

SUPPORTING INFORMATION
NX··Y Halogen Bonds. Comparison with NH··Y H-bonds and CX··Y Halogen Bonds
Binod Nepal and Steve Scheiner

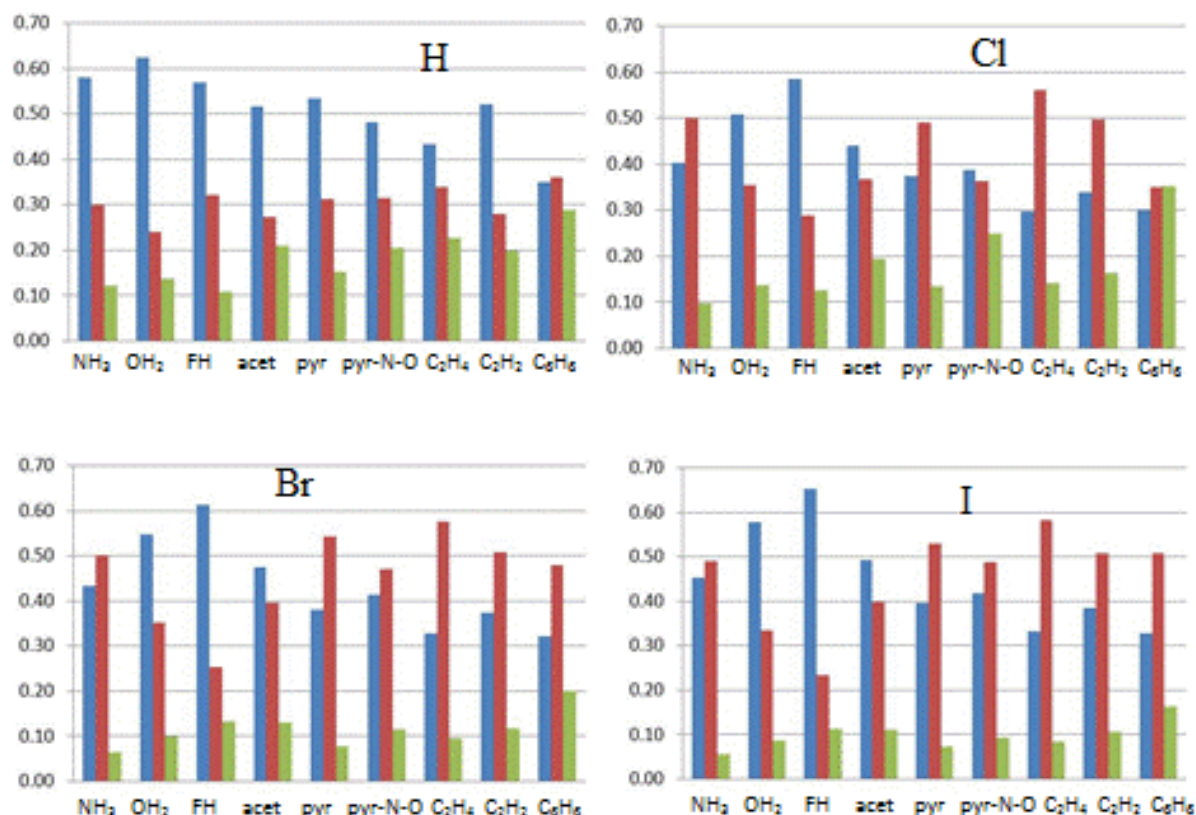


Fig S1. Fractional contributions of electrostatic (blue), induction (red), and dispersion (green) to total attraction energy in complexes with saccharin and its indicated halosubstituted derivatives.

Table S1. SAPT components (kcal/mol) for the H-bonded and X-bonded complexes of succinimide-based systems.

