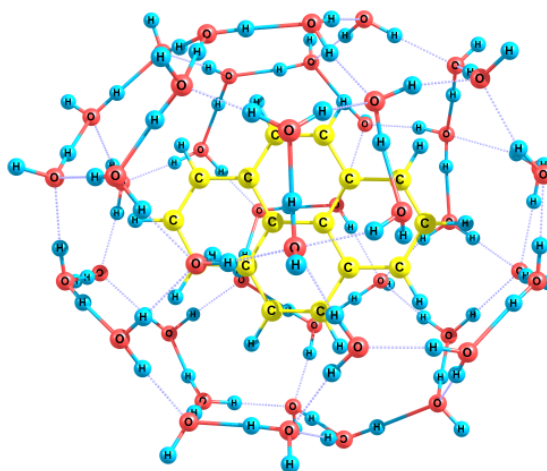


Supplementary material

Ab Initio Simulation of Pyrene Spectra in Water Matrices



The Cartesian coordinates (in Å) of S_0 state of pyrene in water matrix

C	-0.215217104	-2.462430714	-0.146021426
C	-1.150820105	-1.379257257	-0.127795273
C	1.118829634	-2.243081990	-0.057978494
C	-0.660113729	-0.056874846	0.023925020
C	1.643658879	-0.913899517	0.059692434
C	0.734656181	0.178359559	0.116784241
H	-0.591561893	-3.474993666	-0.230800539
C	-2.527393922	-1.576504959	-0.272639559
C	-1.560286327	1.039009307	0.056401383
C	1.222807885	1.503670947	0.256948538
C	-2.923872031	0.795686355	-0.097287102
C	-3.399344230	-0.495374708	-0.260288007
H	-2.909151024	-2.575332411	-0.434197975
C	-1.040377861	2.361674702	0.197240674
H	-3.610340682	1.630567008	-0.096996215
H	-4.454177374	-0.651290761	-0.436012519
C	3.020102819	-0.653480823	0.113441354
C	2.600960912	1.714032696	0.332843977
C	3.483052003	0.649439752	0.243793002
H	1.821168611	-3.069091825	-0.036906873
C	0.290099014	2.585608558	0.294742739
H	-1.732945668	3.194391755	0.198254895
H	2.967484263	2.722414031	0.473793273
H	4.548626867	0.821089041	0.276272574
H	0.673955059	3.591890545	0.386859174
H	3.720942874	-1.475909567	0.040430273
O	5.972739148	2.118527104	-1.771048181
H	5.738111652	2.774334433	-1.079171132
H	6.729334907	2.479750698	-2.237174843
O	3.977405383	1.732755003	-3.708818875
H	3.531801968	0.883953995	-3.529573124
H	4.627846845	1.855028386	-2.997678328
O	2.110495454	3.492044372	-4.044188299
H	2.857033181	2.840019626	-3.894199765
H	2.363496684	4.011779301	-4.809509702

O	1.569166653	5.110963374	-1.875022278
H	0.580465446	5.100149751	-1.832496141
H	1.802877271	4.523450879	-2.616558058
O	3.061732257	5.311983487	0.142359578
H	2.454912241	5.189323611	-0.675329570
H	3.229857500	6.256549416	0.177085669
O	5.313903406	3.857814433	0.223945567
H	4.484514232	4.399524405	0.160136441
H	5.984719400	4.446442943	0.576256781
O	1.486234513	4.856004256	2.496674151
H	1.985973831	4.134872323	2.953703286
H	1.984489811	5.040484557	1.684819072
O	-2.652424138	5.417329130	0.333920292
H	-2.134764067	5.233535112	1.134754623
H	-3.437257659	4.849187838	0.376173241
O	5.279626081	2.118460172	2.588534683
H	5.523178221	1.203902511	2.369628654
H	5.292369503	2.598563562	1.749886614
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H	5.868761309	-1.156303767	-1.368657389
O	2.544564712	-0.556632507	-3.107711506
H	1.728687506	-0.625664040	-3.645127600
H	2.243170509	-0.439580902	-2.199018695
O	-0.128171443	2.028527626	-4.751914032
H	-0.923478105	2.396674614	-4.322878391
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O	-2.230262095	2.614412340	-3.067672619
H	-2.253079169	1.641762481	-2.944806601
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O	6.176355625	-0.533265697	1.801798413
H	6.288125293	-0.574522880	0.812370586
H	7.053330302	-0.670330939	2.165751996
O	-1.091611804	4.929542670	2.678244496
H	-0.096335023	4.832737076	2.547303409
H	-1.183880389	5.744849792	3.176373889
O	4.800061017	-2.127295034	-2.386230899
H	4.422382229	-2.980808038	-2.117365514
H	4.054246306	-1.650091501	-2.781190518
O	2.831651892	2.888548103	3.696480976
H	2.302537836	2.101019698	3.892941220
H	3.689163190	2.568174823	3.358159426
O	-5.812586189	-2.359914670	-1.589571494
H	-5.031198494	-2.769768553	-2.016972828
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O	-0.944882779	-3.061707521	-3.336019681
H	-0.247526896	-3.635758216	-2.982211258
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O	3.563023524	-4.580247941	-1.664331549
H	3.570603094	-4.595392357	-0.653244509
H	4.163374620	-5.279855858	-1.931161641
O	4.531762519	-2.724096409	2.507178113

H	5.125278113	-1.996968365	2.250393148
H	3.776537589	-2.287865315	2.934453281
O	1.312684684	0.672791396	4.597830207
H	0.332692319	0.621882253	4.426419791
H	1.417044949	0.712930921	5.550214025
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H	-1.979462657	3.602596235	3.286025311
H	-2.657179839	3.108487727	4.591378462
O	-3.610960441	-3.724547971	-2.531142944
H	-2.762309551	-3.417140611	-2.892769870
H	-3.371105618	-4.371271947	-1.850011165
O	0.999351207	-4.975695999	-2.482209899
H	1.054922177	-5.581823906	-3.223835216
H	1.931779746	-4.784939293	-2.221679372
O	2.132373961	-1.466743713	3.204765663
H	1.944873968	-0.703133948	3.794702114
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O	-1.261086517	0.459128196	4.177566177
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H	-1.716784668	1.232032620	3.803389546
O	-6.066458314	-2.293488219	0.932695493
H	-5.955427270	-2.349219418	-0.084442521
H	-6.873945379	-2.768432939	1.142162636
O	3.543507312	-4.630216335	0.890227741
H	3.959754880	-3.939251716	1.458516949
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O	-3.887638426	-3.964332981	1.715334435
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H	-3.288735465	-3.374427473	2.203649013
O	-2.259070735	-2.162852777	3.297925898
H	-1.344842699	-2.588702368	3.223538348
H	-2.551802434	-2.389406551	4.185094969
O	0.053388127	-3.266082715	3.364857032
H	0.331618028	-4.035648656	2.835564848
H	0.810490548	-2.648956316	3.344311239
O	-0.301912188	-6.020426816	-0.241076981
H	0.100921981	-5.690211579	-1.063693228
H	-1.255113114	-5.813267264	-0.283132633
O	-2.989778951	-5.410578644	-0.301761230
H	-3.297012396	-4.878889718	0.480524881
H	-3.529254627	-6.203937374	-0.303356064
O	1.053011775	-5.410128552	1.908610710
H	0.515099499	-5.647176383	1.102656756
H	1.115450728	-6.213822854	2.428499265
O	-1.085849602	4.952142014	-1.933100666
H	-1.646582335	5.181771128	-1.169966738
H	-1.401241709	4.084611842	-2.237153999
O	-4.830765217	2.051328900	2.282728717
H	-4.118966576	2.433634665	2.826661931
H	-4.680763094	1.081128660	2.339861917
O	-4.594660842	-0.623357076	2.697940105
H	-3.707770968	-1.009523976	2.685135271
H	-5.115770952	-1.201728975	2.120054109
O	-4.977384692	3.731180152	0.259678116
H	-5.745885438	4.261744294	0.481304169

H	-4.936652840	3.029315720	0.965192776
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H	-5.633722500	3.348031861	-2.853074335
O	-2.444603829	-0.085385875	-3.262106514
H	-1.692438898	-0.412228790	-3.772718249
H	-2.497772165	-0.655199358	-2.487963186
O	-6.265795227	0.309132821	-1.967560515
H	-5.672953932	1.026869598	-2.232180396
H	-6.585735000	0.558504959	-1.083867305
O	-7.022452148	0.542786296	0.727438260
H	-6.602473739	1.089478477	1.399108359
H	-6.765011052	-0.365477784	0.937420036

The Cartesian coordinates (in Å) of L_a state of pyrene in water matrix

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C	-0.598516000	0.029562000	-0.034947000
C	1.542015999	1.237585999	-0.103218000
C	0.809904000	0.008098000	-0.125263000
H	-1.074738000	3.416667998	0.132954000
C	-2.706563999	1.239973999	0.252612000
C	-1.326179999	-1.194141999	-0.040136000
C	1.501858999	-1.231730999	-0.217026000
C	-2.736809999	-1.167904999	0.117935000
C	-3.400230998	0.037509000	0.265729000
H	-3.234858999	2.170005999	0.412507000
C	-0.624027000	-2.405275999	-0.138918000
H	-3.279416999	-2.101791999	0.148404000
H	-4.463832998	0.031495000	0.458417000
C	2.969966999	1.172934999	-0.148960000
C	2.921789999	-1.238835999	-0.287938000
C	3.624178998	-0.048102000	-0.233804000
H	1.395492999	3.380730998	-0.066747000
C	0.760642000	-2.424913999	-0.222368000
H	-1.171346999	-3.339438998	-0.126056000
H	3.432450998	-2.185290999	-0.399849000
H	4.703864998	-0.051916000	-0.260123000
H	1.283478999	-3.369787998	-0.268421000
H	3.538518998	2.093682999	-0.103569000
O	6.293094997	-1.137205000	1.666683999
H	6.171689997	-1.813131999	0.965744000
H	7.062033997	-1.408909999	2.171637999
O	4.181846998	-1.039277000	3.517330998
H	3.603708998	-0.273790000	3.339845998
H	4.854730998	-1.054133000	2.817288999
O	2.680304999	-3.095872999	3.934877998
H	3.288623998	-2.319561999	3.749523998
H	3.047846999	-3.542296998	4.700047998
O	2.398049999	-4.785983998	1.778448999
H	1.420274999	-4.924754998	1.746918999
H	2.543474999	-4.171057998	2.521319999
O	3.887100998	-4.716565998	-0.262024000
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H	4.182531998	-5.626274997	-0.344147000
O	5.903836997	-2.934892999	-0.349519000
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H	-2.643924999	-5.196811998	-0.431368000
O	5.548151997	-1.137679999	-2.656707999
H	5.644912997	-0.201025000	-2.416104999
H	5.647005997	-1.629496999	-1.831091999

