

Supplementary Material

Theoretical investigation of gas-phase molecular complex formation between
2-hydroxy thiophenol and a water molecule

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Z-matrix coordinates in Å of the optimized conformers, transition-states and complexes from MP2/aug-cc-pVTZ calculation.

SG

C						
C	1	1.40310446				
C	2	1.39502054	1	119.51404510		
C	3	1.39005402	2	120.04551987	1	0.46917289
C	4	1.39562825	3	120.59338154	2	0.14373714
C	5	1.39092495	4	119.59161842	3	-0.21107258
S	1	1.78318322	6	120.99558884	5	177.87203025
H	7	1.34132128	1	96.85906171	6	97.20498830
O	2	1.35684633	1	122.25348099	6	179.38000053
H	9	0.97336420	2	106.64098142	1	-4.03281685
H	3	1.08182359	2	118.58189670	1	-179.76824933
H	4	1.08200893	3	119.34804409	2	179.90905602
H	5	1.08132941	4	120.40190075	3	179.66824142
H	6	1.08203765	5	120.97407169	4	179.79779787

SA

C						
C	1	1.40035997				
C	2	1.39284967	1	120.13645847		
C	3	1.39277714	2	120.48432535	1	0.00000000
C	4	1.39310759	3	119.71075399	2	0.00027206
C	5	1.39198137	4	119.82758166	3	0.00000000
S	1	1.76446820	6	118.87267474	5	-179.99804515
H	7	1.33718403	1	95.74588396	6	-179.99144184
O	2	1.37068020	1	117.47909745	6	180.00000000
H	9	0.96456052	2	108.56767199	1	-179.99600583
H	3	1.08471686	2	119.24439756	1	-180.00000000
H	4	1.08151709	3	119.68394073	2	-180.00000000
H	5	1.08144922	4	120.40188577	3	179.99974032
H	6	1.08315633	5	120.18601341	4	179.99895492

AA

C						
C	1	1.40011629				
C	2	1.39207387	1	120.37309299		
C	3	1.39326367	2	120.25096272	1	0.00000000
C	4	1.39287091	3	119.74285535	2	0.00000000
C	5	1.39316518	4	119.96224645	3	0.00000000
S	1	1.76737062	6	123.91526239	5	-180.00000000
H	7	1.33809351	1	94.66544288	6	0.00000000
O	2	1.36753452	1	116.40244718	6	180.00000000
H	9	0.96448484	2	108.89511863	1	180.00000000
H	3	1.08452410	2	119.32883730	1	-180.00000000
H	4	1.08152183	3	119.71496495	2	180.00000000
H	5	1.08152093	4	120.38615757	3	180.00000000
H	6	1.08301661	5	119.93678289	4	180.00000000

TS'_{SG-SG}

C						
C	1	1.40147145				
C	2	1.39290422	1	119.89660784		
C	3	1.39033462	2	120.36169363	1	0.00000000
C	4	1.39429069	3	120.00720269	2	0.00000000
C	5	1.39101449	4	119.81371713	3	0.00000000
S	1	1.77157423	6	123.07205310	5	-180.00000000
H	7	1.33604102	1	95.97531560	6	-0.00080208
O	2	1.36627261	1	123.10003281	6	180.00000000
H	9	0.96556941	2	110.20513507	1	0.00000000
H	3	1.08192531	2	118.14880600	1	-180.00000000
H	4	1.08151386	3	119.64004022	2	-180.00000000
H	5	1.08145823	4	120.52188640	3	180.00000000
H	6	1.08298321	5	120.02926753	4	180.00000000

TS_{SA-SG}

C						
C	1	1.40104489				
C	2	1.39160780	1	120.31347838		
C	3	1.39243763	2	120.35680491	1	-1.49774436
C	4	1.39396563	3	119.63618810	2	0.82347325
C	5	1.39121472	4	120.13555386	3	0.28628172
S	1	1.76463943	6	118.96321105	5	-178.85208275
H	7	1.33852441	1	95.04739517	6	-165.95269233
O	2	1.38741501	1	119.87710619	6	177.51589489
H	9	0.96490628	2	108.55162699	1	94.48709649
H	3	1.08229483	2	118.33482508	1	178.44704660
H	4	1.08153337	3	119.90895415	2	-179.70167614
H	5	1.08178730	4	120.26648366	3	179.60605596
H	6	1.08288993	5	120.23707361	4	178.84319401

