

Supporting Information

S1. Cartesian Coordinates of Optimized Structures

All optimized structures are provided in XYZ format (coordinates in Å). Calculations were performed at the B3LYP-D3(BJ)/def2-TZVP level of theory. Aqueous and zwitterionic environments were modeled using the SMD implicit solvation model (water). All stationary points were confirmed as true minima by vibrational analysis.

The files are organized as follows:

System	Neutral-Gas			Neutral-Aqueous			Zwitterion-Aqueous					
Au₂⁰-Ld	8	2.506330000	-2.085983000	0.021633000	8	2.472294000	-2.072738000	0.661574000	8	2.752466000	-1.402642000	1.125867000
	8	-1.801164000	-0.467206000	-1.611884000	8	-1.847983000	-0.764696000	-1.301996000	8	-1.421395000	-0.992542000	-1.362274000
	8	3.848166000	-0.020905000	-1.040899000	8	3.768579000	-0.457203000	-1.099668000	8	4.058166000	0.130713000	-0.701525000
	8	-2.783996000	-1.569670000	0.083386000	8	-2.914891000	-1.362868000	0.582768000	8	-2.507862000	-1.392133000	0.570710000
	7	-3.671776000	0.902539000	0.988762000	7	-3.604746000	1.336139000	0.908502000	7	-3.634967000	1.073268000	0.456402000
	6	-1.205001000	0.784732000	1.383164000	6	-1.141731000	1.178194000	1.223529000	6	-1.235540000	1.413729000	0.877981000
	6	-2.347428000	0.771018000	0.344453000	6	-2.330531000	0.950095000	0.264221000	6	-2.266011000	0.853425000	-0.114636000
	6	0.159026000	0.611155000	0.771156000	6	0.182471000	0.787927000	0.626103000	6	0.182582000	1.123604000	0.467828000
	6	0.734883000	-0.656569000	0.695600000	6	0.748942000	-0.450657000	0.925173000	6	0.843930000	0.012910000	0.990892000
	6	0.837740000	1.696610000	0.227771000	6	0.834695000	1.626913000	-0.274290000	6	0.836353000	1.919147000	-0.468998000
	6	1.964363000	-0.841398000	0.085072000	6	1.941500000	-0.845124000	0.340071000	6	2.131644000	-0.299555000	0.588004000
	6	-2.353467000	-0.553360000	-0.398594000	6	-2.415654000	-0.511846000	-0.120957000	6	-2.045218000	-0.641623000	-0.359186000
	6	2.073757000	1.520516000	-0.385359000	6	2.031954000	1.237063000	-0.864590000	6	2.130053000	1.611431000	-0.876948000
	6	2.635602000	0.258059000	-0.459879000	6	2.587991000	0.003079000	-0.562496000	6	2.780077000	0.503761000	-0.353858000
	1	-1.398156000	-0.007208000	2.110278000	1	-1.329922000	0.611373000	2.137110000	1	-1.435871000	0.975579000	1.858022000
	1	-1.259458000	1.739430000	1.913221000	1	-1.147673000	2.239813000	1.477342000	1	-1.400651000	2.490592000	0.949307000
	1	-2.217938000	1.583955000	-0.365909000	1	-2.200712000	1.551008000	-0.631597000	1	-2.225241000	1.382872000	-1.061908000
	1	0.231555000	-1.521813000	1.108479000	1	0.260652000	-1.125190000	1.617822000	1	0.356465000	-0.625941000	1.716868000
	1	0.407645000	2.688848000	0.281326000	1	0.408089000	2.591323000	-0.519650000	1	0.336506000	2.784850000	-0.884765000
	1	2.601869000	2.369679000	-0.804430000	1	2.543957000	1.888839000	-1.562696000	1	2.644425000	2.229455000	-1.603400000
	1	-3.641985000	1.619845000	1.706468000	1	-3.515887000	2.289270000	1.253911000	1	-3.764909000	2.055370000	0.711369000
	1	-3.898124000	0.018291000	1.440627000	1	-3.758797000	0.740405000	1.720667000	1	-3.756338000	0.496443000	1.293626000
	1	3.362553000	-2.024637000	-0.423096000	1	3.295777000	-2.197947000	0.167706000	1	3.642433000	-1.477488000	0.751705000
	1	-1.801991000	-1.355963000	-2.003945000	1	-1.874193000	-1.723893000	-1.470623000	1	4.417078000	0.753436000	-1.348296000

	1	4.248355000	0.784670000	-1.384570000	1	4.127703000	0.199862000	-1.711609000	1	-4.362180000	0.815087000	-0.214648000
	79	-7.233643000	1.989087000	-1.934864000	79	-7.448687000	1.145446000	-1.796655000	79	-1.991037000	-3.464914000	0.569145000
	79	-5.320157000	1.393919000	-0.364437000	79	-5.351916000	1.239452000	-0.326452000	79	-1.385467000	-5.945952000	0.676298000
Au₂⁺-Ld	8	2.482184000	-2.010365000	0.647240000	8	2.679678000	-1.919309000	0.735832000	8	2.746052000	-1.555264000	1.868124000
	8	-1.868741000	-0.860744000	-1.271028000	8	-1.792453000	-0.854489000	-1.239500000	8	-4.331870000	-0.589497000	0.443026000
	8	3.756597000	-0.423041000	-1.074705000	8	3.735801000	-0.314660000	-1.131735000	8	4.001870000	-0.238348000	-0.138133000
	8	-2.846141000	-1.390602000	0.688708000	8	-3.161242000	-1.374937000	0.467119000	8	-2.636631000	-1.709645000	-0.436141000
	7	-3.619092000	1.237970000	0.908779000	7	-3.582295000	1.342444000	0.900832000	7	-3.394269000	1.804996000	-0.079943000
	6	-1.139594000	1.184618000	1.202357000	6	-1.149555000	1.003088000	1.271148000	6	-1.392993000	0.859247000	1.034197000
	6	-2.335909000	0.902871000	0.251632000	6	-2.331812000	0.879230000	0.274906000	6	-2.402024000	0.685431000	-0.125265000
	6	0.177964000	0.783647000	0.607780000	6	0.167333000	0.651311000	0.661506000	6	0.026418000	0.520796000	0.677720000
	6	0.743497000	-0.443424000	0.916831000	6	0.830540000	-0.500579000	1.012420000	6	0.733572000	-0.415745000	1.412232000
	6	0.831240000	1.637350000	-0.304198000	6	0.730061000	1.528354000	-0.325421000	6	0.662765000	1.205067000	-0.387863000
	6	1.946523000	-0.827365000	0.336623000	6	2.044085000	-0.813216000	0.400817000	6	2.059665000	-0.701080000	1.102994000
	6	-2.394893000	-0.581938000	-0.077675000	6	-2.498513000	-0.567965000	-0.144767000	6	-3.193146000	-0.627559000	-0.031057000
	6	2.030322000	1.275490000	-0.887049000	6	1.915086000	1.249188000	-0.943102000	6	1.958703000	0.933453000	-0.728939000
	6	2.596721000	0.045066000	-0.576860000	6	2.594810000	0.073720000	-0.601906000	6	2.687698000	-0.034009000	-0.000399000