O	6.331042997	1.599778999	0.788074000
H	6.367056997	0.699904000	1.145589999
H	5.692007997	2.088631999	1.351465999
O	2.412286999	1.031655000	3.055953999
H	1.617240999	0.940332000	3.619346998
H	2.092286999	0.976876000	2.147528999
O	0.245791000	-2.034843999	4.713261998
H	-0.489017000	-2.521290999	4.296222998
H	1.071918999	-2.449488999	4.397748998
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H	0.172788000	-0.494776000	4.540903998
H	0.074371000	0.820037000	5.391975998
O	6.045967997	1.595324999	-1.830765999
H	6.167171997	1.633357999	-0.842366000
H	6.888946997	1.862060999	-2.203147999
O	-0.327153000	-4.860292998	-2.725555999
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H	-0.291788000	-5.669825997	-3.240316999
O	4.490633998	2.861311999	2.388941999
H	3.982572998	3.643477998	2.116161999
H	3.825218998	2.275476999	2.780085999
O	3.219650999	-2.223076999	-3.733711998
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O	-6.072359997	1.497032999	1.618592999
H	-5.353115998	2.012633999	2.043167999
H	-6.038361997	0.575342000	1.947596999
O	-1.370514999	2.828138999	3.313942998
H	-0.758931000	3.485883998	2.947074999
H	-0.826817000	2.058281999	3.515487998
O	2.871407999	5.081763998	1.694177999
H	2.869268999	5.138668998	0.684610000
H	3.340312998	5.865909997	1.988032999
O	4.095797998	3.533226998	-2.501816999
H	4.785044998	2.891929999	-2.255586999
H	3.402726998	3.004079999	-2.929559999
O	1.388674999	-0.248914000	-4.590710998
H	0.413308000	-0.353452000	-4.418191998
H	1.496405999	-0.267303000	-5.543440997
O	-2.079305999	-3.058539999	-3.700256998
H	-1.408704999	-3.683060998	-3.329799998
H	-2.144618999	-3.272725999	-4.633420998
O	-4.100158998	3.150835999	2.563721999
H	-3.211020999	2.950246999	2.903349999
H	-3.963910998	3.851321998	1.907400999
O	0.279302000	5.013085998	2.517854999
H	0.240458000	5.568919997	3.298876999
H	1.229601999	4.986368998	2.254011999
O	1.864779999	2.005942999	-3.215589999
H	1.797921999	1.212578999	-3.791810998
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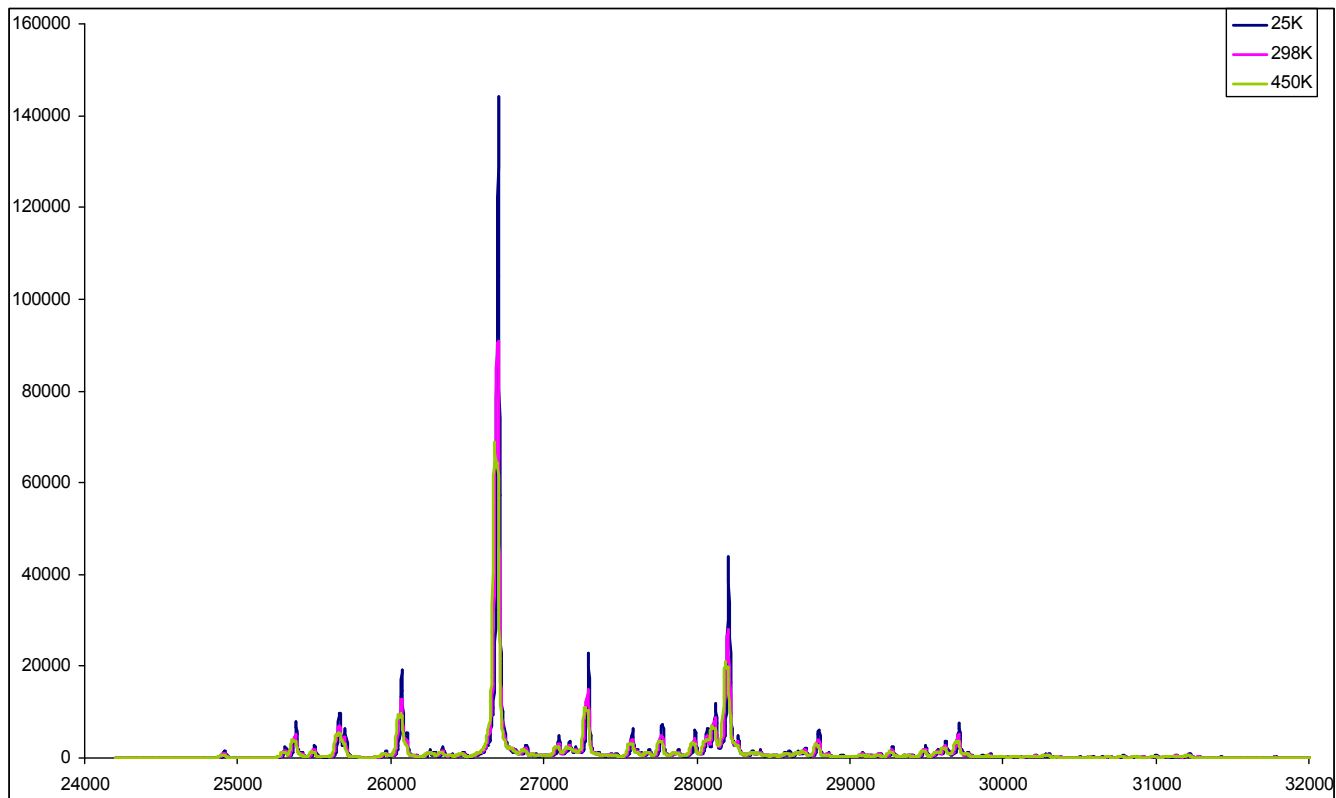
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H	-7.193832997	1.803219999	-1.101135000
O	2.835864999	5.246043998	-0.856915000
H	3.348714998	4.637367998	-1.440344999
H	1.969484999	5.394761998	-1.276016999
O	-4.443877998	3.463905998	-1.636828999
H	-5.104134998	2.791154999	-1.396697999
H	-3.759543998	2.989767999	-2.139217999
O	-2.552536999	1.983592999	-3.251837999
H	-1.718870999	2.553663999	-3.189756999
H	-2.894697999	2.165546999	-4.131590998
O	-0.460522000	3.460747998	-3.363300998
H	-0.296939000	4.243802998	-2.806480999
H	0.384206000	2.968716999	-3.364096998
O	-1.178405999	5.981890997	0.340989000
H	-0.723103000	5.663469997	1.140706999
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O	0.239111000	5.671552997	-1.830605999
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O	-0.261000000	-5.000359998	1.852950999
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H	-0.718581000	-4.219921998	2.209247999
O	-4.444719998	-2.611836999	-2.288722999
H	-3.696649998	-2.869429999	-2.856810999
H	-4.434084998	-1.628433999	-2.316248999
O	-4.599625998	0.069369000	-2.665175999
H	-3.785115998	0.590216000	-2.635414999
H	-5.210789998	0.547371000	-2.083086999
O	-4.333063998	-4.342223998	-0.310125000
H	-5.015075998	-4.973325998	-0.550692000
H	-4.394745998	-3.622737998	-0.997192000
O	-4.423123998	-3.555862998	2.353945999
H	-4.391552998	-3.875626998	1.429831999
H	-5.042903998	-4.128207998	2.810273999
O	-2.394650999	-0.282574000	3.241359999
H	-1.723013999	0.145037000	3.788025998
H	-2.504929999	0.291166000	2.475221999
O	-6.106339997	-1.216345999	1.941215999
H	-5.411809998	-1.838587999	2.199674999
H	-6.385753997	-1.498345999	1.053511000
O	-6.838012997	-1.508046999	-0.753250000
H	-6.346890997	-1.962416999	-1.445476999
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The Cartesian coordinates (in Å) of L_b state of pyrene in water matrix

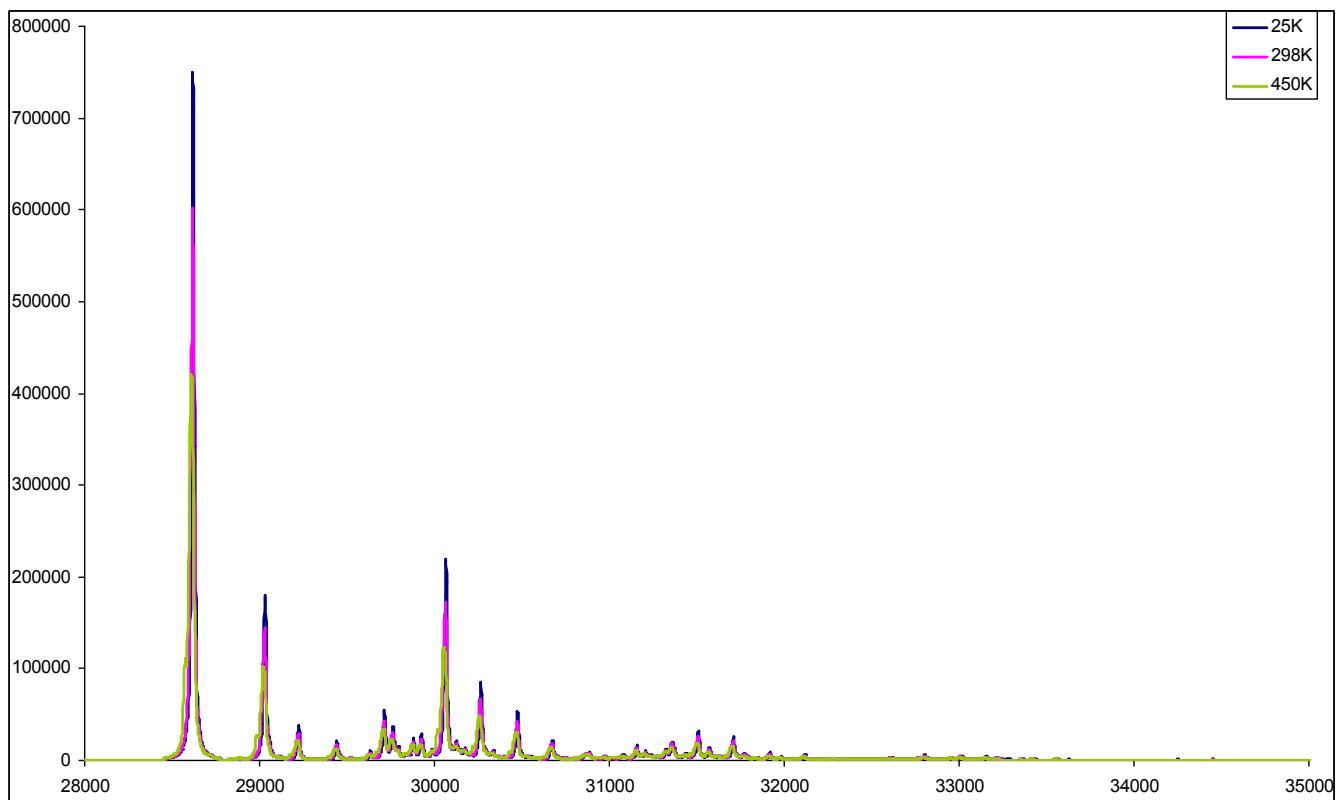
C	-0.551187000	2.495545999	0.081844000
C	-1.307031999	1.292377999	0.092131000
C	0.818075000	2.478544999	-0.008109000
C	-0.599248000	0.043914000	-0.033487000
C	1.537348999	1.253772999	-0.100625000
C	0.782740000	0.021579000	-0.127882000
H	-1.070009000	3.444138998	0.157339000
C	-2.698067999	1.274539999	0.264853000
C	-1.346929999	-1.187074999	-0.038703000
C	1.491909999	-1.229175999	-0.238632000
C	-2.731580999	-1.145717999	0.145210000
C	-3.409144998	0.068950000	0.301637000
H	-3.221782999	2.208734999	0.413591000
C	-0.633585000	-2.405582999	-0.157343000
H	-3.282650998	-2.075394999	0.183593000
H	-4.468718998	0.063533000	0.506231000
C	2.942205999	1.197661999	-0.147616000
C	2.887929999	-1.223921999	-0.307752000
C	3.612753998	-0.026649000	-0.236588000
H	1.379490999	3.406489998	-0.041321000
C	0.734537000	-2.427242999	-0.254193000
H	-1.182287999	-3.339317999	-0.145667000
H	3.402940998	-2.168172999	-0.424393000
H	4.690832998	-0.033821000	-0.256796000
H	1.256794999	-3.371950998	-0.314500000
H	3.507394998	2.120515999	-0.098104000
O	6.341275997	-1.027672000	1.674898999
H	6.208987997	-1.699031999	0.971362000
H	7.156508997	-1.264577999	2.121542999
O	4.310363998	-1.026135000	3.621502998
H	3.724660998	-0.264544000	3.453302998
H	4.974680998	-1.021992000	2.912845999
O	2.775369999	-3.082712999	3.941271998
H	3.397356998	-2.310158999	3.793406998
H	3.119225999	-3.554810998	4.702086998
O	2.497381999	-4.751415998	1.764241999
H	1.521611999	-4.908673998	1.732805999
H	2.635604999	-4.138882998	2.509988999
O	3.970647998	-4.641293998	-0.280793000
H	3.370733998	-4.653269998	0.548572000
H	4.288952998	-5.543140997	-0.363635000
O	5.942170997	-2.812957999	-0.354987000
H	5.224746998	-3.494574998	-0.293122000
H	6.694419997	-3.258808999	-0.749822000
O	2.269209999	-4.354987998	-2.578695999
H	2.634789999	-3.552489998	-3.028827999
H	2.811687999	-4.478246998	-1.784197999
O	-1.668450999	-5.685700997	-0.403950000
H	-1.203563999	-5.386443998	-1.202670999
H	-2.541815999	-5.264024998	-0.419607000
O	5.545917997	-1.049254000	-2.677345999
H	5.618788997	-0.111032000	-2.434701999
H	5.647798997	-1.537092999	-1.849504999