 TS_{SG-SG}^h

C						
C	1	1.40137386				
C	2	1.39481269	1	119.63468892		
C	3	1.38883801	2	120.87433975	1	0.00000000
C	4	1.39425142	3	119.79823522	2	0.00133753
C	5	1.38905634	4	119.59133365	3	-0.00066981
S	1	1.77317735	6	115.25034841	5	-179.99481633
H	7	1.33643743	1	100.27029378	6	-179.98812089
O	2	1.36658325	1	124.43597937	6	-179.99972132
H	9	0.96247139	2	109.84058186	1	-0.02883810
H	3	1.08200843	2	117.73806701	1	180.00000000
H	4	1.08148450	3	119.66617000	2	-179.99968927
H	5	1.08128058	4	120.66363505	3	179.99875362
H	6	1.08345186	5	120.08446533	4	179.99971339

TS_{AA-SA}

C						
C	1	1.40176486				
C	2	1.39619527	1	119.67798887		
C	3	1.39110401	2	120.60602856	1	0.10805887
C	4	1.39316440	3	120.01205316	2	-0.26091721
C	5	1.39169310	4	119.46201415	3	-0.33612590
S	1	1.78277276	6	120.49285864	5	-178.86879832
H	7	1.33897196	1	95.84680220	6	-77.45821932
O	2	1.36386511	1	118.34543222	6	-179.62209291
H	9	0.96480198	2	108.23986864	1	179.40111743
H	3	1.08461058	2	119.30330959	1	179.90255266
H	4	1.08189342	3	119.51634778	2	179.95357405
H	5	1.08135867	4	120.45731349	3	-179.69721987
H	6	1.08213877	5	120.66386528	4	-178.80221971

 TS_{AA-SG}

C						
C	1	1.39930977				
C	2	1.39067883	1	120.58846082		
C	3	1.39297748	2	120.07676714	1	-0.78655019
C	4	1.39393711	3	119.67022224	2	0.57002436
C	5	1.39222212	4	120.29850269	3	-0.00708633
S	1	1.76602318	6	123.98540210	5	-179.90702889
H	7	1.33846484	1	94.79154708	6	5.33908112
O	2	1.38513251	1	118.61242756	6	176.94318507
H	9	0.96458839	2	108.92523008	1	97.26129543
H	3	1.08225893	2	118.52865329	1	178.79361138
H	4	1.08150941	3	119.96004892	2	-179.88561147
H	5	1.08189412	4	120.22335258	3	179.68523341
H	6	1.08281812	5	119.98622154	4	179.55155454

SGw-TL-O

C						
C	1	1.40134124				
C	2	1.39408124	1	120.14310797		
C	3	1.39076574	2	119.45142221	1	0.49650764
C	4	1.39562110	3	120.79126250	2	0.13646165
C	5	1.39100317	4	119.69842357	3	-0.20063121
S	1	1.78347141	6	121.23492717	5	178.03978810
H	7	1.34135959	1	96.85931660	6	95.25135542
O	2	1.36510837	1	121.43070905	6	179.35355490
H	9	0.97451573	2	106.67574621	1	-3.02862343
H	3	1.08244058	2	118.93605712	1	-179.58291889
H	4	1.08194624	3	119.17729901	2	179.97571470
H	5	1.08140336	4	120.37158669	3	179.68359160
H	6	1.08198633	5	121.03919342	4	179.76871360
O	9	2.89351590	2	109.70200504	1	176.34542538
H	15	0.96737533	9	14.30614567	2	171.89443545
H	15	0.96084567	9	116.50683108	2	135.57254518