	1	-1.313250000	0.643958000	2.134088000	1	-1.350415000	0.372766000	2.136938000	1	-1.716377000	0.281005000	1.898174000
	1	-1.141925000	2.253670000	1.426754000	1	-1.128229000	2.046898000	1.593881000	1	-1.411473000	1.912082000	1.329519000
	1	-2.240797000	1.485602000	-0.660671000	1	-2.140070000	1.488415000	-0.604413000	1	-1.911060000	0.757416000	-1.092195000
	1	0.272201000	-1.122067000	1.615682000	1	0.428403000	-1.179975000	1.751073000	1	0.272534000	-0.938130000	2.238672000
	1	0.394255000	2.597422000	-0.546620000	1	0.192122000	2.432033000	-0.579143000	1	0.111142000	1.950506000	-0.944290000
	1	2.531197000	1.941577000	-1.578634000	1	2.341972000	1.908527000	-1.686819000	1	2.459450000	1.458098000	-1.531742000
	1	-3.567134000	2.151233000	1.352213000	1	-3.442499000	2.287769000	1.250841000	1	-2.916877000	2.708937000	-0.103963000
	1	-3.796366000	0.543192000	1.635512000	1	-3.795935000	0.754047000	1.704994000	1	-3.956148000	1.744684000	0.774086000
	1	3.326391000	-2.131929000	0.185636000	1	3.510390000	-2.023583000	0.237482000	1	3.655779000	-1.656987000	1.542683000
	1	-1.907534000	-1.822783000	-1.409186000	1	-1.872396000	-1.805550000	-1.435768000	1	4.363556000	0.257901000	-0.890551000
	1	4.175407000	0.204042000	-1.678832000	1	4.065746000	0.308297000	-1.803862000	1	-4.037700000	1.751361000	-0.873028000
	79	-7.455730000	1.233565000	-1.829958000	79	-7.385724000	1.398151000	-1.874230000	79	-0.640930000	-1.921579000	-1.075149000
	79	-5.343475000	1.228785000	-0.358948000	79	-5.310970000	1.365824000	-0.373651000	79	1.848199000	-2.056016000	-1.626089000
Au₂⁻-Ld	8	1.708340000	-2.851013000	0.898628000	8	2.714021000	-1.490074000	1.710192000	8	2.412985000	-2.243277000	0.418972000
	8	-1.496401000	-0.523726000	-1.904790000	8	-1.064104000	-1.273254000	-1.396259000	8	-1.383502000	-0.446080000	-2.241479000
	8	3.794051000	-1.534772000	-0.041900000	8	4.202139000	-0.059143000	-0.054762000	8	3.969853000	-0.095713000	-0.161373000
	8	-3.100007000	-0.861327000	-0.373746000	8	-2.349528000	-1.766340000	0.377149000	8	-3.273290000	-1.261555000	-1.341834000
	7	-3.248780000	1.947237000	-0.197520000	7	-3.630500000	0.725316000	-0.098425000	7	-3.818423000	1.052390000	-0.091551000
	6	-1.085049000	1.180675000	0.867439000	6	-1.288568000	1.152392000	0.732123000	6	-1.585404000	0.556962000	0.794358000
	6	-1.971791000	1.265378000	-0.405152000	6	-2.205999000	0.525186000	-0.352702000	6	-2.397773000	0.791932000	-0.487821000
	6	0.240159000	0.498780000	0.663291000	6	0.178767000	0.882352000	0.535088000	6	-0.108640000	0.413862000	0.550200000
	6	0.373913000	-0.870905000	0.906883000	6	0.801757000	-0.156866000	1.227286000	6	0.492857000	-0.842381000	0.598595000
	6	1.337083000	1.201144000	0.174548000	6	0.926185000	1.612256000	-0.386963000	6	0.677834000	1.525500000	0.256743000
	6	1.574620000	-1.511112000	0.659119000	6	2.136984000	-0.457176000	1.011322000	6	1.850096000	-0.988675000	0.359000000

	6	-2.273392000	-0.140707000	-0.879457000	6	-1.909304000	-0.955166000	-0.414517000	6	-2.353083000	-0.411692000	-1.446570000
	6	2.549684000	0.565891000	-0.076136000	6	2.267467000	1.317454000	-0.606808000	6	2.039525000	1.385309000	0.012860000
	6	2.673475000	-0.794295000	0.162508000	6	2.878407000	0.287014000	0.091428000	6	2.629596000	0.131246000	0.062093000
	1	-1.668288000	0.669872000	1.638524000	1	-1.614662000	0.767673000	1.700628000	1	-1.972960000	-0.335251000	1.288710000
	1	-0.929502000	2.210291000	1.203021000	1	-1.484755000	2.226277000	0.715527000	1	-1.770876000	1.403239000	1.460397000
	1	-1.411078000	1.778935000	-1.186720000	1	-1.953539000	0.962650000	-1.317066000	1	-2.045550000	1.681827000	-1.003897000
	1	-0.456618000	-1.451637000	1.290786000	1	0.245138000	-0.755160000	1.938057000	1	-0.095667000	-1.723654000	0.821763000
	1	1.256947000	2.265105000	-0.017205000	1	0.461073000	2.417925000	-0.941138000	1	0.227976000	2.509604000	0.216931000
	1	3.398633000	1.123725000	-0.457766000	1	2.851197000	1.886394000	-1.320861000	1	2.654686000	2.248250000	-0.213744000
	1	-3.094744000	2.809628000	0.312708000	1	-3.793608000	1.721680000	0.012982000	1	-3.883583000	1.871123000	0.517233000
	1	-3.845888000	1.356535000	0.372808000	1	-3.859967000	0.300606000	0.796398000	1	-4.197760000	0.243186000	0.432904000
	1	2.627031000	-3.069660000	0.678928000	1	3.613830000	-1.626360000	1.379028000	1	3.359687000	-2.168330000	0.229234000
	1	-1.672756000	-1.464465000	-2.065860000	1	-0.726343000	-2.195632000	-1.266532000	1	4.416628000	0.742066000	-0.344750000
	1	4.581714000	-0.972741000	-0.279070000	1	4.592856000	0.442567000	-0.783278000	1	-4.409237000	1.198502000	-0.911355000
	79	6.468955000	0.170363000	-0.714395000	79	0.659605000	-4.001019000	-0.613057000	79	-4.402205000	0.840285000	3.624182000
	79	5.484759000	2.500304000	-1.595973000	79	2.295168000	-2.510476000	-2.126792000	79	-4.957280000	-1.325236000	2.142424000
Au₃⁰-Ld	8	2.762775000	0.945396000	2.151769000	8	2.811600000	-0.997907000	-1.595632000	8	1.470768000	-1.981456000	2.043014000
	8	-3.850118000	-1.369424000	-1.274772000	8	-3.235746000	-1.871388000	0.861695000	8	-1.979302000	-0.305292000	-1.710773000
	8	3.848596000	1.453585000	-0.266535000	8	4.159733000	-0.383724000	0.666010000	8	3.210898000	-1.391703000	0.035033000
	8	-4.600684000	-0.006018000	0.346870000	8	-2.148961000	-0.455359000	2.216293000	8	-2.992744000	-0.754914000	0.249433000
	7	-2.272574000	1.428253000	0.429665000	7	-3.669786000	0.649028000	-0.501855000	7	-3.831889000	1.891935000	0.281958000
	6	-1.292059000	-0.858882000	0.113579000	6	-1.279588000	1.169066000	0.045558000	6	-1.435307000	1.757732000	0.858169000