O	6.284353997	1.704766999	0.773546000
H	6.329023997	0.808985000	1.140641999
H	5.645883997	2.196506999	1.334310999
O	2.508378999	0.994130000	3.051403999
H	1.675888999	0.914181000	3.561018998
H	2.257868999	0.858829000	2.129494999
O	0.326596000	-2.026535999	4.687358998
H	-0.399674000	-2.538652999	4.286221998
H	1.159696999	-2.435679999	4.383742998
O	-1.692124999	-2.985247999	3.063187999
H	-1.889941999	-2.030070999	2.960227999
H	-2.577241999	-3.382539998	3.067769999
O	0.117888000	0.510177000	4.351007998
H	0.217820000	-0.495144000	4.459346998
H	0.047764000	0.853654000	5.245303998
O	5.990434997	1.692936999	-1.843787999
H	6.113791997	1.728452999	-0.855570000
H	6.828409997	1.973949999	-2.216987999
O	-0.251639000	-4.870354998	-2.741522999
H	0.714446000	-4.605002998	-2.615568999
H	-0.206074000	-5.680198997	-3.254954999
O	4.427641998	2.960316999	2.362286999
H	3.896495998	3.730078998	2.100410999
H	3.786711998	2.351149999	2.760287999
O	3.246073999	-2.185836999	-3.770451998
H	2.589999999	-1.492242999	-3.934680998
H	4.044153998	-1.736583999	-3.431923998
O	-6.127329997	1.409283999	1.668848999
H	-5.411493998	1.938741999	2.079948999
H	-6.061106997	0.488842000	1.996335999
O	-1.396928999	2.870975999	3.299970998
H	-0.814584000	3.573122998	2.969475999
H	-0.836844000	2.090264999	3.369171998
O	2.768250999	5.168355998	1.686471999
H	2.764624999	5.218683998	0.677010000
H	3.248082999	5.947764997	1.975327999
O	3.998239998	3.586325998	-2.495248999
H	4.708724998	2.964644999	-2.258516999
H	3.319641998	3.039612999	-2.924210999
O	1.369435999	-0.240441000	-4.613332998
H	0.394922000	-0.358977000	-4.445023998
H	1.481991999	-0.256427000	-5.565523997
O	-2.033662999	-3.098766999	-3.707098998
H	-1.348739999	-3.708263998	-3.336408999
H	-2.111015999	-3.330231998	-4.635164998
O	-4.149240998	3.098313999	2.575516999
H	-3.250221999	2.930231999	2.906825999
H	-4.042095998	3.799229998	1.914639999
O	0.179268000	5.116545998	2.514905999
H	0.137563000	5.701687997	3.274104998
H	1.129316000	5.088757998	2.249267999
O	1.814655999	1.995988999	-3.207448999
H	1.758603999	1.212066999	-3.798256998
H	1.782954999	1.632355999	-2.313311999
O	-1.203657999	-0.473715000	-4.199091998

H	-1.657577999	0.239868000	-3.727847998
H	-1.512517999	-1.320782999	-3.835177998
O	-6.367342997	1.342209999	-0.858589000
H	-6.273148997	1.398378999	0.159329000
H	-7.246419997	1.666133999	-1.067728999
O	2.724421999	5.300721998	-0.867505000
H	3.245260999	4.692736998	-1.444876999
H	1.858808999	5.438087998	-1.291521999
O	-4.534114998	3.388804998	-1.636070999
H	-5.178324998	2.704901999	-1.383601999
H	-3.847158998	2.926228999	-2.145209999
O	-2.619005999	1.934022999	-3.257011999
H	-1.791662999	2.510615999	-3.187836999
H	-2.954149999	2.110474999	-4.140553998
O	-0.532565000	3.422126998	-3.345804998
H	-0.377567000	4.224461998	-2.814794999
H	0.318730000	2.942079999	-3.343588999
O	-1.301506999	5.972300997	0.306710000
H	-0.839363000	5.699231997	1.119100000
H	-2.207060999	5.610316997	0.354250000
O	-3.855934998	4.935317998	0.393008000
H	-4.088776998	4.376184998	-0.395533000
H	-4.515467998	5.631481997	0.421356000
O	0.126419000	5.676570997	-1.861946999
H	-0.439736000	5.796707997	-1.049732000
H	0.052065000	6.494019997	-2.358281999
O	-0.151134000	-5.034019998	1.843005999
H	-0.685814000	-5.337088998	1.086429999
H	-0.614648000	-4.255364998	2.194615999
O	-4.374405998	-2.683354999	-2.253732999
H	-3.631640998	-2.931250999	-2.833289999
H	-4.389097998	-1.700520999	-2.292053999
O	-4.612471998	-0.010366000	-2.633933999
H	-3.812260998	0.533494000	-2.635455999
H	-5.217461998	0.453370000	-2.034636999
O	-4.236352998	-4.414645998	-0.278394000
H	-4.915356998	-5.047525998	-0.522729000
H	-4.300341998	-3.693713998	-0.963013000
O	-4.344829998	-3.633405998	2.384822999
H	-4.304544998	-3.953123998	1.461024999
H	-4.964726998	-4.209328998	2.836364999
O	-2.406471999	-0.375582000	3.290569998
H	-1.677445999	0.105192000	3.705449998
H	-2.658159999	0.141436000	2.518451999
O	-6.051143997	-1.308232999	1.982336999
H	-5.350563998	-1.922178999	2.244392999
H	-6.324587997	-1.596290999	1.094567000
O	-6.784027997	-1.638133999	-0.706878000
H	-6.272956997	-2.082878999	-1.391088999
H	-6.713616997	-0.694624000	-0.905845000



a



b

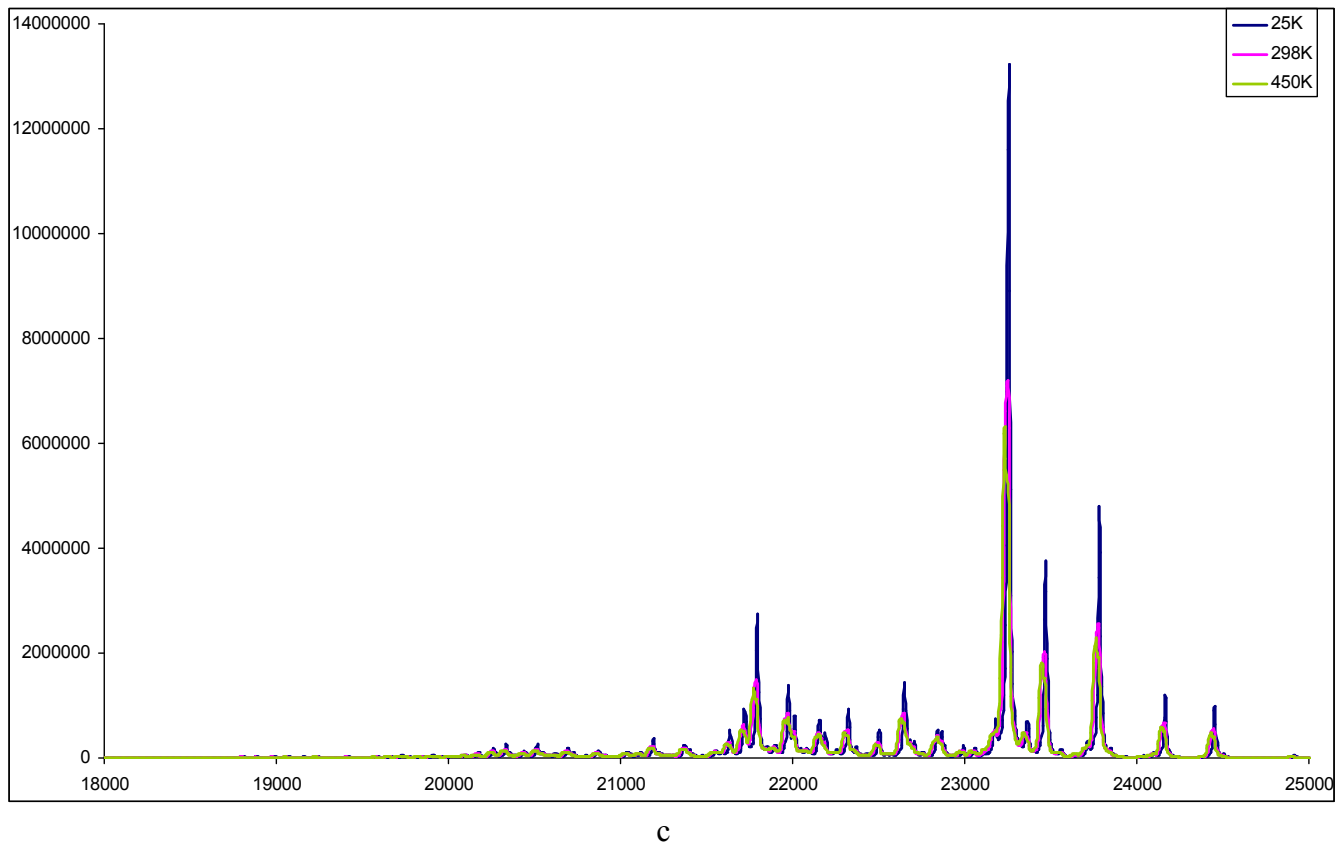


Figure S1. Temperature dependence of the Herzberg–Teller spectra of (a) $S_0 \rightarrow S_1$, (b) $S_0 \rightarrow S_2$, and (c) $S_1 \rightarrow S_0$ transitions of pyrene in absolute scale. Procedure 2, Lorentzian broadening with HWHM $\sim 5 \text{ cm}^{-1}$.