	ELST	EXCH	IND	EX-IND	DISP	EX-DISP	E _{TOT}	E _{int} ^a
H								
NH ₃	-17.80	16.52	-8.02	5.08	-3.82	0.81	-7.22	-8.28
OH ₂	-17.57	14.81	-6.88	4.11	-3.71	0.73	-8.52	-8.32
FH	-22.18	21.04	-12.32	6.82	-3.97	0.83	-9.78	-9.83
acetone	-14.36	13.46	-6.03	3.19	-4.24	0.69	-7.28	-6.80
pyridine	-19.55	20.68	-9.86	5.65	-5.52	0.98	-7.62	-9.39
Pyridine-N-oxide	-21.49	20.10	-9.73	5.05	-5.72	1.01	-10.78	-9.85
ethene	-6.34	7.81	-4.09	3.09	-3.15	0.53	-2.14	-2.50
acetylene	-8.50	8.32	-3.87	2.66	-2.94	0.49	-3.83	-3.56
benzene	-6.30	10.74	-4.77	3.37	-6.10	0.92	-2.14	-3.30
Cl								
NH ₃	-10.18	11.55	-12.16	10.57	-2.47	0.61	-2.07	-3.64
OH ₂	-5.24	5.07	-3.52	2.82	-1.45	0.25	-2.08	-2.36
FH	-12.83	10.29	-5.82	2.71	-2.34	0.37	-7.63	-7.01
acetone	-7.75	9.02	-6.34	5.19	-3.22	0.53	-2.59	-2.69
pyridine	-11.81	15.26	-14.57	12.66	-4.27	0.86	-1.86	-4.21
Pyridine-N-oxide	-11.14	14.37	-9.99	8.37	-5.99	1.09	-3.29	-3.74
ethene	-5.75	8.82	-10.54	9.97	-2.74	0.59	0.36	-1.10
acetylene	-4.45	6.25	-6.23	5.83	-2.04	0.39	-0.24	-1.07
benzene	-3.92	8.81	-6.07	5.50	-4.31	0.70	0.70	-0.97
Br								
NH ₃	-20.23	29.21	-22.21	13.32	-3.11	0.76	-2.26	-5.32
OH ₂	-8.75	10.38	-5.44	3.38	-1.62	0.32	-1.74	-3.05
FH	-3.75	3.86	-1.53	1.04	-0.80	0.12	-1.06	-1.32
acetone	-12.89	18.20	-10.28	6.46	-3.54	0.68	-1.37	-2.95
pyridine	-29.50	48.90	-38.67	22.07	-6.29	1.36	-2.14	-5.61
Pyridine-N-oxide	-20.94	30.38	-22.24	14.90	-6.07	1.39	-2.58	-4.32
ethene	-11.22	21.66	-18.89	12.63	-3.33	0.75	1.60	-0.38
acetylene	-7.38	13.17	-9.39	6.38	-2.27	0.44	0.96	-0.63
benzene	-7.64	17.27	-11.44	8.00	-4.43	0.86	2.62	0.02
I								
NH ₃	-28.19	35.16	-28.44	15.24	-3.64	0.81	-9.06	-9.43
OH ₂	-12.33	12.35	-6.73	3.94	-1.84	0.36	-4.25	-5.12
FH	-4.69	3.90	-1.65	1.05	-0.82	0.12	-2.09	-2.16
acetone	-17.81	22.23	-13.56	7.86	-4.13	0.82	-4.60	-5.21
pyridine	-37.06	53.14	-46.29	23.43	-7.27	1.47	-12.58	-10.66
Pyridine-N-oxide	-29.54	37.58	-32.50	19.69	-6.94	1.63	-10.08	-8.31
ethene	-14.88	26.29	-24.30	14.92	-3.95	0.80	-1.13	-1.5
acetylene	-9.12	14.55	-10.93	6.89	-2.51	0.43	-0.69	-1.47
benzene	-10.00	20.01	-14.55	9.54	-5.06	0.98	0.91	-1.04

^acounterpoise-corrected interaction energy computed at MP2 level

Table S2. SAPT components (kcal/mol) for the H-bonded and X-bonded complexes of saccharin-based systems.