	6	-2.305602000	0.196187000	-0.382524000	6	-2.358790000	0.096186000	-0.142494000	6	-2.483887000	1.499764000	-0.241213000
	6	0.133211000	-0.388807000	0.004419000	6	0.125220000	0.686594000	0.280271000	6	-0.159962000	0.984185000	0.643453000
	6	0.845848000	-0.026368000	1.144915000	6	0.776814000	-0.123669000	-0.696042000	6	0.107899000	-0.128389000	1.439388000
	6	0.715874000	-0.216077000	-1.247856000	6	0.845701000	1.085335000	1.390923000	6	0.727680000	1.308447000	-0.379841000
	6	2.103747000	0.553477000	1.037256000	6	2.152034000	-0.429064000	-0.556266000	6	1.235949000	-0.903274000	1.224890000
	6	-3.712758000	-0.381094000	-0.374318000	6	-2.545735000	-0.748980000	1.108470000	6	-2.491865000	0.023273000	-0.640623000
	6	1.968413000	0.371505000	-1.361669000	6	2.188740000	0.731105000	1.554481000	6	1.856887000	0.529823000	-0.606705000
	6	2.645950000	0.783623000	-0.227732000	6	2.844353000	-0.021010000	0.602946000	6	2.115283000	-0.576366000	0.190395000
	1	-1.448710000	-1.757741000	-0.483382000	1	-1.575380000	1.822296000	0.867485000	1	-1.868325000	1.463259000	1.815195000
	1	-1.532470000	-1.114451000	1.149352000	1	-1.290913000	1.770690000	-0.867703000	1	-1.246023000	2.832170000	0.892230000
	1	-2.055720000	0.465252000	-1.409485000	1	-2.063902000	-0.586953000	-0.940024000	1	-2.296324000	2.105733000	-1.121876000
	1	0.417969000	-0.143251000	2.132348000	1	0.323511000	-0.267976000	-1.669614000	1	-0.570747000	-0.409741000	2.234206000
	1	0.179048000	-0.501801000	-2.143692000	1	0.366574000	1.694094000	2.145619000	1	0.533892000	2.164118000	-1.014048000
	1	2.411341000	0.541177000	-2.333820000	1	2.734879000	1.053712000	2.432625000	1	2.547989000	0.775223000	-1.404352000
	1	-2.395366000	1.186456000	1.409592000	1	-3.583114000	1.101730000	-1.406436000	1	-3.819207000	2.856533000	0.623432000
	1	-3.077405000	2.002691000	0.195444000	1	-3.905609000	1.382616000	0.161875000	1	-4.097020000	1.276492000	1.056483000
	1	3.538150000	1.451174000	1.864942000	1	3.722977000	-1.194464000	-1.327532000	1	2.218831000	-2.485821000	1.691071000
	1	-4.760949000	-1.700417000	-1.216101000	1	-3.325198000	-2.376082000	1.689164000	1	3.707774000	-1.126390000	-0.750908000
	1	3.776117000	2.176680000	-0.905855000	1	4.553199000	-0.070330000	1.492781000	1	-4.547278000	1.816845000	-0.445102000
	79	1.499243000	4.301680000	0.879244000	79	2.078764000	-4.031004000	1.561200000	79	-2.266164000	-2.766705000	0.191939000

	79	-0.511818000	2.722950000	0.268012000	79	-0.686141000	-4.332785000	1.198761000	79	0.202376000	-3.572661000	-0.907999000
	79	1.149732000	3.614346000	-1.780758000	79	0.490667000	-2.160978000	0.294361000	79	-1.582341000	-5.269400000	0.414161000
Au₃⁺-Ld	8	3.457550000	-0.623919000	2.163453000	8	2.347558000	-2.046071000	-0.443971000	8	2.791357000	-2.319106000	0.626658000
	8	-1.709197000	-0.607487000	-2.373754000	8	-2.366185000	0.657703000	-2.129615000	8	-3.075124000	0.909248000	-2.228714000
	8	4.446182000	0.195675000	-0.170968000	8	4.166099000	-0.048642000	-0.160107000	8	4.242618000	-0.022566000	0.520332000
	8	-2.461263000	-1.905591000	-0.707259000	8	-2.628377000	-1.005277000	-0.655727000	8	-4.508449000	1.029809000	-0.537439000
	7	-3.568922000	0.568579000	0.160031000	7	-3.562491000	1.537754000	0.671452000	7	-2.727340000	1.913118000	1.237336000
	6	-1.151452000	0.351403000	0.855256000	6	-1.269581000	0.723027000	1.341278000	6	-1.448714000	0.007307000	0.274962000
	6	-2.193258000	0.444176000	-0.285097000	6	-2.206289000	1.212054000	0.222381000	6	-2.193030000	1.313713000	-0.024837000
	6	0.308748000	0.255366000	0.474636000	6	0.165772000	0.546791000	0.929164000	6	0.054874000	0.090896000	0.417266000
	6	1.217137000	-0.326884000	1.418521000	6	0.630794000	-0.657543000	0.420629000	6	0.769060000	-1.094518000	0.504277000
	6	0.827889000	0.779528000	-0.692171000	6	1.076756000	1.611909000	1.063594000	6	0.774632000	1.303545000	0.397562000
	6	2.613315000	-0.277942000	1.185391000	6	1.961073000	-0.832421000	0.044794000	6	2.159620000	-1.115641000	0.546733000
	6	-2.137502000	-0.803404000	-1.143004000	6	-2.395312000	0.155572000	-0.847922000	6	-3.361642000	1.076109000	-0.985709000
	6	2.205582000	0.758062000	-0.951260000	6	2.439785000	1.447417000	0.690746000	6	2.197125000	1.288925000	0.408192000
	6	3.094487000	0.231814000	-0.041187000	6	2.876157000	0.209997000	0.184231000	6	2.884941000	0.075772000	0.485206000
	1	-1.420399000	-0.495250000	1.490085000	1	-1.665955000	-0.214459000	1.735406000	1	-1.656740000	-0.695925000	-0.531748000
	1	-1.292588000	1.249814000	1.464711000	1	-1.329129000	1.470916000	2.133151000	1	-1.881609000	-0.443170000	1.171932000
	1	-1.973695000	1.296037000	-0.926371000	1	-1.783086000	2.106375000	-0.232595000	1	-1.545907000	2.066978000	-0.463536000
	1	0.892741000	-0.501599000	2.438902000	1	-0.041416000	-1.498859000	0.311935000	1	0.246641000	-2.043195000	0.511591000
	1	0.180742000	1.227748000	-1.431230000	1	0.782678000	2.507989000	1.593441000	1	0.275074000	2.252537000	0.536709000
	1	2.578448000	1.175478000	-1.879157000	1	3.179121000	2.185209000	0.979768000	1	2.747596000	2.214740000	0.518899000
	1	-3.760908000	1.485017000	0.541808000	1	-3.507557000	2.343386000	1.286771000	1	-1.981447000	2.029024000	1.927839000
	1	-3.817311000	-0.139069000	0.840576000	1	-3.918716000	0.765642000	1.228782000	1	-3.455679000	1.310459000	1.629952000
	1	4.371596000	-0.535329000	1.850940000	1	3.290043000	-2.018889000	-0.669417000	1	3.750886000	-2.183646000	0.606770000