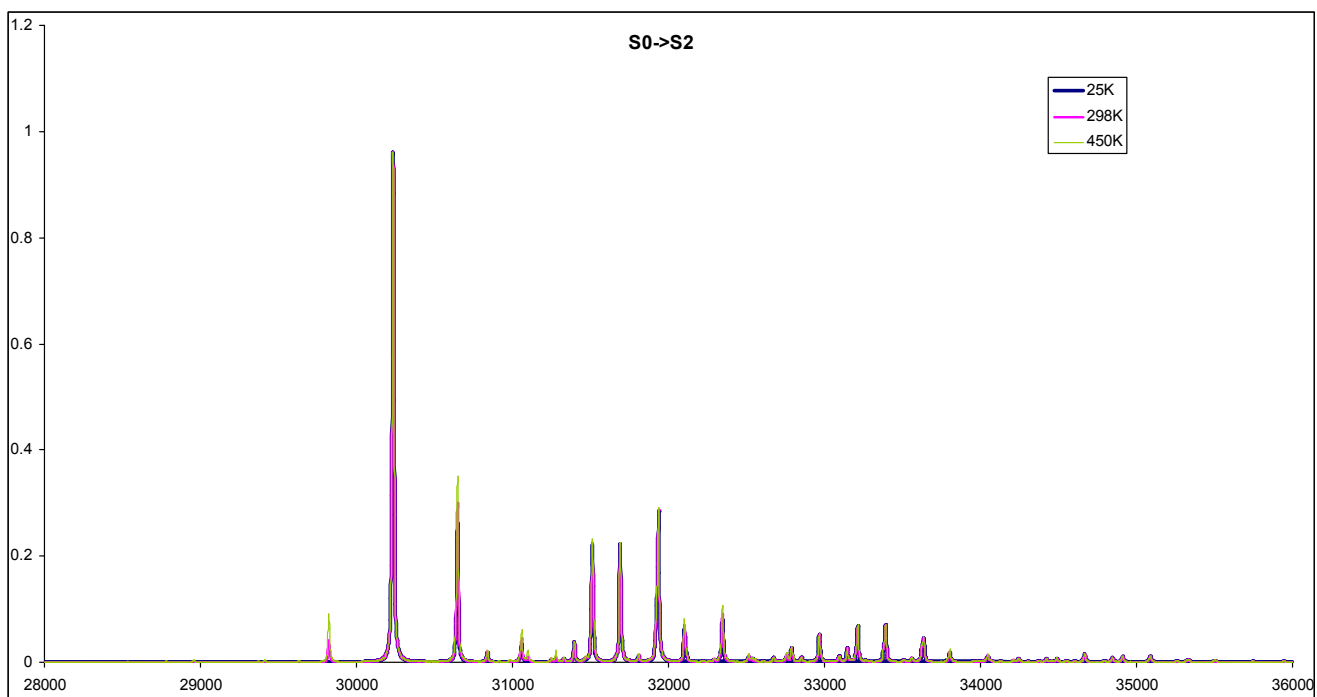
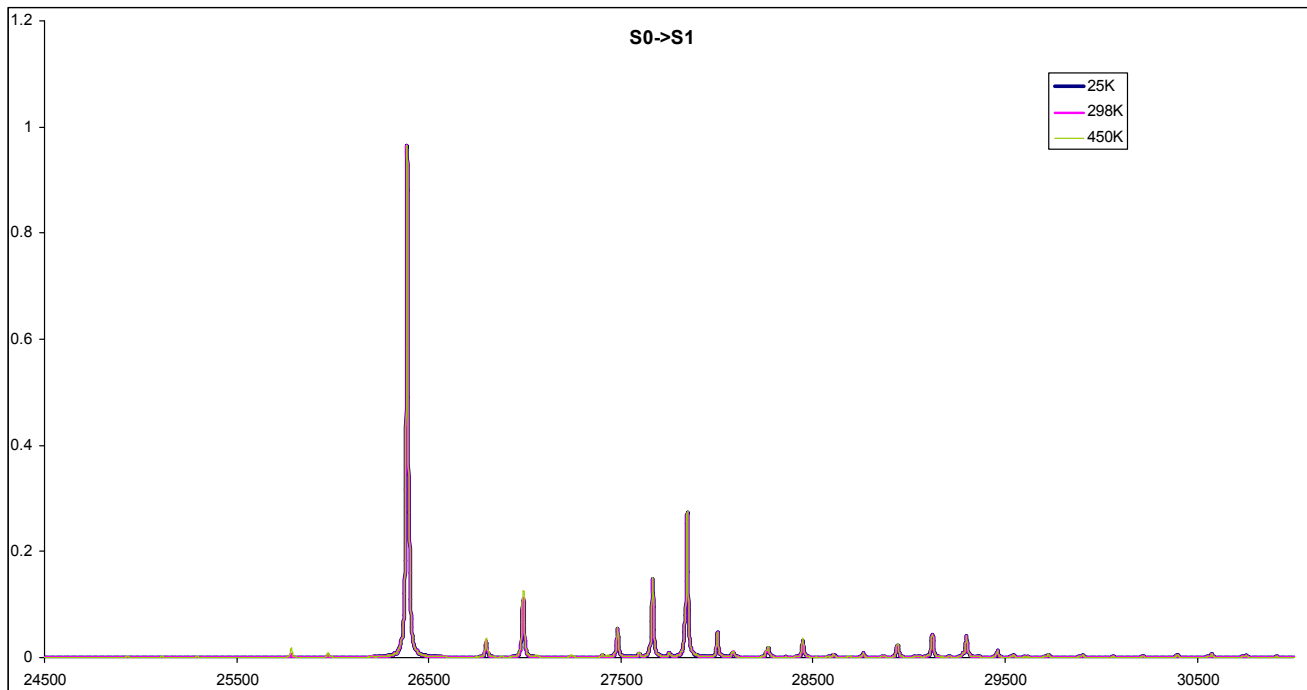


Figure S2. Temperature dependence of the Franck–Condon spectra of the S₀→S₁ and S₀→S₂ transitions of pyrene normalized to unit height. Procedure 1, Lorentzian broadening with HWHM ~5 cm⁻¹.

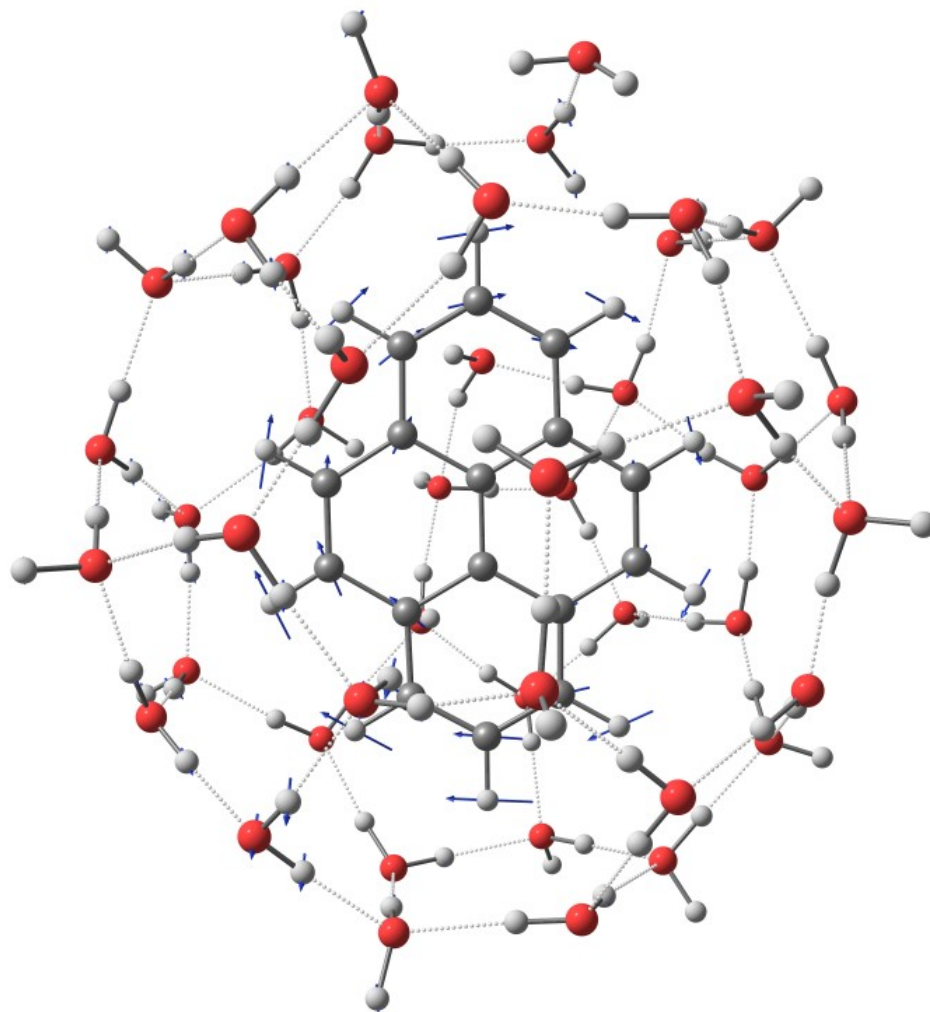


Figure S3. The mode (15 cm^{-1}) of $\text{Py} \cdot 44\text{H}_2\text{O}$ cluster with the largest HR factor.