SAw-TL-O

C						
C	1	1.40255865				
C	2	1.39533984	1	119.73987231		
C	3	1.39295062	2	120.49712821	1	0.00000000
C	4	1.39316837	3	119.94164248	2	0.00000000
C	5	1.39204501	4	119.70354173	3	0.00000000
S	1	1.76489955	6	119.02955656	5	180.00000000
H	7	1.33768147	1	95.29784895	6	179.99766017
O	2	1.36307534	1	117.77153206	6	179.99971498
H	9	0.97485522	2	109.44934403	1	-179.99879804
H	3	1.08337475	2	118.87115115	1	-179.99971282
H	4	1.08190127	3	119.58700360	2	-180.00000000
H	5	1.08158977	4	120.48921576	3	-180.00000000
H	6	1.08326666	5	120.22516748	4	-180.00000000
O	9	2.80605723	2	112.04342038	1	-179.98595759
H	15	0.96272151	9	115.83404393	2	-118.28377519
H	15	0.96272362	9	115.77952139	2	118.24011388

AAw-TL-O

C						
C	1	1.40194395				
C	2	1.39462025	1	119.98710693		
C	3	1.39340097	2	120.25438339	1	-0.00034260
C	4	1.39296680	3	119.97537862	2	0.00028973
C	5	1.39326483	4	119.83951254	3	0.00000000
S	1	1.76797769	6	123.91434069	5	-180.00000000
H	7	1.33844703	1	94.68637319	6	0.00000000
O	2	1.35987771	1	116.73509744	6	179.99961869
H	9	0.97467075	2	109.61546072	1	179.99399585
H	3	1.08332827	2	118.96003597	1	179.99935007
H	4	1.08189766	3	119.63248444	2	-180.00000000
H	5	1.08167313	4	120.46146088	3	180.00000000
H	6	1.08314835	5	119.98149228	4	180.00000000
O	9	2.80923205	2	112.22045208	1	179.99758505
H	15	0.96279837	9	114.13195724	2	-119.72682658
H	15	0.96279904	9	114.10448219	2	119.75059709

SGw-TL-S

C						
C	1	1.40298489				
C	2	1.39483974	1	119.36373441		
C	3	1.38983462	2	120.03576708	1	0.27026819
C	4	1.39552550	3	120.58603738	2	0.16063892
C	5	1.39103927	4	119.83085263	3	-0.10082899
S	1	1.78592755	6	121.17909247	5	178.12856744
H	7	1.34168403	1	97.25782323	6	93.15111757
O	2	1.35806483	1	122.61141673	6	179.66406277
H	9	0.97210739	2	107.04313529	1	-3.25775815
H	3	1.08180537	2	118.53352137	1	-179.81187882
H	4	1.08206447	3	119.31941284	2	179.97715926
H	5	1.08133863	4	120.40292417	3	179.78339425
H	6	1.08237332	5	120.83086180	4	179.65571604
O	7	3.41828253	1	91.70723473	6	0.51562031
H	15	0.96646919	7	17.29144042	1	-153.78265236
H	15	0.96161280	7	120.78290639	1	-131.53613737

SAw-TL-S

C						
C	1	1.39950971				
C	2	1.39234184	1	119.96468937		
C	3	1.39273795	2	120.34055278	1	0.35549325
C	4	1.39284057	3	119.86409375	2	-0.48752835
C	5	1.39182904	4	119.94352670	3	-0.00162381
S	1	1.76915267	6	119.02517274	5	178.03677978
H	7	1.33826746	1	95.94337438	6	163.29373467
O	2	1.37087362	1	117.44386693	6	-179.40128571
H	9	0.96458027	2	108.53113429	1	179.00859518
H	3	1.08458342	2	119.34202725	1	-179.86959988
H	4	1.08157045	3	119.59341573	2	179.88966564
H	5	1.08124031	4	120.39762038	3	-179.21176329
H	6	1.08262294	5	120.36299766	4	-178.00797059
O	6	3.31559697	5	129.14569330	4	-120.79206938
H	15	0.96711462	6	64.09083587	5	145.86768006
H	15	0.96157584	6	163.94438982	5	-168.86890740