	1	-1.722489000	-1.443580000	-2.872665000	1	-2.554713000	-0.062245000	-2.761413000	1	4.645715000	0.856753000	0.481838000
	1	4.744119000	0.641695000	-0.972815000	1	4.715874000	0.740005000	-0.044698000	1	-3.147372000	2.827342000	1.055912000
	79	1.187090000	-2.427536000	0.611967000	79	-0.718107000	2.057000000	-2.760743000	79	1.056799000	1.612711000	-4.451835000
	79	-1.011962000	-3.562016000	-0.557283000	79	1.432650000	2.478294000	-1.111758000	79	-1.158919000	1.205776000	-3.087152000
	79	1.093907000	-5.017302000	-0.070225000	79	1.219630000	3.643476000	-3.490857000	79	1.308870000	1.485997000	-1.834118000
Au₃⁻-Ld	8	2.228143000	-1.936053000	1.468825000	8	2.378073000	-2.181102000	0.173914000	8	2.449868000	-2.269386000	0.176536000
	8	-1.417198000	-0.709600000	-1.526590000	8	-2.083044000	-0.675680000	-1.058630000	8	-1.647371000	-0.520144000	-1.599286000
	8	3.867827000	-0.312809000	-0.281227000	8	3.564472000	-0.447512000	-1.547131000	8	4.067835000	-0.186491000	-0.473452000
	8	-2.973565000	-1.327544000	-0.018075000	8	-2.884251000	-1.317236000	0.938475000	8	-3.537902000	-0.791098000	-0.417212000
	7	-3.771272000	1.330475000	0.082588000	7	-3.473759000	1.402029000	1.391842000	7	-3.443551000	1.650221000	0.576615000
	6	-1.432176000	1.237299000	1.020072000	6	-0.988026000	1.141308000	1.444578000	6	-1.237665000	0.764052000	1.304198000
	6	-2.376281000	0.991527000	-0.189358000	6	-2.287009000	0.994136000	0.620461000	6	-2.147529000	1.070110000	0.105804000
	6	0.001161000	0.864824000	0.761371000	6	0.248005000	0.760205000	0.675878000	6	0.186972000	0.526106000	0.878539000
	6	0.506910000	-0.346963000	1.219826000	6	0.779776000	-0.524504000	0.789369000	6	0.691521000	-0.766213000	0.749601000
	6	0.819373000	1.665540000	-0.031048000	6	0.845383000	1.659421000	-0.204178000	6	1.008265000	1.603901000	0.557741000
	6	1.790167000	-0.774750000	0.902706000	6	1.881145000	-0.905169000	0.039712000	6	1.984892000	-0.979247000	0.299222000

	6	-2.307177000	-0.481568000	-0.570235000	6	-2.468185000	-0.449531000	0.200892000	6	-2.474937000	-0.188469000	-0.720759000
	6	2.092909000	1.239990000	-0.377707000	6	1.953139000	1.284564000	-0.956958000	6	2.306415000	1.397478000	0.104808000
	6	2.591820000	0.021903000	0.069437000	6	2.472960000	0.004478000	-0.840103000	6	2.797710000	0.108168000	-0.029418000
	1	-1.825915000	0.668957000	1.866255000	1	-1.083888000	0.528144000	2.342537000	1	-1.631221000	-0.096813000	1.847644000
	1	-1.513123000	2.300275000	1.271810000	1	-0.935310000	2.186604000	1.754020000	1	-1.271671000	1.624449000	1.977544000
	1	-2.012095000	1.576364000	-1.035563000	1	-2.223707000	1.616137000	-0.269073000	1	-1.683113000	1.820035000	-0.532041000
	1	-0.103615000	-1.005954000	1.824674000	1	0.332603000	-1.246472000	1.461788000	1	0.073936000	-1.623851000	0.985434000
	1	0.450342000	2.612832000	-0.407589000	1	0.445376000	2.660398000	-0.305903000	1	0.631065000	2.614154000	0.648379000
	1	2.731426000	1.842570000	-1.011217000	1	2.422733000	1.982902000	-1.639697000	1	2.945441000	2.235086000	-0.147818000
	1	-3.821634000	2.149595000	0.677688000	1	-3.334311000	2.350012000	1.731032000	1	-3.312702000	2.306685000	1.347829000
	1	-4.191315000	0.554967000	0.586490000	1	-3.565314000	0.802886000	2.209354000	1	-4.055967000	0.877779000	0.858921000
	1	2.788701000	-2.446397000	0.849907000	1	3.131194000	-2.287091000	-0.425697000	1	3.359654000	-2.242631000	-0.154059000
	1	-1.274889000	-1.685847000	-1.657371000	1	-2.164439000	-1.627500000	-1.250016000	1	4.532579000	0.631010000	-0.699160000
	1	3.957873000	-1.281903000	-0.409302000	1	3.889944000	0.253774000	-2.128011000	1	-3.901227000	2.145847000	-0.206895000
	79	1.665643000	-3.585766000	-1.557517000	79	-7.588431000	1.263588000	-1.119599000	79	-1.879426000	3.018872000	-2.804302000
	79	-0.819472000	-3.846338000	-2.274801000	79	-9.871622000	1.180639000	-2.546593000	79	-4.464963000	3.129732000	-2.444397000
	79	4.172305000	-3.574829000	-0.786958000	79	-5.396453000	1.337294000	0.243004000	79	0.701875000	2.754339000	-2.943600000
Au₄⁰-Ld	8	2.667445000	-1.740284000	0.687950000	8	2.704619000	-1.756756000	0.632955000	8	2.210578000	-2.053076000	-0.757743000
	8	-2.165012000	-1.396823000	-0.733351000	8	-1.977951000	-1.323353000	-0.828804000	8	-1.977235000	0.297114000	-2.097579000
	8	3.592640000	-0.244569000	-1.336975000	8	3.614529000	-0.135852000	-1.345706000	8	4.108200000	-0.207642000	-0.163313000
	8	-2.495641000	-1.609312000	1.490387000	8	-2.583307000	-1.744399000	1.293605000	8	-3.331499000	-0.723838000	-0.665248000
	7	-3.702663000	0.888164000	1.244195000	7	-3.709317000	0.854554000	1.264766000	7	-3.549425000	1.557722000	0.771724000
	6	-1.214061000	1.162782000	1.304213000	6	-1.228096000	1.072897000	1.352034000	6	-1.317976000	0.670876000	1.259492000
	6	-2.419874000	0.581445000	0.552364000	6	-2.440717000	0.543904000	0.562447000	6	-2.228642000	1.214273000	0.146540000
	6	0.087768000	0.843502000	0.616624000	6	0.077158000	0.798906000	0.654076000	6	0.121204000	0.478083000	0.865799000
	6	0.811410000	-0.290938000	0.982028000	6	0.821515000	-0.336958000	0.972881000	6	0.535189000	-0.686608000	0.222620000
	6	0.549516000	1.635150000	-0.429534000	6	0.531619000	1.639291000	-0.359038000	6	1.070411000	1.458998000	1.151014000
	6	1.976338000	-0.632280000	0.314823000	6	1.993839000	-0.628912000	0.294333000	6	1.860257000	-0.886153000	-0.134602000
	6	-2.352905000	-0.943167000	0.494835000	6	-2.351540000	-0.961727000	0.397878000	6	-2.535731000	0.179664000	-0.954780000
	6	1.718539000	1.299815000	-1.104447000	6	1.708539000	1.352667000	-1.042116000	6	2.426381000	1.281961000	0.787934000