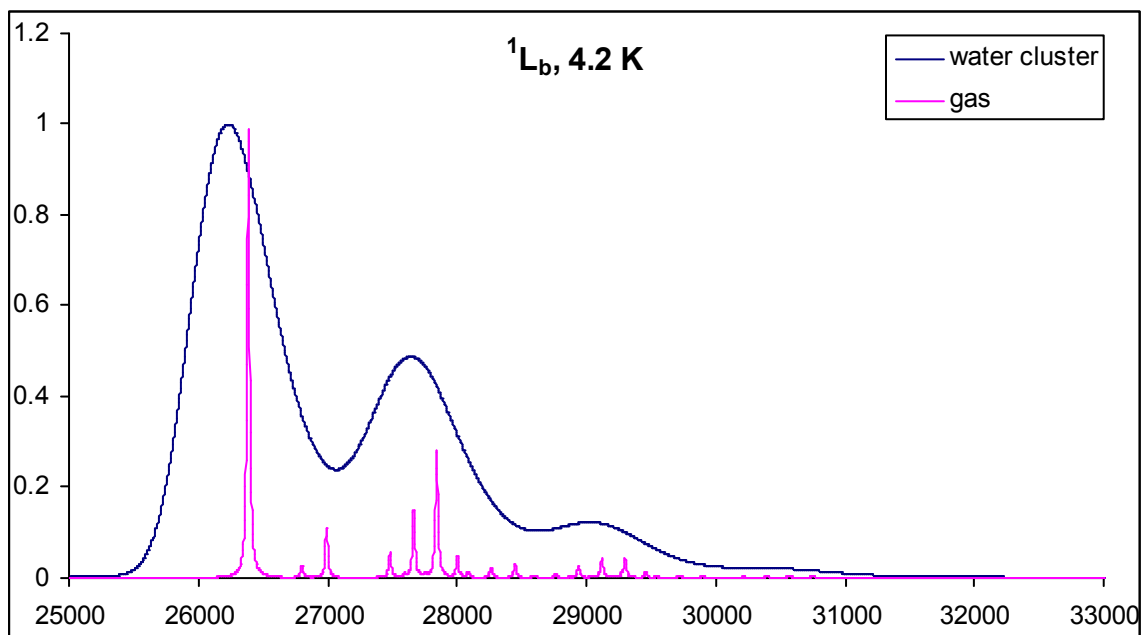
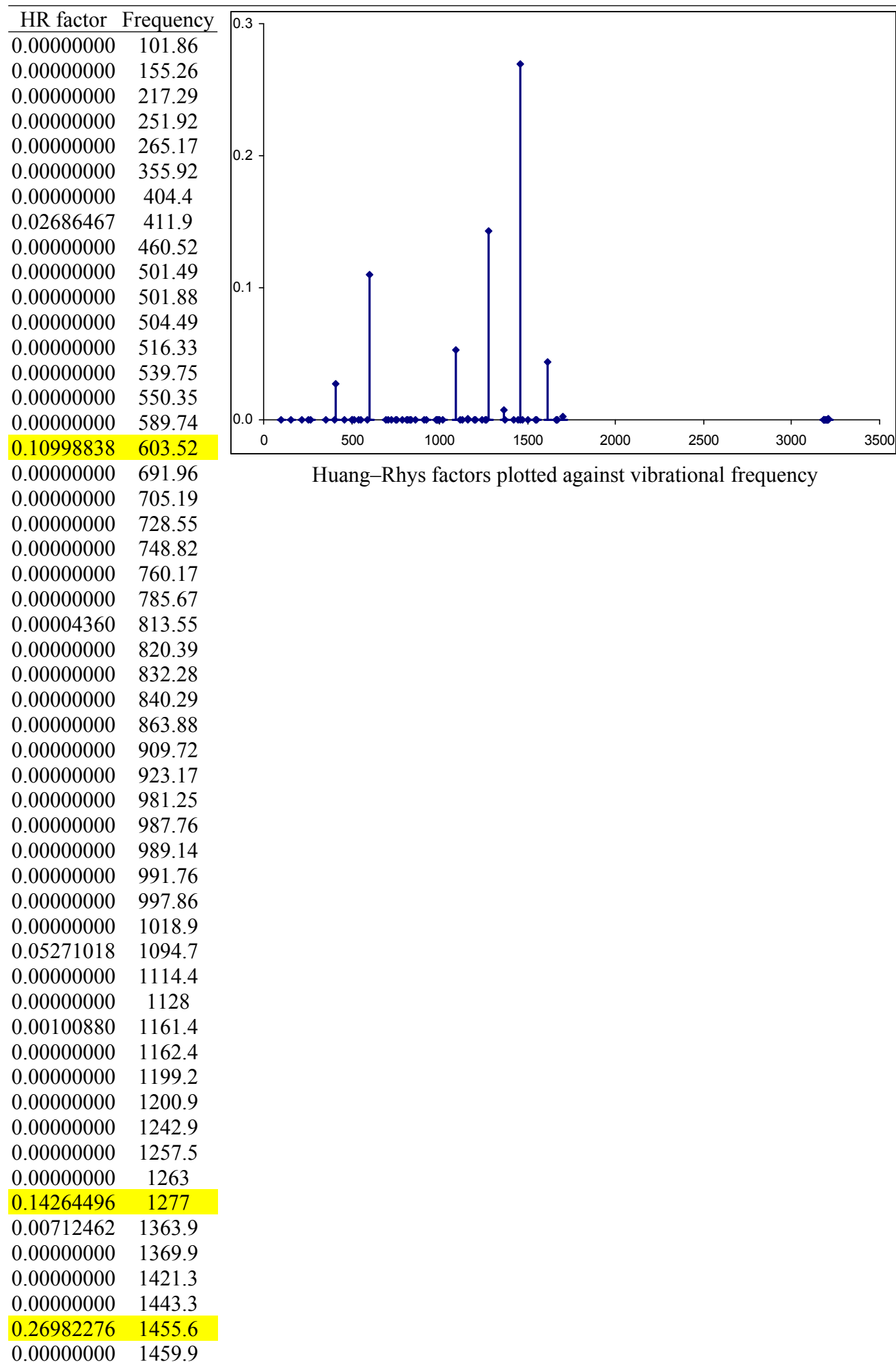


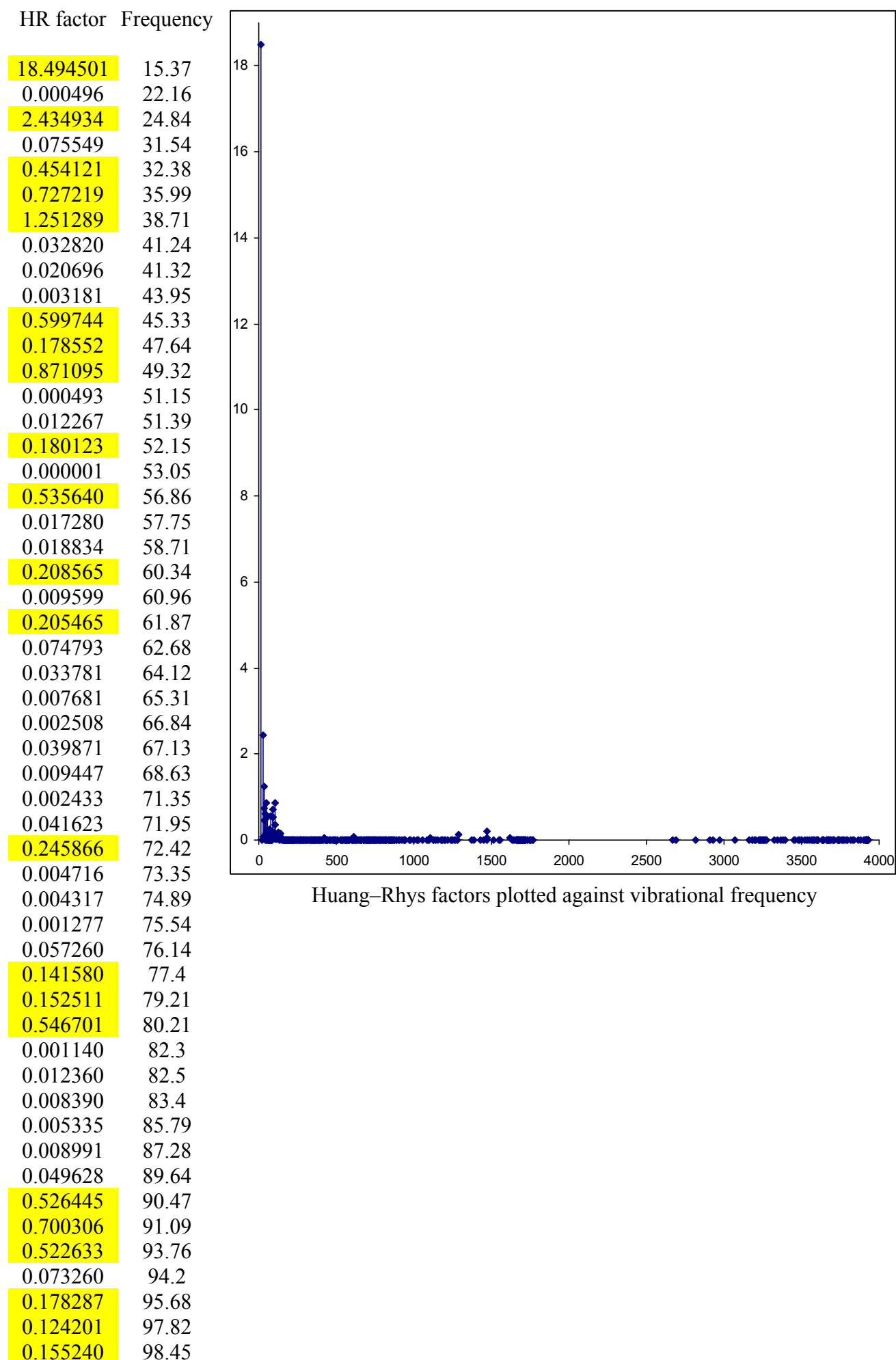
Figure S4. Vibronic profile of $S_0 \rightarrow S_1$ transition of pyrene (pink line) and $\text{Py} \cdot 44\text{H}_2\text{O}$ cluster (blue line).

Figure S5. Huang–Rhys factors for S0→S1 transition of pyrene (Procedure 1)

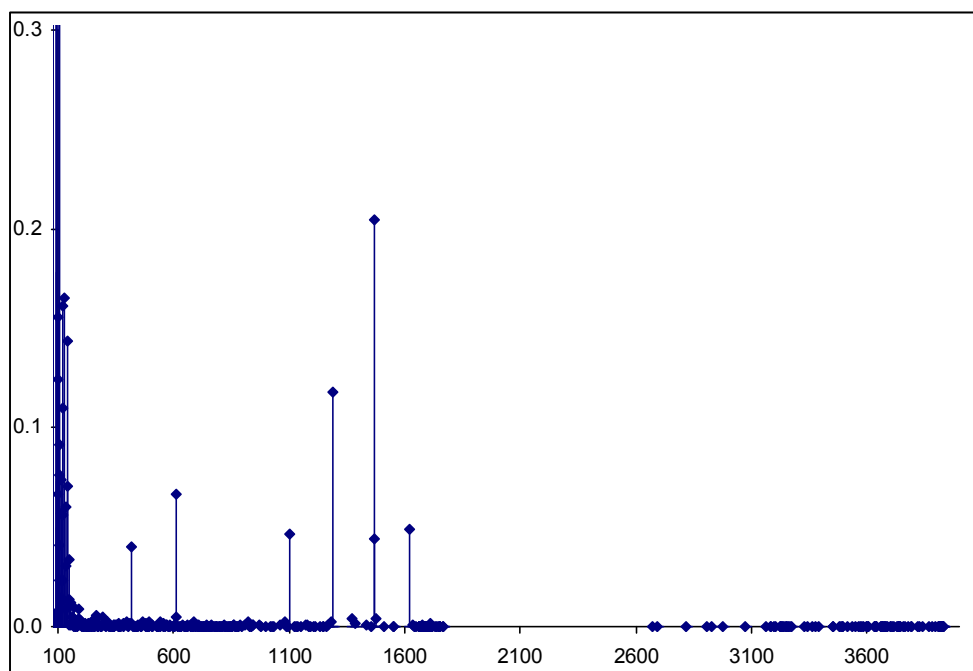


0.00000000	1471.8
0.00000000	1504.4
0.00000000	1545.1
0.00000000	1552.1
0.04420957	1614.7
0.00000000	1660.9
0.00000000	1661
0.00000000	1670.8
0.00251489	1700.2
0.00000000	3182.4
0.00000000	3182.5
0.00000000	3184.8
0.00000026	3185.1
0.00000000	3192.6
0.00000000	3193.3
0.00000000	3201.7
0.00002871	3202.1
0.00000000	3210.2
0.00086641	3211.2