AAw-TL-S

C						
C	1	1.40047077				
C	2	1.39191117	1	120.43785719		
C	3	1.39346179	2	120.24252057	1	0.00000000
C	4	1.39288561	3	119.66816395	2	0.00000000
C	5	1.39326260	4	120.12847051	3	0.00000000
S	1	1.76654844	6	123.48419188	5	180.00000000
H	7	1.34134708	1	94.56578184	6	-0.00030397
O	2	1.36910537	1	116.55983872	6	180.00000000
H	9	0.96431600	2	108.69943380	1	179.99920726
H	3	1.08464580	2	119.35165930	1	180.00000000
H	4	1.08167870	3	119.72478182	2	-180.00000000
H	5	1.08182557	4	120.27521982	3	-180.00000000
H	6	1.08257657	5	120.41576306	4	-180.00000000
O	6	3.51109102	5	139.67336654	4	179.99621627
H	15	0.96238454	6	126.54005025	5	-79.74658266
H	15	0.96238425	6	126.55270559	5	79.74538369

SGw-CY

C						
C	1	1.40176141				
C	2	1.39232506	1	120.25110086		
C	3	1.39162830	2	119.71834762	1	0.87404314
C	4	1.39493602	3	120.42493522	2	0.22583552
C	5	1.39215313	4	119.80354860	3	-0.78628986
S	1	1.78006049	6	121.27147508	5	178.33197881
H	7	1.34671970	1	95.32264249	6	113.41449650
O	2	1.36754010	1	121.32670396	6	179.83530973
H	9	0.97628246	2	106.05549476	1	-14.01307473
H	3	1.08204024	2	118.83962033	1	-179.85771627
H	4	1.08192597	3	119.44545517	2	179.78179618
H	5	1.08145029	4	120.28406757	3	179.63196228
H	6	1.08206456	5	120.91654393	4	-179.14192092
O	9	2.91575635	2	94.28876541	1	64.84898350
H	15	0.96733882	9	25.72431287	2	105.00395294
H	15	0.96157598	9	126.62303584	2	67.86220566

SAw-CY

C						
C	1	1.39912574				
C	2	1.39139670	1	120.45197823		
C	3	1.39235238	2	120.24738242	1	-0.59264396
C	4	1.39296331	3	119.76585305	2	0.16352190
C	5	1.39154496	4	119.89288863	3	0.46950514
S	1	1.76674914	6	118.79319594	5	-178.45691715
H	7	1.33817243	1	96.09995213	6	-163.58797844
O	2	1.37650381	1	117.35185398	6	-179.37440516
H	9	0.96563008	2	108.61563884	1	-176.51781100
H	3	1.08445086	2	119.40080651	1	179.98420139
H	4	1.08136353	3	119.65109062	2	-179.75868646
H	5	1.08133488	4	120.35546654	3	179.91767953
H	6	1.08290985	5	120.30283645	4	178.93038864
O	9	3.01238669	2	102.18342191	1	68.04272065
H	15	0.96538789	9	4.75947989	2	-155.78592388
H	15	0.96246151	9	101.97020661	2	-54.13033709

AAw-CY

C						
C	1	1.39891386				
C	2	1.39037722	1	120.71278954		
C	3	1.39283828	2	120.02744992	1	0.05976347
C	4	1.39276545	3	119.76801323	2	-0.17847761
C	5	1.39257020	4	120.04622102	3	0.23597927
S	1	1.76840467	6	123.86829656	5	179.54879706
H	7	1.33814585	1	94.79020852	6	5.38178939
O	2	1.37426377	1	116.36043762	6	-179.61225895
H	9	0.96551977	2	108.99076360	1	-177.25661464
H	3	1.08422166	2	119.46504927	1	-179.63674300
H	4	1.08133548	3	119.70449431	2	-179.95622022
H	5	1.08143763	4	120.33047702	3	-179.85921749
H	6	1.08284324	5	119.98826792	4	179.64186003
O	9	2.98825628	2	104.62661468	1	71.08081227
H	15	0.96590529	9	7.98999341	2	-119.97727964
H	15	0.96172812	9	107.70161017	2	-63.82083444