	6	2.428902000	0.170456000	-0.737496000	6	2.440971000	0.220270000	-0.721139000	6	2.820754000	0.086728000	0.159969000
	1	-1.216167000	0.757755000	2.318583000	1	-1.237639000	0.612763000	2.341818000	1	-1.741314000	-0.271939000	1.612651000
	1	-1.345375000	2.246109000	1.377167000	1	-1.375071000	2.147207000	1.475740000	1	-1.360613000	1.383416000	2.085616000
	1	-2.473155000	0.981262000	-0.457153000	1	-2.476673000	1.009668000	-0.418474000	1	-1.828665000	2.133595000	-0.272251000
	1	0.472395000	-0.932647000	1.785244000	1	0.490438000	-1.010974000	1.753548000	1	-0.179240000	-1.466890000	-0.008532000
	1	0.001307000	2.521045000	-0.725009000	1	-0.034558000	2.524439000	-0.620239000	1	0.786929000	2.345322000	1.701407000
	1	2.078401000	1.920637000	-1.917288000	1	2.067226000	2.007121000	-1.827855000	1	3.189928000	1.953624000	1.163499000
	1	-3.787398000	1.887388000	1.402731000	1	-3.790075000	1.864872000	1.358922000	1	-3.421822000	2.146086000	1.598385000
	1	-3.684784000	0.426360000	2.152311000	1	-3.674661000	0.468998000	2.207543000	1	-4.027502000	0.693467000	1.044786000
	1	3.435439000	-1.831788000	0.108012000	1	3.485812000	-1.814975000	0.063467000	1	3.161121000	-2.044315000	-0.945246000
	1	-2.380700000	-2.363847000	-0.774613000	1	-1.978477000	-2.298305000	-0.890075000	1	4.693396000	0.531358000	0.057518000
	1	3.812221000	0.332172000	-2.076022000	1	3.825509000	0.507166000	-2.036561000	1	-4.150829000	2.054680000	0.110815000

	79	-5.435684000	0.093133000	0.216682000	79	-5.451884000	0.080957000	0.305220000	79	1.308801000	3.509452000	-3.563147000
	79	-7.594233000	-0.744583000	-0.981688000	79	-7.688585000	-0.684904000	-0.815427000	79	-0.407554000	1.708489000	-2.543642000
	79	-3.707086000	-4.283139000	-1.262694000	79	-3.977693000	-4.325069000	-1.498870000	79	1.912137000	5.090803000	-5.568765000
	79	-5.505524000	-2.447439000	-1.029230000	79	-5.633471000	-2.397135000	-1.044276000	79	1.763504000	2.412320000	-1.166512000
Au₄⁺-Ld	8	3.474545000	-0.256642000	2.035174000	8	2.944534000	-1.625270000	0.716052000	8	2.326726000	-2.072460000	-0.460573000
	8	-2.729381000	0.994541000	-2.357329000	8	-1.525659000	-1.359909000	-1.045983000	8	-1.613887000	0.074148000	-1.969582000
	8	4.296534000	0.493618000	-0.383130000	8	3.844527000	0.157340000	-1.127874000	8	4.204877000	-0.124440000	-0.243890000
	8	-2.355991000	-1.035762000	-1.568184000	8	-2.679156000	-2.062319000	0.737582000	8	-3.008589000	-0.870621000	-0.530972000
	7	-3.648551000	0.845146000	0.494113000	7	-3.718790000	0.549985000	1.035842000	7	-3.456910000	1.527119000	0.676400000
	6	-1.239711000	0.340293000	0.922172000	6	-1.268312000	0.808284000	1.237692000	6	-1.180744000	0.843771000	1.295188000
	6	-2.292404000	0.896253000	-0.034850000	6	-2.434642000	0.314354000	0.339876000	6	-2.099375000	1.221549000	0.122383000
	6	0.202894000	0.359921000	0.475811000	6	0.091840000	0.671855000	0.612426000	6	0.247623000	0.608746000	0.892497000
	6	1.188332000	-0.117729000	1.397211000	6	0.914682000	-0.401973000	0.950120000	6	0.664351000	-0.619989000	0.404372000
	6	0.630348000	0.856572000	-0.738893000	6	0.536973000	1.591857000	-0.333050000	6	1.190988000	1.644463000	1.007381000
	6	2.562987000	-0.004404000	1.089814000	6	2.157988000	-0.555306000	0.358274000	6	1.983521000	-0.841464000	0.015313000
	6	-2.422967000	0.172065000	-1.370486000	6	-2.250661000	-1.150381000	0.031402000	6	-2.269617000	0.058369000	-0.867206000
	6	1.992533000	0.897563000	-1.069977000	6	1.783794000	1.443697000	-0.930139000	6	2.540360000	1.430613000	0.618015000
	6	2.952886000	0.465744000	-0.183907000	6	2.597469000	0.373812000	-0.588623000	6	2.929657000	0.176044000	0.123625000
	1	-1.519595000	-0.680331000	1.199279000	1	-1.312756000	0.257315000	2.178737000	1	-1.589994000	-0.049244000	1.771419000
	1	-1.327463000	0.928217000	1.840681000	1	-1.482220000	1.857162000	1.449756000	1	-1.222043000	1.661761000	2.016692000
	1	-2.065066000	1.934699000	-0.274897000	1	-2.438424000	0.870413000	-0.593953000	1	-1.746037000	2.122985000	-0.370259000
	1	0.925320000	-0.263773000	2.439429000	1	0.590370000	-1.134846000	1.678929000	1	-0.036177000	-1.440583000	0.313684000
	1	-0.073217000	1.243787000	-1.461399000	1	-0.089556000	2.431255000	-0.607247000	1	0.929632000	2.556481000	1.527162000
	1	2.294168000	1.287797000	-2.034756000	1	2.136728000	2.159858000	-1.662893000	1	3.304580000	2.155748000	0.870154000
	1	-3.917760000	1.686097000	0.982773000	1	-3.748772000	1.533097000	1.301870000	1	-3.392587000	2.180514000	1.460925000
	1	-3.818065000	0.033321000	1.072495000	1	-3.732088000	0.017142000	1.905728000	1	-3.896323000	0.659136000	0.999306000
	1	4.364189000	-0.134956000	1.668543000	1	3.773957000	-1.585823000	0.217558000	1	3.264510000	-2.074201000	-0.706652000
	1	-2.923977000	0.480917000	-3.160784000	1	-1.371125000	-2.316522000	-1.162289000	1	4.777590000	0.650544000	-0.151281000
	1	4.528447000	0.904790000	-1.224362000	1	4.057152000	0.858694000	-1.759220000	1	-4.060090000	1.938833000	-0.039519000
	79	1.212130000	-2.291242000	0.723883000	79	-5.584898000	0.150750000	0.047518000	79	1.106390000	3.688079000	-3.530636000
	79	-1.185117000	-2.688815000	-0.712675000	79	-7.931239000	0.404427000	-1.138571000	79	-1.028560000	3.189721000	-5.137267000
	79	2.766873000	-4.496894000	1.063494000	79	-4.887371000	-2.605256000	0.280177000	79	1.498526000	2.513956000	-1.185485000
79	0.280642000	-4.756195000	-0.010073000	79	-7.351742000	-2.124446000	-0.484039000	79	-0.649132000	1.734574000	-2.866781000	
