49440400-0.82182400-0.88734500	30.096632.028651.5855 120.7538172.3757193.6265 198.5282205.3356209.0021 218.3504246.1852267.8218 277.5575353.9903362.8443 392.1980417.6094566.1053 612.1177650.8167656.2706 736.7245918.2735938.9996 1638.37221642.40081642.5231 1651.75871664.06303580.3759 3611.60143657.11703659.2408 3681.57643703.76663951.4313 3952.79683953.41103953.8751
P11	O1.676397001.963876001.06345700 H2.625466001.838694000.99733400 H1.280040001.089629000.89319800 O0.000000002.55748100-1.07637700 H0.661660002.65651400-0.36707500 H-0.654467003.24173100-0.92097400 O0.000000000.000000000.01557800 H0.22106000-0.75282100-0.56143300 H-0.221060000.75282100-0.56143300 O-1.67639700-1.963876001.06345700 H-1.28004000-1.089629000.89319800 H-2.62546600-1.838694000.99733400 O0.00000000-2.55748100-1.07637700 H-0.66166000-2.65651400-0.36707500 H0.65446700-3.24173100-0.92097400	29.855035.478552.0884 121.3352168.0086184.6148 187.2451202.4534207.0242 215.4835235.0732249.7204 275.9573357.5242363.3673 388.4493416.8815556.2752 598.7464639.0072695.2407 723.3716919.3317925.6893 1634.35421641.26291641.8906 1654.56211663.16913587.2958 3615.74323660.22233661.3033 3686.17113710.81553952.8041 3952.99603953.28513954.6283
P12	O-1.752232001.46389400-0.56365300 H-2.110493000.58763000-0.31658300 H-2.483988002.08039800-0.50417000 O0.45197400-1.44243800-0.10536300	26.882038.532861.9402 88.6143130.3157152.0477 171.9788194.4346214.6337 225.6807238.5970261.5665

	H0.50219000-1.31384300-1.05761500 H0.47542000-0.528522000.27174200 O-2.32224300-1.160525000.13351900 H-1.39327700-1.462554000.11486700 H-2.64062700-1.372700001.01379200 O0.574065001.081237000.83563700 H1.400944001.331298000.40554700 H-0.158578001.490897000.33870600 O3.037373000.05638500-0.32532600 H2.56324100-0.74361700-0.06326200 H3.93367100-0.05741000-0.00154200	287.4466348.4199374.6951 439.1676451.6574505.5790 572.6226592.3016709.9776 744.5990789.35231082.0913 1611.00691631.71611655.2916 1667.64061680.65793351.4136 3560.80573617.45743642.3836 3808.52433867.68923910.5711 3947.70093961.76583964.6594
P13	O0.22117300-1.79994100-0.04747800 H1.04993100-1.31399800-0.14820000 H-0.36377600-1.42633800-0.72236500 O2.567685000.00001900-0.09325100 H3.018621000.000064000.75579400 H3.26352900-0.00007800-0.75589300 O-1.754248000.00003700-1.19783100 H-2.594345000.00003600-1.66019500 H-1.95540100-0.00000100-0.23683100 O-1.43114500-0.000056001.50714900 H-0.85077100-0.759442001.33433900 H-0.850773000.759346001.33440400 O0.221148001.79993800-0.04740400 H1.049921001.31404700-0.14824400 H-0.363844001.42638800-0.72228300	41.545583.1816114.1594 126.3543160.1592162.2601 170.3975193.1086199.2227 199.2565220.1519255.3351 263.9772401.1011417.2479 443.9117477.8299522.8927 557.2055585.4324603.9518 653.0985839.8141951.8575 1630.29431643.10941655.6525 1683.64071696.25543507.4566 3714.29533744.57363774.0008 3783.98353840.87033859.0528 3877.39763955.64393978.1069
P14	O0.32179300-0.78494000-1.25609700 H-0.054198000.07329900-1.49379700 H1.27486700-0.62075200-1.16748800 O-1.125434001.59729100-0.44740800 H-1.276938002.54402800-0.47153500 H-0.594527001.415432000.34717300 O-2.35378900-0.991374000.28060800 H-2.27980000-0.08163300-0.03776400 H-1.82397400-1.49218900-0.34807000 O2.744927000.03972700-0.02783800 H2.204109000.089907000.77499300 H3.54667800-0.423689000.22334900 O0.310460000.047961001.39433200 H-0.32263200-0.290237002.03410200 H0.14277000-0.483490000.59025600	26.733046.158779.8826 123.1934152.3967156.6827 166.6144180.6440189.2251 203.8608219.8076269.4489 303.2909348.2086355.8470 387.9350409.3679443.8067 484.6436518.1608551.5440 730.5133763.8435923.3029 1633.62121636.01391648.3395 1660.99151678.56143575.1583 3683.72083722.00843762.3689 3801.98743842.48403918.5939 3923.24303960.28243962.9292
P15	O-1.35406400-2.02767900-0.53511900 H-1.85589700-2.14355900-1.34426800 H-0.59250000-1.47014600-0.77034700 O0.57808400-0.00104700-0.40798100 H0.17820300-0.000784000.48463800 H1.54086400-0.00160200-0.28829900	24.028044.920051.3158 59.5808108.5229125.6761 141.7519165.4300195.4035 197.7286212.7437233.6462 239.4948267.7705341.7634 394.9498398.7573525.7138

	O-1.357737000.001552001.54405100 H-1.70252300-0.762045001.05675100 H-1.699779000.765523001.05528700 O-1.351038002.02921700-0.53687800 H-1.859252002.13293800-1.34372500 H-0.590450001.46968600-0.77059900 O3.38003700-0.001163000.04480900 H3.70932400-0.763129000.52910600 H3.709751000.766081000.52040600	545.5480590.8904602.2145 784.9121839.6006931.3869 1623.26541637.64151641.8391 1665.50221671.71973559.2904 3674.93363702.66813731.6110 3750.45553817.13653874.0613 3960.41953962.53423982.2641
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