SGw-PI

C						
C	1	1.40350219				
C	2	1.39593280	1	119.57252743		
C	3	1.39055976	2	120.06743046	1	0.66354952
C	4	1.39666985	3	120.54295267	2	0.12184984
C	5	1.39260069	4	119.57719639	3	-0.43109232
S	1	1.78233156	6	121.01980212	5	176.80758837
H	7	1.34153842	1	96.53375576	6	98.41592426
O	2	1.35504879	1	122.22612763	6	178.68311183
H	9	0.97404595	2	106.66033703	1	-4.19157847
H	3	1.08205525	2	118.60554264	1	-179.70260573
H	4	1.08192618	3	119.40603970	2	179.60820592
H	5	1.08129683	4	120.41003615	3	179.43881665
H	6	1.08207168	5	120.92012073	4	179.53636028
O	6	3.43553020	5	81.53285914	4	72.35988670
H	15	0.96496623	6	19.20491386	5	-1.95598245
H	15	0.96182257	6	107.87705250	5	-81.55934220

SAw-PI

C						
C	1	1.40099776				
C	2	1.39243591	1	120.07804902		
C	3	1.39286998	2	120.45761850	1	-0.27952109
C	4	1.39391798	3	119.79466760	2	0.61482479
C	5	1.39244037	4	119.80021254	3	-0.25859377
S	1	1.76405839	6	118.84995236	5	-176.58704444
H	7	1.33783028	1	95.67441556	6	-178.45336403
O	2	1.36785310	1	117.32613234	6	-179.56903387
H	9	0.96477303	2	108.80494300	1	175.07019679
H	3	1.08434051	2	119.29408927	1	-179.46742082
H	4	1.08144213	3	119.66618053	2	-179.42025403
H	5	1.08139114	4	120.41348407	3	179.85087849
H	6	1.08319459	5	120.23655444	4	-179.43470480
O	1	3.25446289	6	86.27524981	5	-78.95879569
H	15	0.96412910	1	51.42505283	6	37.28987685
H	15	0.96359163	1	53.88164794	6	-122.49547760

AAw-PI

C						
C	1	1.40083449				
C	2	1.39181846	1	120.30229011		
C	3	1.39334068	2	120.19714756	1	-0.06976820
C	4	1.39336667	3	119.85277791	2	0.36442292
C	5	1.39345756	4	119.95360618	3	-0.22845434
S	1	1.76754803	6	124.00347361	5	-176.99164259
H	7	1.33872559	1	94.67006208	6	0.94205693
O	2	1.36526696	1	116.21787583	6	-179.53568265
H	9	0.96473144	2	109.16527114	1	175.22148388
H	3	1.08415366	2	119.38444175	1	-179.48686111
H	4	1.08140341	3	119.67987256	2	-179.59589000
H	5	1.08142504	4	120.39057247	3	179.96626971
H	6	1.08291737	5	120.00979576	4	-179.38098986
O	1	3.22199424	6	90.75859924	5	-85.19331353
H	15	0.96362319	1	47.93130178	6	38.46304076
H	15	0.96435195	1	55.25563673	6	-134.37125609

SG-SA-w

C						
C	1	1.40557957				
C	2	1.39510902	1	118.95525123		
C	3	1.39136706	2	120.88133997	1	-2.10798941
C	4	1.39404019	3	120.01255932	2	0.22225229
C	5	1.39126107	4	119.69584228	3	1.37727474
S	1	1.77542238	6	118.19224450	5	179.35247710
H	7	1.34141392	1	95.65839678	6	-148.37413768
O	2	1.36455489	1	122.54304359	6	178.83304585
H	9	0.98097485	2	109.22097947	1	53.25061174
H	3	1.08211559	2	117.75374790	1	178.67393364
H	4	1.08186406	3	119.69778653	2	-179.51668645
H	5	1.08159959	4	120.49738442	3	-179.91374119
H	6	1.08280396	5	120.45463434	4	177.38552851
O	9	2.76721620	2	105.21031590	1	53.95309654
H	15	0.96989788	9	93.89323700	2	-41.57145578
H	15	0.96259920	9	118.48041310	2	68.61096221