	ELST	EXCH	IND	EX-IND	DISP	EX-DISP	E _{TOT}	E _{int} ^a
H								
NH ₃	-21.72	21.22	-11.18	6.98	-4.53	0.97	-8.27	-10.14
OH ₂	-16.87	13.91	-6.47	3.76	-3.71	0.67	-8.70	-8.23
FH	-21.73	21.06	-12.26	6.73	-4.12	0.85	-9.47	-9.63
acetone	-16.69	17.39	-8.85	5.34	-6.80	1.06	-8.54	-7.44
pyridine	-24.13	27.79	-14.05	7.94	-6.91	1.22	-8.13	-11.5
Pyridine-N-oxide	-27.14	33.51	-17.70	10.96	-11.54	2.02	-9.89	-11.6
ethene	-8.09	10.05	-6.31	4.88	-4.24	0.72	-3.00	-3.15
acetylene	-8.79	9.42	-4.73	3.27	-3.36	0.55	-3.65	-3.75
benzene	-10.60	17.21	-10.94	8.51	-8.71	1.45	-3.07	-4.64
Cl								
NH ₃	-11.86	13.70	-14.71	12.76	-2.86	0.72	-2.25	-4.18
OH ₂	-5.88	5.66	-4.10	3.33	-1.59	0.28	-2.30	-2.52
FH	-10.05	8.37	-4.96	2.28	-2.17	0.30	-6.21	-5.39
acetone	-8.82	10.53	-7.37	6.02	-3.88	0.63	-2.89	-2.90
pyridine	-14.08	18.92	-18.49	16.01	-5.09	1.05	-1.68	-4.65
Pyridine-N-oxide	-12.45	17.39	-11.65	9.99	-7.98	1.40	-3.29	-4.03
ethene	-6.61	10.23	-12.43	11.72	-3.13	0.68	0.46	-1.32
acetylene	-4.77	6.94	-7.01	6.54	-2.30	0.44	-0.17	-1.13
benzene	-5.96	12.31	-6.94	6.38	-6.98	1.21	0.02	-1.13
Br								
NH ₃	-24.66	36.16	-28.51	16.67	-3.69	0.88	-3.14	-6.61
OH ₂	-9.78	11.62	-6.31	3.92	-1.79	0.35	-1.99	-3.40
FH	-3.98	4.02	-1.64	1.09	-0.86	0.13	-1.24	-1.45
acetone	-14.53	20.76	-12.11	7.55	-3.98	0.76	-1.54	-3.41
pyridine	-37.71	63.79	-53.74	29.05	-7.62	1.60	-4.63	-7.72
Pyridine-N-oxide	-24.34	36.08	-27.59	17.99	-6.77	1.54	-3.10	-5.26
ethene	-13.46	26.26	-23.71	15.57	-3.92	0.87	1.61	-0.61
acetylene	-8.20	14.99	-11.10	7.47	-2.58	0.50	1.08	-0.72
benzene	-8.36	19.23	-12.43	8.70	-5.19	1.01	2.95	-0.10
I								
NH ₃	-33.59	42.11	-36.38	18.58	-4.21	0.90	-12.61	-11.67
OH ₂	-14.05	14.22	-8.12	4.65	-2.09	0.40	-4.99	-5.84
FH	-5.17	4.20	-1.85	1.13	-0.90	0.13	-2.46	-2.45
acetone	-20.92	26.14	-16.94	9.52	-4.69	0.91	-5.97	-6.39
pyridine	-43.86	62.81	-58.72	28.01	-8.22	1.57	-18.41	-13.84
Pyridine-N-oxide	-34.77	43.99	-40.55	23.53	-7.69	1.75	-13.73	-10.82
ethene	-18.43	32.99	-32.38	19.17	-4.72	0.95	-2.43	-2.09
acetylene	-10.58	17.38	-13.91	8.56	-2.93	0.50	-0.98	-1.75
benzene	-11.49	23.02	-17.76	11.37	-5.71	1.09	0.53	-1.55

^acounterpoise-corrected interaction energy computed at MP2 level

Atomic Coordinates

Succinimide-H...NH3

6	1.290492000	-1.458036000	0.000333000
6	2.088647000	-0.141119000	-0.001050000
6	1.034505000	0.968880000	0.000060000
7	-0.219972000	0.357802000	0.000774000
6	-0.176783000	-1.030708000	0.000292000
1	1.470162000	-2.081697000	0.888327000
1	2.724012000	-0.013220000	-0.889557000
1	2.727065000	-0.012720000	0.885162000
8	1.232949000	2.176155000	0.000374000
1	-1.131339000	0.850734000	0.000318000
1	1.469862000	-2.083677000	-0.886313000
8	-1.161892000	-1.765691000	0.000022000
7	-3.065499000	0.796958000	-0.000562000
1	-3.042611000	-0.226481000	-0.001267000
1	-3.605376000	1.083628000	-0.816883000
1	-3.603105000	1.082296000	0.817753000

Succinimide-H...OH2

6	0.994868000	1.588370000	0.010905000
6	2.027358000	0.445591000	0.021691000
6	1.203792000	-0.842618000	-0.005843000
7	-0.146801000	-0.474068000	-0.020125000
6	-0.363824000	0.895361000	-0.013287000
1	1.066864000	2.238880000	-0.873030000
1	2.657437000	0.432855000	0.922848000
1	2.695233000	0.448368000	-0.851798000
8	1.617239000	-1.991720000	-0.014696000
1	-0.928427000	-1.136695000	-0.036356000
1	1.039223000	2.232206000	0.901418000
8	-1.468381000	1.438866000	-0.025701000
8	-2.914064000	-0.975915000	0.082714000
1	-2.798601000	-0.009632000	0.001734000
1	-3.755648000	-1.177580000	-0.343260000

Succinimide-H...FH

6	0.806613000	1.632391000	-0.000247000
6	1.967162000	0.619045000	0.000049000
6	1.302518000	-0.757004000	0.000037000
7	-0.088478000	-0.545148000	0.000369000
6	-0.456487000	0.784756000	0.000131000
1	0.787190000	2.281460000	-0.887855000
1	2.611512000	0.691662000	0.887971000
1	2.612003000	0.691560000	-0.887510000
8	1.837664000	-1.851812000	-0.000161000
1	-0.779064000	-1.298230000	0.000328000
1	0.787340000	2.282231000	0.886792000
8	-1.619796000	1.201941000	0.000098000
9	-2.915045000	-1.021930000	-0.000176000