Au₄-Ld	8	2.377374000	-0.700123000	2.807062000	8	2.553600000	-2.037947000	0.710372000	8	2.106795000	-2.257571000	1.172684000
	8	-0.777204000	-1.807189000	-0.844772000	8	-1.901235000	-0.939681000	-1.062818000	8	-1.776826000	-0.960791000	-1.468084000
	8	4.146360000	-0.233730000	0.858163000	8	3.763656000	-0.578286000	-1.242898000	8	3.810901000	-0.762878000	-0.338085000
	8	-2.279054000	-1.695731000	0.834334000	8	-2.763458000	-1.327113000	0.974687000	8	-3.403430000	-1.103821000	0.078251000
	7	-3.510646000	0.346526000	-0.664351000	7	-3.498592000	1.393298000	1.002137000	7	-3.667154000	1.547322000	0.177212000
	6	-1.297109000	1.194849000	0.202522000	6	-1.013096000	1.277734000	1.194227000	6	-1.353896000	1.192115000	0.936620000
	6	-2.061506000	0.161853000	-0.673912000	6	-2.258223000	0.941212000	0.344528000	6	-2.332140000	0.998653000	-0.230738000
	6	0.170399000	0.903599000	0.370136000	6	0.276577000	0.829640000	0.562382000	6	0.035558000	0.710492000	0.617482000

6	0.622356000	0.294273000	1.540104000	6	0.853536000	-0.385762000	0.929628000	6	0.463214000	-0.544541000	1.047446000
6	1.075776000	1.136178000	-0.661340000	6	0.886436000	1.589503000	-0.432938000	6	0.901362000	1.491143000	-0.144600000
6	1.948602000	-0.081567000	1.673549000	6	2.012872000	-0.835284000	0.317955000	6	1.725315000	-1.016914000	0.722111000
6	-1.741020000	-1.226770000	-0.143151000	6	-2.352737000	-0.555965000	0.134358000	6	-2.526037000	-0.490554000	-0.582458000
6	2.409379000	0.767843000	-0.531006000	6	2.050334000	1.144336000	-1.050489000	6	2.167818000	1.023474000	-0.476410000
6	2.849716000	0.156868000	0.632349000	6	2.615285000	-0.067254000	-0.681744000	6	2.583431000	-0.229628000	-0.050716000
1	-1.784745000	1.209246000	1.180064000	1	-1.137736000	0.814802000	2.175186000	1	-1.746024000	0.661945000	1.807084000
1	-1.447431000	2.178060000	-0.255250000	1	-1.014012000	2.360545000	1.330793000	1	-1.331748000	2.257811000	1.176735000
1	-1.690520000	0.225598000	-1.697407000	1	-2.184770000	1.431166000	-0.623115000	1	-2.004194000	1.555218000	-1.104283000
1	-0.065380000	0.059771000	2.342542000	1	0.399509000	-0.999361000	1.698089000	1	-0.191283000	-1.174070000	1.637632000
1	0.738169000	1.581628000	-1.589155000	1	0.453194000	2.536219000	-0.730153000	1	0.587902000	2.469986000	-0.485278000
1	3.107768000	0.923379000	-1.342080000	1	2.529662000	1.735649000	-1.821789000	1	2.845506000	1.627280000	-1.068420000
1	-3.736213000	1.334336000	-0.703304000	1	-3.420446000	2.388035000	1.198124000	1	-3.580182000	2.440863000	0.665361000
1	-3.870517000	-0.016857000	0.213331000	1	-3.594421000	0.919974000	1.898321000	1	-4.113908000	0.855269000	0.789133000
1	3.275613000	-1.013291000	2.618837000	1	3.358510000	-2.203589000	0.198398000	1	3.008192000	-2.463245000	0.869612000
1	-0.381726000	-2.573617000	-0.359532000	1	-1.935408000	-1.911612000	-1.119251000	1	4.344764000	-0.134150000	-0.842792000
1	4.512846000	-0.651438000	0.047045000	1	4.092267000	0.026437000	-1.922238000	1	-4.272110000	1.677474000	-0.635741000
79	5.107218000	-1.791303000	-1.926763000	79	-8.061478000	1.750647000	1.061819000	79	5.702274000	-3.077466000	1.726403000
79	1.272770000	-3.888246000	0.734671000	79	-10.199490000	1.275250000	-0.663587000	79	4.384602000	-4.799838000	0.049252000
79	2.881729000	-1.457198000	-3.534337000	79	-5.355413000	1.069017000	-0.153616000	79	7.580222000	-1.439340000	0.591406000
79	2.630847000	-2.732659000	-1.148484000	79	-7.554366000	0.723989000	-1.510473000	79	6.318464000	-3.213854000	-1.061776000

	Cationic				Neutral				Anionic			
Au₁₀-Ld - Zwitterionic (PEH)	8	1.303924153	-1.417496744	2.999292289	8	1.583945012	-1.361367510	3.100994601	8	1.607373950	-1.332539173	3.118736896
	8	-2.004704946	-0.734538242	-1.520328892	8	-2.270178937	-0.711583483	-1.757662287	8	-2.297528456	-0.694971269	-1.786843515
	8	3.134016104	-1.644138079	1.016938667	8	3.299280954	-1.543294502	1.009899545	8	3.301106768	-1.529766296	1.008007941
	8	-3.099390400	-0.644832286	0.458648590	8	-3.459036123	-0.636881163	0.155649957	8	-3.462167803	-0.644184853	0.140080844
	7	-3.725632067	2.003514486	-0.166318428	7	-3.629387781	2.138635559	-0.319856318	7	-3.630338450	2.137229458	-0.322301273
	6	-1.342552247	1.799113310	0.449174491	6	-1.450194634	1.541262481	0.623420004	6	-1.465425703	1.536342671	0.647361940
	6	-2.429177231	1.376388209	-0.568325132	6	-2.382724153	1.349192206	-0.580540603	6	-2.378818046	1.349008596	-0.569706652
	6	-0.153116363	0.873519748	0.540455109	6	-0.212484761	0.678352147	0.644278601	6	-0.218624322	0.686942245	0.667496591
	6	0.039240203	0.121159558	1.699235591	6	0.116406033	0.004357522	1.819849299	6	0.125864030	0.026923223	1.846407735
	6	0.760592198	0.738081910	-0.503068170	6	0.640066770	0.560889904	-0.452013602	6	0.623230401	0.564347086	-0.436378009
	6	1.134807194	-0.718683414	1.832698008	6	1.283717526	-0.736586746	1.916948200	6	1.295080555	-0.712504637	1.935943124
	6	-2.549197247	-0.140509487	-0.557848849	6	-2.752451594	-0.124054540	-0.755873682	6	-2.757563472	-0.122235771	-0.768729093
	6	1.854822971	-0.112268732	-0.380655638	6	1.809616273	-0.187976568	-0.362481781	6	1.794397195	-0.181774110	-0.353352381
	6	2.058088479	-0.827430863	0.791224236	6	2.145525306	-0.823991252	0.823006595	6	2.142379817	-0.810738211	0.832069722
	1	-1.814814403	1.849010356	1.431271356	1	-2.026941413	1.345659870	1.528487120	1	-2.049534734	1.322058275	1.543636685
	1	-1.027357188	2.808853489	0.180749316	1	-1.168226679	2.598316562	0.640636377	1	-1.195699117	2.596400637	0.683798991