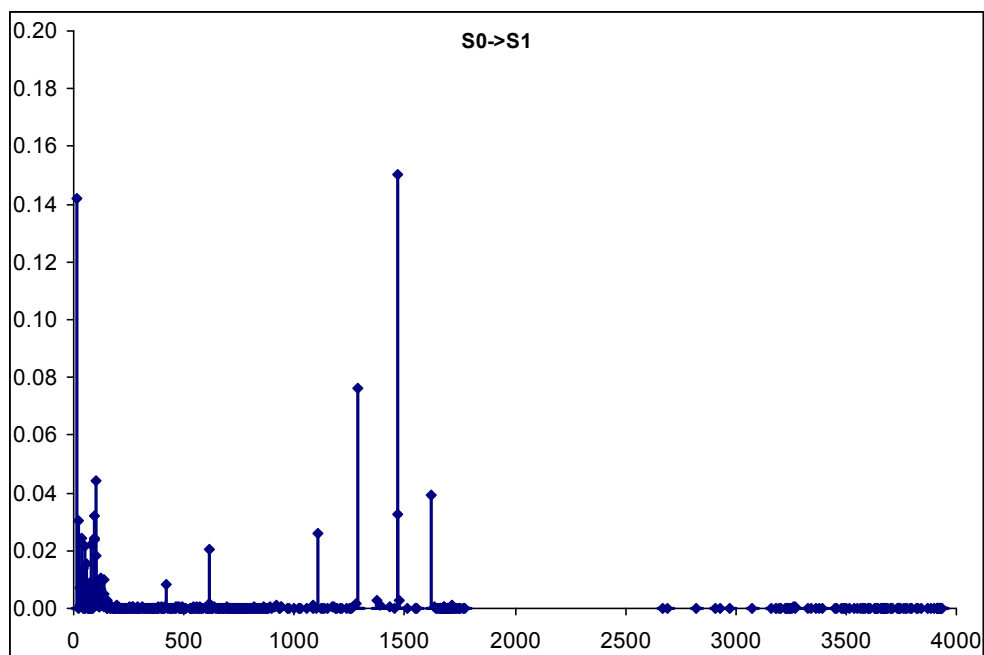
Figure S6. Huang–Rhys factors for S₀→S₁ transition of Py·4H₂O cluster (Procedure 1)



0.066327	100.31
0.863753	102.8
0.091615	103.77
0.353524	104.59
0.076054	106.17
0.023129	107.72
0.040966	109.35
0.014389	112.57
0.057035	113.06
0.012748	114.86
0.073841	116.32
0.022871	118.66
0.056399	121.06
0.161578	122.5
0.109760	123.64
0.165470	126.07
0.059886	132.87
0.009090	133.83
0.030845	137.63
0.143965	138.95
0.070963	140.72
0.013777	146.06
0.033633	148.81
0.000794	150.77
0.000570	153.91
0.011644	158.59
0.004707	160.7
0.001318	164.61
0.004149	166.09
0.000103	169.41
0.009268	172.48
0.001013	174.79
0.001937	178.14
0.000314	179.5
0.000291	180.44
0.001183	183.98
0.002457	185.93
0.004225	188.21
0.001060	189.38
0.008761	191.85
0.000488	195.51
0.002846	199.89
0.000654	202.38
0.000047	204.33
0.000024	211.14
0.000027	212.43
0.000562	213.2
0.000124	216.41
0.000937	219.61
0.001826	220.51
0.000060	224.76
0.000006	228.73
0.000190	229.97
0.000045	231.31
0.001681	234.06



Enlarged view of the 100–4000 cm^{-1} region



Contributions of individual modes to the total reorganization energy

0.000034	238.67
0.000348	243.28
0.000058	245.39
0.000010	249.68
0.003490	253.32
0.001939	259.47
0.000118	261.44
0.001347	265.18
0.004278	266.24
0.005655	268.31
0.000145	272.71
0.000026	274.15
0.000028	276.21
0.000484	281.71
0.000019	286.82
0.000002	288.18
0.000008	289.97
0.004830	292.2
0.000809	298.25
0.001072	299.44
0.000370	304.04
0.000649	308.91
0.002038	311.2
0.000432	319.05
0.000267	322.2
0.000061	328
0.000303	332.55
0.000002	337.08
0.000086	340.15
0.000704	340.48
0.000557	342.2
0.000099	344.94
0.000928	351.53
0.000594	353.95
0.000576	356.85
0.000084	360.19
0.001398	361.77
0.000061	364.27
0.000163	367.84
0.000005	371.05
0.000297	372.42
0.000436	377.53
0.000583	383.92
0.000839	384.44
0.000322	385.26
0.001724	385.92
0.000762	394.42
0.002328	397.18
0.001352	399.68
0.000985	402.72
0.000018	405.79
0.001221	412.18
0.001918	414.88
0.040428	420.29
0.000000	427.8

0.000093	431.37
0.000227	437.98
0.000011	439.41
0.000606	444.14
0.000067	445.16
0.000103	457.37
0.000340	460.39
0.001448	464.23
0.002367	466.87
0.000149	478.74
0.001406	480.69
0.000002	486.8
0.000315	488.18
0.000001	490.95
0.002081	493.56
0.000422	494.73
0.000836	505.43
0.000022	507.06
0.000000	507.47
0.000264	526.4
0.000007	527.83
0.000013	533.51
0.000523	536.78
0.000271	542.94
0.002218	543.26
0.000166	552.95
0.000657	554.58
0.001514	559.44
0.000109	564.58
0.000451	565.82
0.000478	569.41
0.001038	571.53
0.000030	578.31
0.000507	581.58
0.000003	586.86
0.000118	596.76
0.000289	606.22
0.000544	606.39
0.001065	607.16
0.066225	611.24
0.005026	612.99
0.000547	614.76
0.000011	620.86
0.000098	623.87
0.000010	629.94
0.000017	632.77
0.000962	638.88
0.000055	647.29
0.000268	652.47
0.000023	655.49
0.000003	660.17
0.000023	661.16
0.000657	662.73
0.000103	672.54
0.000517	672.97

0.000010	677.74
0.000376	682.16
0.000159	687.51
0.002215	691.15
0.000025	695.09
0.000466	697.84
0.000207	700.65
0.000434	701.83
0.000053	706.33
0.000089	707.65
0.000003	709.34
0.000048	710.7
0.000556	710.86
0.000301	715.4
0.000073	721.78
0.000053	724.24
0.000005	727.66
0.000375	731.68
0.000207	737.72
0.000240	739.59
0.000133	740.61
0.000549	744.91
0.000000	746.98
0.000372	749.7
0.000211	753.98
0.000039	756.8
0.000546	760.51
0.000191	763.83
0.000280	765.97
0.000082	773.14
0.000005	774.42
0.000149	781.13
0.000018	782.18
0.000139	786.05
0.000064	788.52
0.000047	799.22
0.000044	801.53
0.000000	803.84
0.000140	807.29
0.000238	813.69
0.001098	817.4
0.000222	818.58
0.000000	822.78
0.000044	824.19
0.000053	835.14
0.000095	838.48
0.000354	842.12
0.000331	848.29
0.000027	849.96
0.000010	852.18
0.000123	855.28
0.000428	857.67
0.000925	861.81
0.000005	866.96
0.000140	871.01

0.000000	872.05
0.000240	876.5
0.000019	884.5
0.000859	889.97
0.000190	898.13
0.001041	909.52
0.002599	921.25
0.000103	933.17
0.000232	934.4
0.000863	940.51
0.000764	941.58
0.000409	971.24
0.000076	977.04
0.000001	997.54
0.000023	1023.08
0.000106	1028.69
0.000219	1030.5
0.000442	1059.12
0.002049	1084.5
0.000245	1088.07
0.000031	1097.69
0.046737	1103.42
0.000000	1123.71
0.000000	1127.32
0.000224	1137.37
0.000031	1152.38
0.000760	1172.84
0.000831	1181.36
0.000022	1186.58
0.000103	1195.87
0.000233	1207.41
0.000198	1216.01
0.000001	1237.36
0.000058	1248.8
0.000391	1249
0.000046	1259.57
0.000531	1268.16
0.002656	1279.28
0.118196	1288.35
0.004065	1373.08
0.001752	1385.25
0.000407	1431.88
0.000073	1452.2
0.204187	1469.72
0.044005	1471.55
0.003847	1475.23
0.000015	1512.2
0.000009	1550.92
0.000020	1554.15
0.048612	1619.85
0.000507	1636.62
0.000082	1643.26
0.000004	1649.81
0.000025	1659.57
0.000051	1660.46

0.000037	1662.01
0.000003	1662.72
0.000287	1665.21
0.000031	1666.08
0.000011	1666.66
0.000005	1667.61
0.000016	1670.67
0.000003	1672.52
0.000006	1674.74
0.000339	1675.08
0.000000	1676.61
0.000058	1678.29
0.000659	1678.64
0.000165	1679.28
0.000045	1685.57
0.000082	1685.94
0.000197	1688.32
0.000147	1689.5
0.000003	1691.4
0.000019	1693.52
0.000003	1693.7
0.000003	1696.64
0.000055	1699.74
0.000021	1700.91
0.000000	1702.16
0.000000	1703.56
0.000004	1704.7
0.000020	1708.02
0.000081	1708.63
0.001580	1710.89
0.000581	1711.16
0.000004	1717.7
0.000027	1718.33
0.000002	1718.82
0.000000	1720.96
0.000019	1729.4
0.000003	1735.87
0.000018	1744.3
0.000003	1750.24
0.000006	1751.18
0.000000	1753.12
0.000000	1768.26
0.000005	1769.63
0.000005	2668.96
0.000001	2689.99
0.000000	2820.35
0.000000	2909.64
0.000000	2928.92
0.000000	2973.89
0.000005	3073.27
0.000000	3163.15
0.000000	3181.83
0.000002	3185.54
0.000003	3195.08
0.000000	3207.69

0.000010	3224.31
0.000011	3224.85
0.000006	3230.03
0.000005	3233.62
0.000002	3237.2
0.000006	3245.9
0.000013	3251.27
0.000006	3254.96
0.000344	3262.81
0.000262	3265.91
0.000022	3272.88
0.000008	3326.6
0.000005	3342.54
0.000000	3364.88
0.000003	3377.98
0.000002	3391.48
0.000003	3453.08
0.000003	3455.66
0.000006	3482.29
0.000001	3489.17
0.000002	3496.93
0.000002	3498.57
0.000000	3518.43
0.000000	3535.21
0.000000	3549.97
0.000000	3565.36
0.000002	3569.98
0.000000	3578.76
0.000000	3584.38
0.000000	3599.57
0.000001	3601.77
0.000003	3605.25
0.000000	3607.48
0.000002	3630.52
0.000000	3633.97
0.000000	3637.46
0.000002	3640.66
0.000001	3643.64
0.000000	3659.71
0.000000	3662.78
0.000000	3667.38
0.000001	3668.65
0.000002	3669.45
0.000000	3673.17
0.000000	3677.57
0.000001	3681.79
0.000001	3683.54
0.000002	3690.83
0.000000	3702.32
0.000000	3705.32
0.000004	3706.17
0.000000	3713.8
0.000003	3729.4
0.000000	3736.11
0.000001	3737.28

0.000001	3738.56
0.000000	3740.3
0.000001	3742.92
0.000000	3746.04
0.000000	3759.34
0.000003	3765.74
0.000000	3777.75
0.000000	3791.56
0.000001	3794.88
0.000015	3817.79
0.000004	3829.7
0.000001	3839.91
0.000006	3867.52
0.000000	3881.94
0.000004	3898.53
0.000001	3910.85
0.000000	3912.86
0.000003	3915.88
0.000001	3916.07
0.000001	3916.7
0.000001	3918.45
0.000002	3921.67
0.000001	3922.09
0.000002	3922.66
0.000002	3922.96
0.000002	3924.62
0.000001	3925.24
0.000001	3926.87
0.000002	3929.91
0.000002	3930.34
0.000001	3932.08