SG-AA-w

C						
C	1	1.40419292				
C	2	1.39450437	1	119.20066480		
C	3	1.39149169	2	120.79674781	1	-1.16090602
C	4	1.39394033	3	119.88900597	2	-0.34040114
C	5	1.39171848	4	119.86220816	3	1.11866036
S	1	1.77590345	6	122.34783080	5	176.29259308
H	7	1.33809723	1	95.29024312	6	12.86417915
O	2	1.36524136	1	121.97124676	6	178.63576378
H	9	0.98033385	2	109.50628841	1	54.80753160
H	3	1.08207053	2	117.74417357	1	179.12770861
H	4	1.08174708	3	119.81427056	2	-179.89608174
H	5	1.08171366	4	120.49968217	3	-179.60572327
H	6	1.08311801	5	120.00096905	4	178.30592853
O	9	2.77269295	2	105.11810503	1	55.65158807
H	15	0.96867050	9	94.56464418	2	-46.76423589
H	15	0.96258176	9	116.96203387	2	63.18268836

Table S 1: Enthalpies of formation ($\Delta H_{298.15K}^\theta$), $T\Delta S$, Gibbs free energies of formation ($\Delta G_{298.15K}^\theta$) in kJ mol^{-1} of the complexes and equilibrium constants (K_{eq}) at 298.15 K obtained from MP2/aug-cc-pVTZ method.

Complex	$\Delta H_{298.15K}^\theta$	$T\Delta S$	$\Delta G_{298.15K}^\theta$	K_{eq}
SGw-TL-O	-16.21	-37.18	20.97	2.119×10^{-4}
SAw-TL-O	-18.95	-35.58	16.63	12.205×10^{-4}
AAw-TL-O	-13.94	-36.05	22.11	1.338×10^{-4}
SGw-TL-S	-11.04	-36.21	25.17	0.389×10^{-4}
SAw-TL-S	-3.12	-35.14	32.02	0.025×10^{-4}
AAw-TL-S	1.24	-32.71	33.95	0.011×10^{-4}
SGw-CY	-20.77	-38.69	17.92	7.253×10^{-4}
SAw-CY	-5.96	-36.78	30.83	0.040×10^{-4}
AAw-CY	-2.47	-36.05	33.58	0.013×10^{-4}
SGw-PI	-12.51	-33.98	21.46	1.739×10^{-4}
SAw-PI	-6.71	-34.10	27.39	0.159×10^{-4}
AAw-PI	-2.45	-34.91	32.46	0.021×10^{-4}
SG-SA-w	-19.25	-40.17	20.92	2.163×10^{-4}
SG-AA-w	-13.49	-39.11	25.61	0.326×10^{-4}

Table S 2: Interaction energies (kJ mol^{-1}) of 2-hydroxy thiophenol-water complexes calculated by different DFT methods using aug-cc-pVTZ basis set.

Complex	wB97XD		M06-2X		B3LYP-D3	
	E_{int}	E_{def}	E_{int}	E_{def}	E_{int}	E_{def}
SGw-TL-O	-12.12	0.40	-13.45	0.43	-14.49	0.41
SAw-TL-O	-23.02	0.67	-25.59	0.52	-24.80	0.59
AAw-TL-O	-23.13	0.62	-24.48	0.49	-24.24	0.56
SGw-TL-S	-8.86	0.25	-10.29	0.26	-10.80	0.25
SAw-TL-S	-8.18	1.30	-10.37	1.14	-9.92	1.37
AAw-TL-S	-8.95	0.10	-8.56	0.12	-10.42	0.08
SGw-CY	-14.20	1.90	-16.78	1.38	-16.61	1.91
SAw-CY	-10.85	0.97	-12.00	0.76	-12.67	1.01
AAw-CY	-11.61	0.45	-12.73	0.39	-13.84	0.43
SGw-PI	-10.24	0.15	-9.87	0.20	-10.63	0.15
SAw-PI	-11.72	0.44	-13.71	0.76	-12.42	0.41
AAw-PI	-12.22	0.39	-11.97	0.66	-12.67	0.36
SG-SA-w	-13.79	13.94	-17.67	13.27	-16.95	13.65
SG-AA-w	-7.59	20.56	-12.09	18.32	-10.86	19.00

Table S 3: Calculated SAPT decomposition of interaction energy (kJ mol^{-1}) for various complexes obtained at the sSAPT0/aug-cc-pVDZ level.