	1	-2.201144087	1.719161201	-1.571656158	1	-1.946866425	1.732719823	-1.497133334	1	-1.931525466	1.740936013	-1.477311192
	1	-0.660263197	0.191432000	2.522229567	1	-0.536864466	0.054491985	2.681176705	1	-0.518647243	0.081906040	2.714107967
	1	0.622797542	1.296479635	-1.419748239	1	0.403755681	1.058371777	-1.383082164	1	0.376014767	1.052434238	-1.369557843
	1	2.567745510	-0.216428522	-1.189247362	1	2.473841091	-0.278217735	-1.213004734	1	2.448508856	-0.280103076	-1.210445273
	1	-3.613660141	3.014865395	-0.054836343	1	-3.400271269	3.107761375	-0.084295235	1	-3.406562483	3.104679503	-0.075382567
	1	-4.041739471	1.613790584	0.726814981	1	-4.143718102	1.726943584	0.464594395	1	-4.155470971	1.718631996	0.451188836
	1	2.035619962	-2.044073497	2.889473044	1	2.293990596	-2.002988289	2.944429470	1	2.310676162	-1.979887853	2.953069731
	1	3.619142986	-1.803357512	0.194801342	1	3.689478716	-1.783052523	0.157005955	1	3.619615630	-1.864784145	0.156804174
	1	-4.452367016	1.836673981	-0.867031403	1	-4.241540492	2.142271818	-1.139227501	1	-4.230047483	2.146382146	-1.150661650
	79	5.295850375	-5.452397320	1.140473832	79	5.322019040	-5.415793339	1.101725673	79	5.237163114	-5.435750986	1.118218633
	79	4.220553986	-4.680298056	-1.274860654	79	4.112412017	-4.591025757	-1.295048349	79	4.126348255	-4.562548929	-1.329756084
	79	3.663226656	-5.628325289	3.391250804	79	3.754333164	-5.594012912	3.339138775	79	3.747921609	-5.585322948	3.444625158
	79	2.655555777	-4.762071618	1.011739198	79	2.639088633	-4.716255082	1.017136073	79	2.572078139	-4.837165847	0.977984057
	79	1.591999128	-3.865814278	-1.324112284	79	1.517737725	-3.740224184	-1.308282285	79	1.552379867	-3.743473392	-1.422210940
	79	1.034679585	-4.997050426	3.281652599	79	1.091865605	-4.909266383	3.321465104	79	1.120654941	-4.867426423	3.345990080
	79	-0.026595679	-3.970389855	0.938589212	79	-0.006056813	-3.773918693	0.993039002	79	0.035532317	-3.840399940	0.945165460
	79	-0.623219147	-2.412114295	-1.203082129	79	-0.812161334	-2.421290058	-1.236432027	79	-0.769560388	-2.445772601	-1.342579153
	79	-1.625456890	-4.315318237	3.163750167	79	-1.455789531	-3.911147525	3.288804880	79	-1.383157746	-3.793090986	3.341418866
	79	-2.285373090	-2.457087108	1.374558279	79	-2.365285633	-2.378878371	1.247147569	79	-2.268752489	-2.402360684	1.177003194

Au₁₀-Ld - Zwitterionic (FF)	8	1.929337000	-2.753188000	0.977337000	8	1.442655000	-2.804818000	1.253009000	8	0.954520000	-3.070908000	1.006860000
	8	-3.300151000	1.427735000	-1.866232000	8	-3.458527000	0.751539000	-1.581267000	8	-3.152474000	0.408794000	-1.526150000
	8	2.299991000	-2.516588000	-1.697187000	8	1.847097000	-2.840223000	-1.443388000	8	1.791084000	-2.824443000	-1.575310000
	8	-4.106316000	0.159138000	-0.194333000	8	-3.582552000	-0.182770000	0.461702000	8	-3.433377000	-0.276422000	0.599305000
	7	-3.184291000	2.420694000	1.339902000	7	-3.220709000	2.639377000	1.188804000	7	-3.210525000	2.515465000	1.180231000
	6	-1.492838000	0.685154000	1.069142000	6	-1.169248000	1.300424000	1.020883000	6	-1.029291000	1.385248000	0.990617000
	6	-2.354998000	1.694009000	0.319510000	6	-2.367446000	1.846158000	0.242916000	6	-2.308019000	1.776880000	0.237233000
	6	-0.518878000	-0.123464000	0.247601000	6	-0.386651000	0.224239000	0.307060000	6	-0.237319000	0.310734000	0.289183000
	6	0.237174000	-1.091194000	0.920564000	6	0.144265000	-0.825427000	1.057490000	6	0.017622000	-0.889624000	0.947121000
	6	-0.332083000	0.027260000	-1.118664000	6	-0.157333000	0.242104000	-1.065097000	6	0.210324000	0.466920000	-1.021584000
	6	1.174563000	-1.870579000	0.262738000	6	0.896102000	-1.825457000	0.463570000	6	0.705297000	-1.915101000	0.316270000
	6	-3.325326000	1.055873000	-0.694120000	6	-3.218857000	0.725031000	-0.372508000	6	-3.039644000	0.541060000	-0.303954000
	6	0.585389000	-0.788456000	-1.813213000	6	0.577961000	-0.773293000	-1.673732000	6	0.885974000	-0.563571000	-1.663044000
	6	1.351737000	-1.731546000	-1.120152000	6	1.104526000	-1.812845000	-0.918554000	6	1.125387000	-1.761392000	-1.004381000
	1	-2.154117000	-0.002000000	1.602894000	1	-1.529531000	0.892900000	1.966718000	1	-1.309950000	1.023036000	1.980603000
	1	-0.933871000	1.235542000	1.831416000	1	-0.519080000	2.146473000	1.263354000	1	-0.431476000	2.289912000	1.126782000
	1	-1.755184000	2.446644000	-0.184162000	1	-2.067057000	2.530838000	-0.544086000	1	-2.098952000	2.452671000	-0.585767000
	1	0.116631000	-1.229876000	1.987600000	1	-0.023431000	-0.873777000	2.126110000	1	-0.333252000	-1.047622000	1.958871000
	1	-0.860703000	0.779807000	-1.683158000	1	-0.546643000	1.041689000	-1.679755000	1	0.022759000	1.390250000	-1.554479000
	1	0.836625000	-0.565981000	-2.842562000	1	0.778260000	-0.742088000	-2.736053000	1	1.224178000	-0.447737000	-2.684216000
	1	-2.584281000	2.859839000	2.042896000	1	-2.663237000	3.362873000	1.650688000	1	-2.717321000	3.305754000	1.603750000
	1	-3.813528000	1.768150000	1.816878000	1	-3.612675000	2.029832000	1.912485000	1	-3.522705000	1.892205000	1.930438000
	1	2.479421000	-3.272740000	0.370969000	1	1.765738000	-3.524498000	0.688997000	1	1.228558000	-3.759246000	0.380280000
	1	2.282457000	-2.417196000	-2.661169000	1	1.743870000	-2.859142000	-2.406371000	1	1.557897000	-2.886646000	-2.517257000
	1	-3.752169000	3.150228000	0.902068000	1	-3.993026000	3.095447000	0.697079000	1	-4.035988000	2.874089000	0.695110000
	79	0.091766000	-5.158581000	1.353701000	79	0.217856000	-6.049602000	1.012112000	79	-0.188929000	-6.462206000	1.115661000