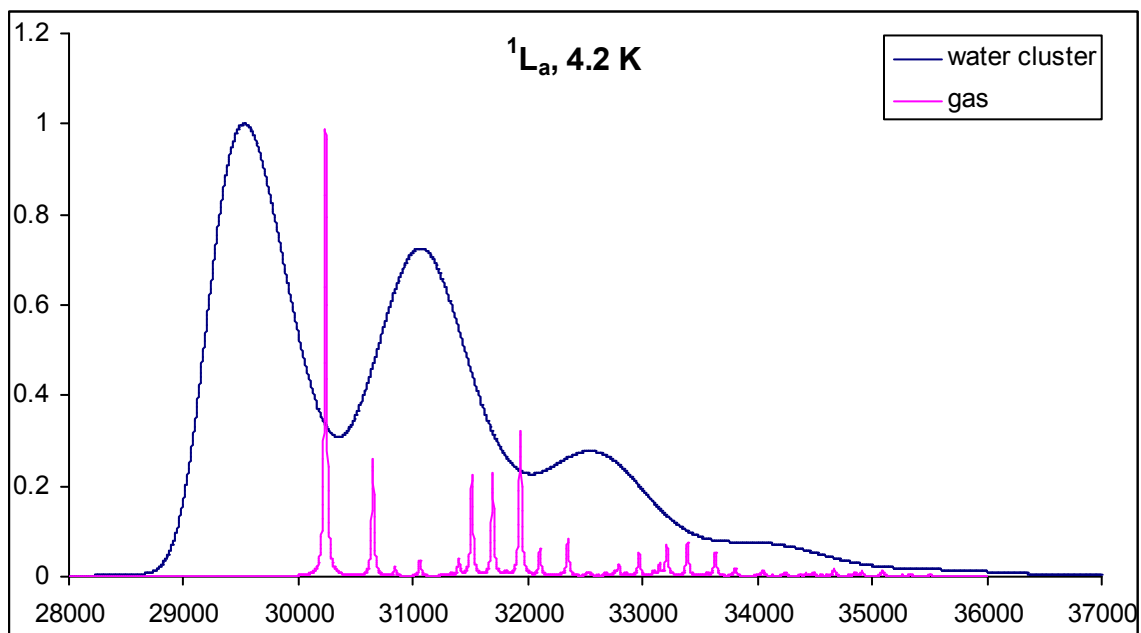
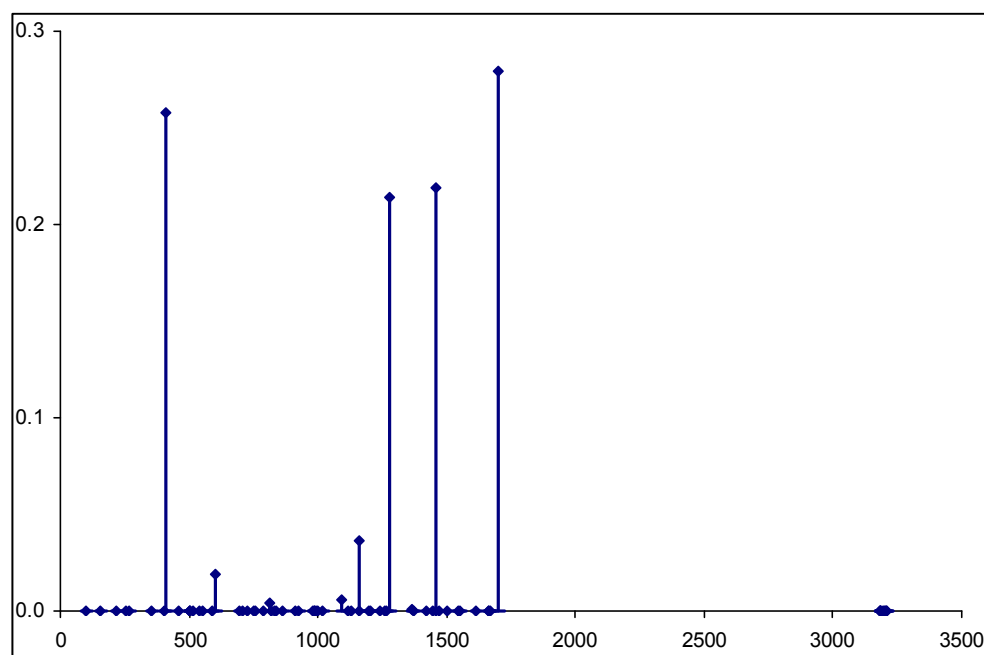


Figure S7. Vibronic profile of $S_0 \rightarrow S_2$ transition of pyrene (pink line) and $\text{Py} \cdot 44\text{H}_2\text{O}$ cluster (blue line).

Figure S8. Huang–Rhys factors for S₀→S₂ transition of pyrene (Procedure 1)

HR factor	Frequency
0.00000000	101.86
0.00000000	155.26
0.00000000	217.29
0.00000000	251.92
0.00000000	265.17
0.00000000	355.92
0.00000000	404.4
0.25787022	411.9
0.00000000	460.52
0.00000000	501.49
0.00000000	501.88
0.00000000	504.49
0.00000000	516.33
0.00000000	539.75
0.00000000	550.35
0.00000000	589.74
0.01884109	603.52
0.00000000	691.96
0.00000000	705.19
0.00000000	728.55
0.00000000	748.82
0.00000000	760.17
0.00000000	785.67
0.00377267	813.55
0.00000000	820.39
0.00000000	832.28
0.00000000	840.29
0.00000000	863.88
0.00000000	909.72
0.00000000	923.17
0.00000000	981.25
0.00000000	987.76
0.00000000	989.14
0.00000000	991.76
0.00000000	997.86
0.00000000	1018.9
0.00574195	1094.7
0.00000000	1114.4
0.00000000	1128
0.03676667	1161.4
0.00000000	1162.4
0.00000000	1199.2
0.00000000	1200.9
0.00000000	1242.9
0.00000000	1257.5
0.00000000	1263
0.21443311	1277
0.00097600	1363.9
0.00000000	1369.9
0.00000000	1421.3
0.00000000	1443.3
0.21926115	1455.6
0.00000000	1459.9

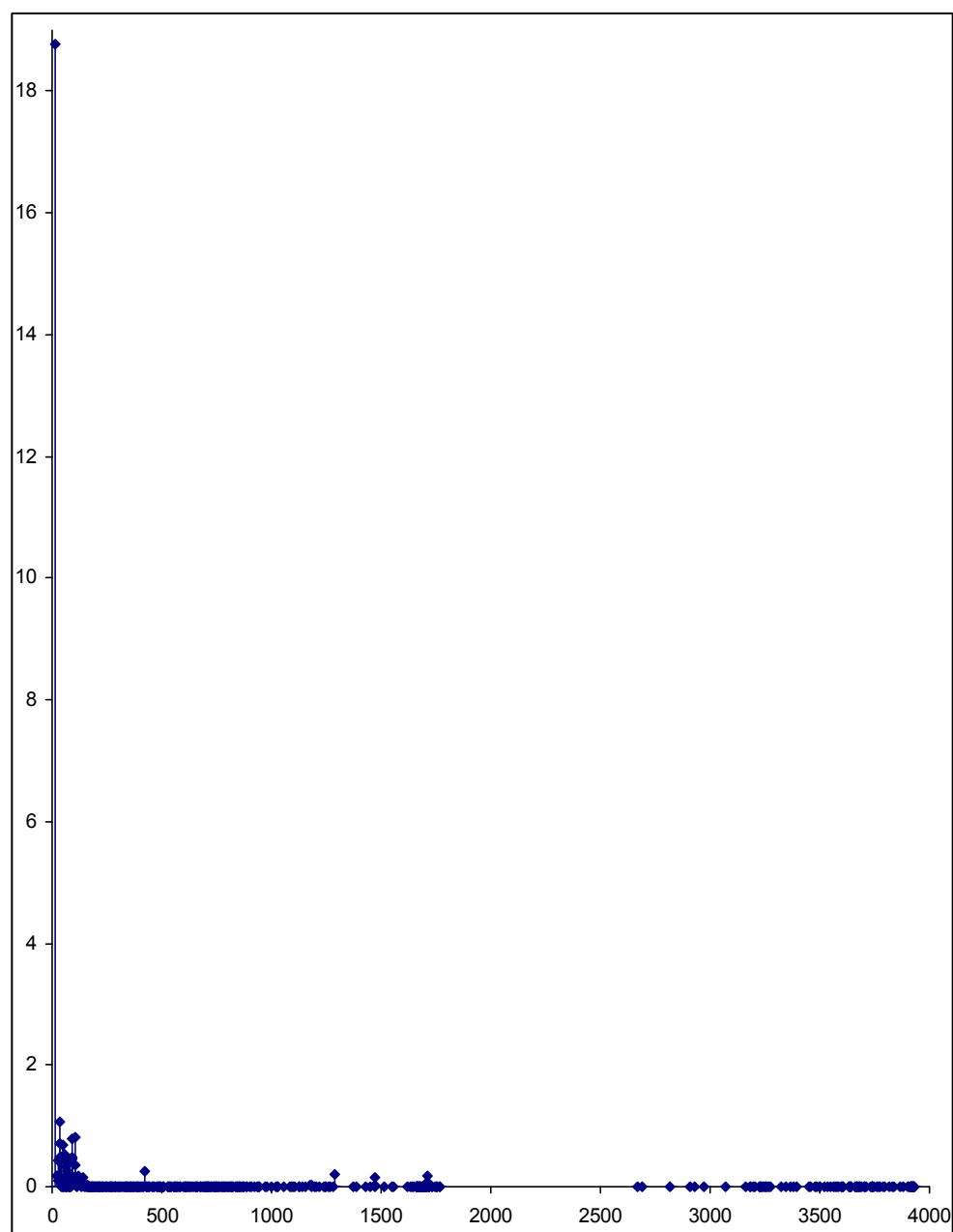


Huang–Rhys factors plotted against vibrational frequency

0.00000000	1471.8
0.00000000	1504.4
0.00000000	1545.1
0.00000000	1552.1
0.00005087	1614.7
0.00000000	1660.9
0.00000000	1661
0.00000000	1670.8
0.27937304	1700.2
0.00000000	3182.4
0.00000000	3182.5
0.00000000	3184.8
0.00014250	3185.1
0.00000000	3192.6
0.00000000	3193.3
0.00000000	3201.7
0.00019902	3202.1
0.00000000	3210.2
0.00026754	3211.2