Complex	E_{elst}	E_{exch}	E_{ind}	E_{disp}	E_{int}^{sSAPT0}	CT
SGw-TL-O	-35.02	29.02	-7.65	-7.81	-21.46	-1.97
SAw-TL-O	-56.98	43.78	-13.89	-7.10	-34.19	-5.04
AAw-TL-O	-56.34	43.29	-13.57	-6.97	-33.59	-5.01
SGw-TL-S	-26.39	27.98	-8.00	-7.23	-13.65	-2.06
SAw-TL-S	-23.50	25.33	-7.82	-7.54	-13.54	-1.92
AAw-TL-S	-25.92	25.77	-10.14	-5.45	-15.73	-1.15
SGw-CY	-41.60	39.55	-11.10	-10.67	-23.82	-2.23
SAw-CY	-29.22	24.83	-5.69	-8.41	-18.48	-1.48
AAw-CY	-30.27	23.97	-5.68	-7.78	-19.76	-1.61
SGw-PI	-14.75	18.39	-5.47	-9.84	-11.67	-0.86
SAw-PI	-17.96	18.09	-5.17	-10.25	-15.29	-0.45
AAw-PI	-18.73	18.34	-5.32	-10.11	-15.83	-0.47
SG-SA-w	-80.30	79.49	-20.56	-12.92	-34.28	-8.22
SG-AA-w	-75.56	76.03	-19.39	-12.08	-31.00	-7.80

Table S 4: Calculated SAPT decomposition of interaction energy (kJ mol^{-1}) for various complexes obtained at the SAPT2+/aug-cc-pVDZ level.

Complex	E_{elst}	E_{exch}	E_{ind}	E_{disp}	E_{int}^{SAPT2+}	CT
SGw-TL-O	-32.88	37.42	-10.13	-12.73	-18.33	-2.73
SAw-TL-O	-50.87	51.76	-16.77	-13.13	-29.01	-5.05
AAw-TL-O	-50.56	51.35	-16.34	-12.92	-28.47	-5.07
SGw-TL-S	-23.94	32.01	-9.19	-12.09	-13.23	-2.14
SAw-TL-S	-20.98	28.63	-9.01	-12.13	-13.49	-1.88
AAw-TL-S	-22.77	26.35	-7.69	-9.87	-13.99	-1.69
SGw-CY	-40.51	46.23	-11.53	-17.77	-23.57	-3.05
SAw-CY	-28.31	33.01	-8.18	-13.86	-17.34	-2.03
AAw-CY	-27.93	31.34	-8.04	-12.85	-17.48	-2.15
SGw-PI	-14.79	22.92	-7.13	-14.32	-13.32	-0.99
SAw-PI	-18.33	23.45	-6.58	-15.45	-16.91	-0.81
AAw-PI	-19.00	23.83	-6.64	-15.35	-17.17	-0.84
SG-SA-w	-78.73	94.92	-26.57	-22.36	-32.73	-8.37
SG-AA-w	-73.83	89.66	-24.68	-21.27	-30.11	-7.92

Table S 5: Difference in NBO charges (Δq) of selected atoms of the complexes from the respective monomers.

Complex	Δq (S7)	Δq (H8)	Δq (O9)	Δq (H10)
SGw-TL-O	0.000	0.002	-0.031	0.008
SAw-TL-O	-0.012	0.002	-0.036	0.036
AAw-TL-O	-0.007	-0.003	-0.036	0.036
SGw-TL-S	-0.023	0.008	0.001	-0.001
SAw-TL-S	-0.019	0.001	0.000	0.000
AAw-TL-S	-0.037	0.037	0.000	-0.003
SGw-CY	-0.023	0.047	-0.024	0.005
SAw-CY	-0.001	-0.006	-0.015	0.007
AAw-CY	-0.012	0.007	-0.019	0.008
SGw-PI	0.013	0.000	0.001	0.002
SAw-PI	-0.002	0.004	0.002	0.003
AAw-PI	-0.002	0.003	0.001	0.004
SG-SA-w	0.002	0.019	-0.045	0.030
SG-AA-w	0.030	-0.007	-0.041	0.029