	79	-1.216574000	-2.402974000	-2.390918000	79	-1.590846000	-2.776113000	-2.527129000	79	-1.852510000	-3.071845000	-2.383135000
	79	-5.300792000	-6.020499000	-2.275888000	79	-5.219010000	-6.358355000	-2.864481000	79	-5.040300000	-6.411991000	-3.086929000
	79	-0.056561000	-2.932360000	-4.807901000	79	-0.333571000	-2.489967000	-4.876498000	79	-0.442925000	-2.297525000	-4.552970000
	79	-3.314573000	-4.224153000	-2.067928000	79	-3.734126000	-4.451761000	-1.723651000	79	-4.214405000	-4.579941000	-1.339349000
	79	-2.779956000	-6.900349000	-2.799792000	79	-2.548446000	-6.615026000	-3.134084000	79	-2.372829000	-5.946710000	-3.115046000
	79	-3.547619000	-1.827014000	-0.895100000	79	-3.151773000	-2.169745000	-0.342025000	79	-3.389450000	-2.387481000	-0.044408000
	79	-1.012779000	-6.107444000	-0.867874000	79	-0.308947000	-6.420574000	-1.606481000	79	-0.091716000	-6.227820000	-1.583934000
	79	-1.703570000	-3.557751000	0.180740000	79	-1.450599000	-4.292938000	-0.117117000	79	-1.814627000	-4.625867000	0.027865000
	79	-0.824442000	-5.067551000	-3.446466000	79	-0.505522000	-4.991915000	-3.901560000	79	0.073991000	-4.884753000	-3.896557000

Au₁₀-Ld - Zwitterionic (CTP)	8	-0.412156000	-3.394031000	0.322866000	8	-0.770004000	-3.636891000	0.118290000	8	-1.984206000	-3.511946000	1.157097000
	8	-3.367664000	0.578457000	-0.948263000	8	-2.906163000	0.500981000	-1.367764000	8	-2.354345000	0.752708000	-1.638595000
	8	0.321939000	-3.022849000	-2.274593000	8	1.017211000	-3.178280000	-1.912099000	8	0.182752000	-3.913972000	-0.430646000
	8	-3.712120000	0.130457000	1.240531000	8	-3.908901000	0.304502000	0.653498000	8	-3.950205000	1.137855000	-0.083147000
	7	-2.890429000	2.709012000	1.816489000	7	-2.870031000	2.738059000	1.356316000	7	-2.514253000	3.313062000	0.780883000
	6	-0.940720000	1.405707000	1.028043000	6	-1.005633000	1.124038000	1.172490000	6	-1.185011000	1.303987000	1.320490000
	6	-2.332968000	1.961592000	0.648072000	6	-2.134987000	1.842467000	0.409587000	6	-1.811208000	2.135488000	0.182929000
	6	-0.510141000	0.260133000	0.149581000	6	-0.413101000	-0.005053000	0.372347000	6	-0.763384000	-0.072062000	0.874447000
	6	-0.609724000	-1.045697000	0.626680000	6	-0.827156000	-1.315569000	0.605171000	6	-1.536244000	-1.177101000	1.226252000
	6	-0.096924000	0.469260000	-1.163889000	6	0.480377000	0.245245000	-0.665213000	6	0.343689000	-0.259805000	0.050216000
	6	-0.310493000	-2.126473000	-0.188264000	6	-0.351968000	-2.362871000	-0.169474000	6	-1.209798000	-2.446929000	0.775229000
	6	-3.247127000	0.798999000	0.280988000	6	-3.090325000	0.801261000	-0.162553000	6	-2.814741000	1.281033000	-0.589679000
	6	0.189161000	-0.608871000	-1.991070000	6	0.958299000	-0.797558000	-1.447882000	6	0.672747000	-1.528747000	-0.410447000
	6	0.077739000	-1.904318000	-1.510090000	6	0.554058000	-2.102410000	-1.201575000	6	-0.096622000	-2.625014000	-0.047909000
	1	-0.988125000	1.063019000	2.062639000	1	-1.419846000	0.736288000	2.104435000	1	-1.924947000	1.211535000	2.117365000
	1	-0.232050000	2.233420000	0.976680000	1	-0.248143000	1.869516000	1.419847000	1	-0.336513000	1.868079000	1.712480000
	1	-2.272387000	2.655326000	-0.183942000	1	-1.740985000	2.463055000	-0.388860000	1	-1.051882000	2.518586000	-0.491301000
	1	-0.929915000	-1.236852000	1.642728000	1	-1.538918000	-1.536875000	1.390437000	1	-2.413441000	-1.058255000	1.848728000
	1	-0.019933000	1.476128000	-1.553510000	1	0.801692000	1.258623000	-0.870022000	1	0.948236000	0.588177000	-0.245428000
	1	0.493023000	-0.454724000	-3.019352000	1	1.659788000	-0.610794000	-2.252391000	1	1.532494000	-1.680710000	-1.051815000
	1	-2.215466000	3.400095000	2.154686000	1	-2.217581000	3.349731000	1.853247000	1	-1.897071000	3.818814000	1.420890000
	1	-3.098437000	2.058805000	2.580656000	1	-3.377630000	2.173306000	2.043902000	1	-3.336688000	2.993672000	1.301116000
	1	-0.169268000	-4.038379000	-0.358280000	1	-0.544075000	-4.236717000	-0.613667000	1	-1.744421000	-4.287230000	0.625260000
	1	0.589691000	-2.764603000	-3.168472000	1	1.554118000	-2.874502000	-2.656886000	1	0.805019000	-3.915346000	-1.171200000
	1	-3.753067000	3.197966000	1.566113000	1	-3.546511000	3.324729000	0.862231000	1	-2.829713000	3.962254000	0.056552000
	79	-6.605872000	-5.588944000	-3.762189000	79	-5.790605000	-5.891382000	-1.981865000	79	-1.510445000	-6.538414000	-2.534976000
	79	-4.084098000	-2.033424000	1.031491000	79	-4.944254000	-1.619070000	0.244790000	79	-4.936338000	-1.018854000	-0.286971000
	79	-5.555464000	-5.687376000	-1.212190000	79	-4.514307000	-4.281117000	-0.087808000	79	-2.190464000	-3.894929000	-2.598035000
	79	-3.709369000	-1.410950000	-1.838996000	79	-6.864908000	-3.057054000	-0.922571000	79	-5.254752000	-3.520741000	-0.808873000
	79	-2.400588000	-3.573280000	-2.766617000	79	-5.051491000	-3.324549000	-3.197256000	79	-5.565779000	-5.186661000	-3.012780000
	79	-4.299623000	-4.623862000	0.959632000	79	-3.330556000	-1.472972000	-2.278273000	79	-2.832612000	-1.286460000	-2.417696000
	79	-2.791108000	-5.817102000	-0.962426000	79	-2.416156000	-3.909046000	-2.972572000	79	-4.136132000	-2.841239000	-4.173234000
	79	-1.275022000	-6.078277000	-3.251178000	79	-0.739345000	-6.004548000	-2.669243000	79	-5.622729000	-4.460778000	-5.719278000
	79	-3.934444000	-5.978175000	-3.651685000	79	-3.170524000	-6.226707000	-1.485290000	79	-3.254892000	-5.799055000	-4.603831000
	79	-5.115300000	-3.392276000	-2.939636000	79	-7.648581000	-4.276984000	-3.253576000	79	-3.783244000	-5.850154000	-1.084344000