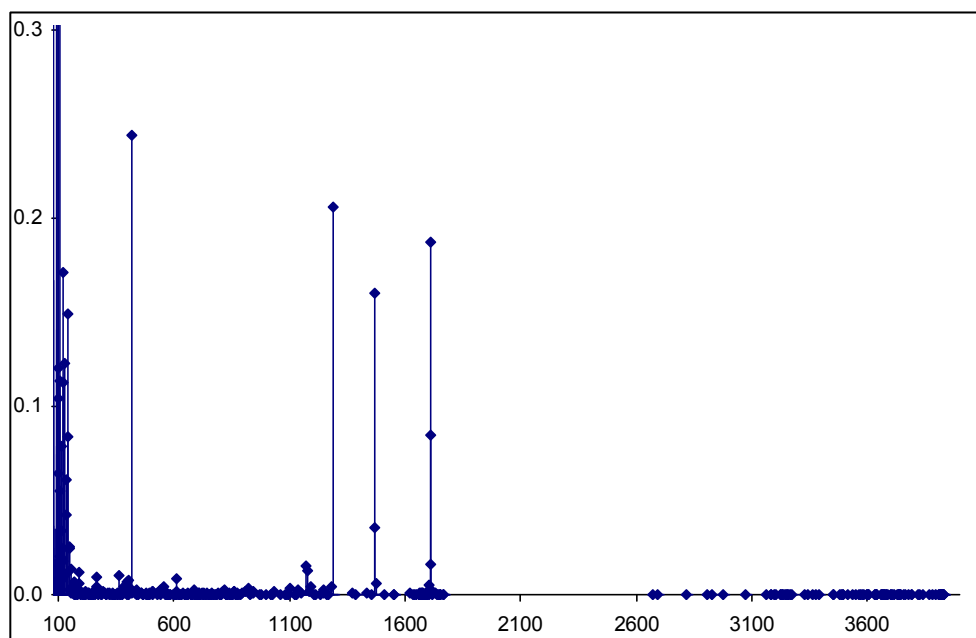
Figure S9. Huang–Rhys factors for S₀→S₂ transition of Py·44H₂O cluster (Procedure 1)

HR factor	Frequency
18.776969	15.37
0.179430	22.16
0.430061	24.84
0.092862	31.54
0.489711	32.38
0.719757	35.99
1.056164	38.71
0.054511	41.24
0.035329	41.32
0.010947	43.95
0.445200	45.33
0.089036	47.64
0.688723	49.32
0.000895	51.15
0.008505	51.39
0.119882	52.15
0.001721	53.05
0.544933	56.86
0.022723	57.75
0.022625	58.71
0.326485	60.34
0.005742	60.96
0.162294	61.87
0.156402	62.68
0.038788	64.12
0.000297	65.31
0.001571	66.84
0.017013	67.13
0.036141	68.63
0.003705	71.35
0.105826	71.95
0.266584	72.42
0.014132	73.35
0.000258	74.89
0.000505	75.54
0.024956	76.14
0.104648	77.4
0.166781	79.21
0.431578	80.21
0.000210	82.3
0.036504	82.5
0.018731	83.4
0.034412	85.79
0.009155	87.28
0.078742	89.64
0.492232	90.47
0.782891	91.09
0.450542	93.76
0.074934	94.2
0.140772	95.68
0.104282	97.82
0.120189	98.45
0.064202	100.31

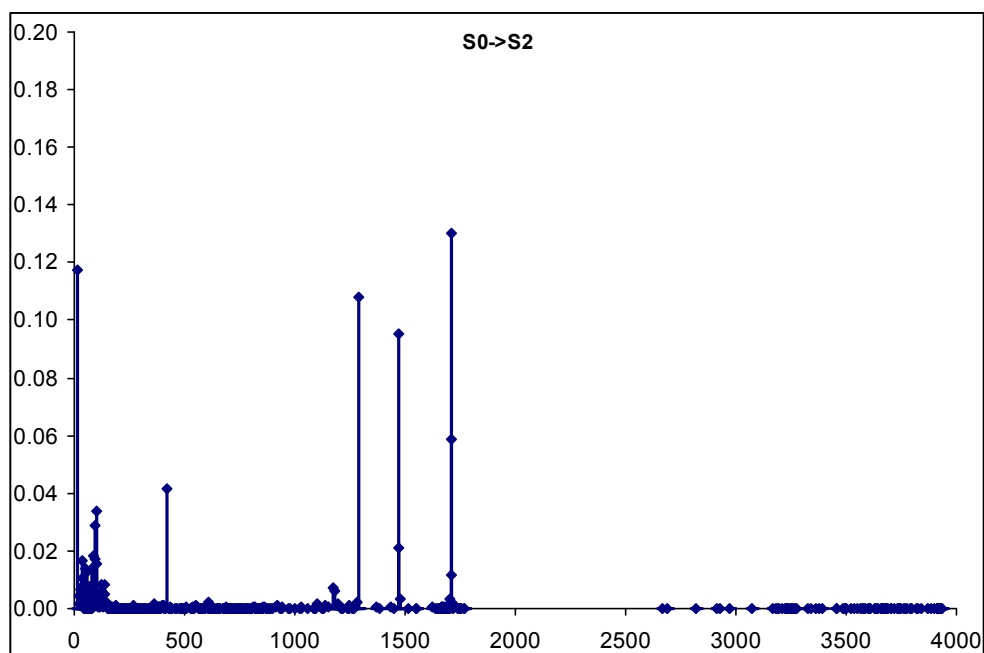


Huang–Rhys factors plotted against vibrational frequency

0.813009	102.8
0.113392	103.77
0.360378	104.59
0.055488	106.17
0.015100	107.72
0.020165	109.35
0.019615	112.57
0.033829	113.06
0.007939	114.86
0.078610	116.32
0.017835	118.66
0.024621	121.06
0.171302	122.5
0.113037	123.64
0.123229	126.07
0.060753	132.87
0.011102	133.83
0.042583	137.63
0.148769	138.95
0.084004	140.72
0.025018	146.06
0.024172	148.81
0.002331	150.77
0.000700	153.91
0.013149	158.59
0.001258	160.7
0.001421	164.61
0.006896	166.09
0.000018	169.41
0.004895	172.48
0.002910	174.79
0.003302	178.14
0.000089	179.5
0.000721	180.44
0.000009	183.98
0.001828	185.93
0.006233	188.21
0.000845	189.38
0.012077	191.85
0.000130	195.51
0.002110	199.89
0.000238	202.38
0.001121	204.33
0.000003	211.14
0.000460	212.43
0.000363	213.2
0.000090	216.41
0.000119	219.61
0.001460	220.51
0.000702	224.76
0.000048	228.73
0.000384	229.97
0.000635	231.31
0.000903	234.06
0.000183	238.67



Enlarged view of the 100–4000 cm^{-1} region



Contributions of individual modes to the total reorganization energy

0.000005	243.28
0.000148	245.39
0.000002	249.68
0.001585	253.32
0.000546	259.47
0.000010	261.44
0.001221	265.18
0.003838	266.24
0.009718	268.31
0.000727	272.71
0.000584	274.15
0.000233	276.21
0.000925	281.71
0.000587	286.82
0.000094	288.18
0.000254	289.97
0.001610	292.2
0.000958	298.25
0.000536	299.44
0.000007	304.04
0.000206	308.91
0.001009	311.2
0.000257	319.05
0.000863	322.2
0.000001	328
0.000183	332.55
0.000504	337.08
0.000000	340.15
0.000126	340.48
0.000030	342.2
0.000289	344.94
0.000025	351.53
0.000123	353.95
0.000852	356.85
0.009869	360.19
0.000970	361.77
0.000077	364.27
0.000635	367.84
0.000045	371.05
0.000493	372.42
0.000003	377.53
0.000554	383.92
0.001989	384.44
0.002279	385.26
0.003832	385.92
0.000120	394.42
0.007051	397.18
0.002138	399.68
0.007944	402.72
0.000414	405.79
0.003190	412.18
0.000771	414.88
0.243823	420.29
0.001393	427.8
0.001172	431.37

0.002171	437.98
0.000303	439.41
0.001255	444.14
0.000152	445.16
0.000522	457.37
0.000432	460.39
0.000063	464.23
0.000015	466.87
0.000355	478.74
0.000547	480.69
0.000052	486.8
0.000027	488.18
0.000112	490.95
0.000055	493.56
0.000537	494.73
0.002033	505.43
0.001271	507.06
0.000084	507.47
0.000454	526.4
0.000009	527.83
0.000429	533.51
0.001636	536.78
0.000275	542.94
0.002630	543.26
0.004121	552.95
0.001789	554.58
0.002207	559.44
0.000938	564.58
0.000017	565.82
0.000254	569.41
0.000257	571.53
0.000096	578.31
0.000246	581.58
0.000128	586.86
0.000000	596.76
0.000303	606.22
0.000018	606.39
0.000001	607.16
0.008359	611.24
0.000137	612.99
0.001280	614.76
0.000026	620.86
0.000005	623.87
0.000005	629.94
0.000037	632.77
0.000725	638.88
0.000363	647.29
0.000011	652.47
0.000004	655.49
0.000069	660.17
0.000191	661.16
0.000597	662.73
0.000030	672.54
0.000405	672.97
0.000056	677.74

0.000624	682.16
0.000004	687.51
0.002922	691.15
0.000083	695.09
0.000279	697.84
0.000082	700.65
0.000078	701.83
0.000586	706.33
0.000004	707.65
0.000095	709.34
0.000078	710.7
0.000457	710.86
0.000197	715.4
0.000452	721.78
0.000061	724.24
0.000114	727.66
0.000525	731.68
0.000161	737.72
0.000000	739.59
0.000137	740.61
0.000661	744.91
0.000067	746.98
0.000294	749.7
0.000330	753.98
0.000037	756.8
0.000176	760.51
0.000124	763.83
0.000871	765.97
0.000323	773.14
0.000000	774.42
0.000336	781.13
0.000001	782.18
0.000036	786.05
0.000546	788.52
0.000009	799.22
0.000000	801.53
0.000086	803.84
0.000597	807.29
0.001473	813.69
0.000759	817.4
0.002139	818.58
0.000193	822.78
0.000232	824.19
0.000032	835.14
0.000606	838.48
0.000132	842.12
0.000078	848.29
0.000361	849.96
0.000076	852.18
0.000197	855.28
0.001618	857.67
0.001479	861.81
0.000118	866.96
0.000403	871.01
0.000001	872.05

0.000522	876.5
0.000017	884.5
0.000002	889.97
0.000486	898.13
0.001331	909.52
0.002999	921.25
0.000106	933.17
0.000508	934.4
0.001756	940.51
0.000565	941.58
0.000065	971.24
0.000077	977.04
0.000043	997.54
0.000002	1023.08
0.000039	1028.69
0.001330	1030.5
0.000033	1059.12
0.000172	1084.5
0.000085	1088.07
0.000001	1097.69
0.003802	1103.42
0.000028	1123.71
0.000053	1127.32
0.002214	1137.37
0.000668	1152.38
0.015416	1172.84
0.013006	1181.36
0.001729	1186.58
0.003920	1195.87
0.000000	1207.41
0.000314	1216.01
0.000092	1237.36
0.000532	1248.8
0.002451	1249
0.000400	1259.57
0.000364	1268.16
0.004359	1279.28
0.206349	1288.35
0.000688	1373.08
0.000014	1385.25
0.000485	1431.88
0.000297	1452.2
0.160057	1469.72
0.035228	1471.55
0.005838	1475.23
0.000336	1512.2
0.000378	1550.92
0.000022	1554.15
0.000570	1619.85
0.000004	1636.62
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0.000032	1649.81
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0.000263	1660.46
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0.000165	1665.21
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0.000661	1666.66
0.000887	1667.61
0.000008	1670.67
0.000021	1672.52
0.000461	1674.74
0.000002	1675.08
0.000260	1676.61
0.000018	1678.29
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0.000702	1693.7
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0.000288	1699.74
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0.001276	1703.56
0.005154	1704.7
0.002924	1708.02
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0.187303	1710.89
0.084878	1711.16
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0.000660	1718.33
0.000003	1718.82
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0.000069	1751.18
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0.000004	3207.69
0.000078	3224.31

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