1	-2.626005000	-0.111431000	-0.000046000
Succinimide-H...Acetone			
6	-3.282082000	-0.339675000	-0.009015000
6	-2.856180000	1.138870000	0.023348000
6	-1.327954000	1.113054000	0.029615000
7	-0.921442000	-0.215256000	0.005662000
6	-1.974265000	-1.134347000	-0.018585000
1	-3.858316000	-0.612243000	-0.905165000
1	-3.196194000	1.676473000	0.920616000
1	-3.188729000	1.713390000	-0.853591000
8	-0.576338000	2.083664000	0.051753000
1	0.072997000	-0.489535000	0.005913000
1	-3.867444000	-0.648525000	0.869264000
8	-1.849616000	-2.350431000	-0.043132000
6	2.872613000	-0.180250000	-0.004513000
8	1.876686000	-0.912208000	0.026883000
6	2.762900000	1.323639000	-0.114538000
6	4.265002000	-0.770279000	0.064693000
1	1.715845000	1.650134000	-0.062889000
1	4.213920000	-1.865936000	0.061996000
1	3.208439000	1.643568000	-1.071708000
1	3.352123000	1.798967000	0.686574000
1	4.762782000	-0.420848000	0.984505000
1	4.868617000	-0.412934000	-0.785226000
Succinimide-H...Pyridine			
6	3.710816000	0.463567000	-0.000708000
6	3.409619000	-1.046307000	0.001777000
6	1.883374000	-1.145643000	-0.000269000
7	1.368452000	0.143797000	-0.000769000
6	2.339077000	1.143166000	0.000083000
1	4.263766000	0.800446000	-0.889803000
1	3.789796000	-1.570225000	0.891064000
1	3.793031000	-1.574361000	-0.883627000
8	1.211861000	-2.174544000	-0.000990000
1	0.340083000	0.331737000	-0.000756000
1	4.267094000	0.803471000	0.885088000
8	2.111680000	2.347187000	0.000840000
6	-4.247427000	-0.182441000	0.000745000
6	-3.746008000	1.130482000	0.000183000
6	-2.354429000	1.322900000	-0.000584000
7	-1.472236000	0.298641000	-0.000806000
6	-1.957151000	-0.965382000	-0.000235000
6	-3.333339000	-1.249557000	0.000525000
1	-5.325188000	-0.368674000	0.001335000
1	-4.417060000	1.993443000	0.000364000
1	-1.922887000	2.328718000	-0.001070000
1	-1.202664000	-1.759649000	-0.000395000
1	-3.675004000	-2.287816000	0.000921000

Succinimide-H...Pyridine-N-oxide

6	-3.477500000	-1.385246000	0.000354000
6	-4.119950000	0.012703000	-0.000325000
6	-2.944176000	0.993236000	-0.000168000
7	-1.764328000	0.241771000	-0.000213000
6	-1.971846000	-1.127085000	0.000081000
1	-3.725871000	-1.986492000	-0.886583000
1	-4.737924000	0.213715000	0.886857000
1	-4.737022000	0.213100000	-0.888287000
8	-3.003570000	2.214149000	-0.000092000
1	-0.812166000	0.660115000	-0.000022000
1	-3.725605000	-1.985403000	0.888110000
8	-1.084245000	-1.980303000	0.000143000
6	4.333519000	-0.769894000	-0.000241000
6	3.092048000	-1.429745000	-0.000213000
6	1.893849000	-0.714588000	-0.000007000
7	1.908684000	0.666284000	0.000172000
6	3.114874000	1.335615000	0.000147000
6	4.321247000	0.635536000	-0.000048000
1	5.272174000	-1.327514000	-0.000404000
1	3.030170000	-2.520886000	-0.000356000
1	0.898272000	-1.167270000	0.000024000
1	3.014056000	2.420916000	0.000293000
1	5.249892000	1.211758000	-0.000054000
8	0.814209000	1.342201000	0.000353000

Succinimide-H...Ethene

6	2.448403000	0.085507000	-0.000143000
6	1.822217000	-1.322174000	0.000001000
6	0.311226000	-1.091319000	-0.000021000
7	0.099362000	0.287267000	0.000170000
6	1.266195000	1.055664000	0.000057000
1	3.064060000	0.292209000	-0.887625000
1	2.080341000	-1.918396000	0.887396000
1	2.080368000	-1.918640000	-0.887215000
8	-0.573400000	-1.938340000	-0.000126000
1	-0.841053000	0.685907000	0.000096000
1	3.064462000	0.292246000	0.887045000
8	1.304076000	2.277547000	0.000078000
6	-3.191555000	0.343413000	0.675879000
6	-3.191847000	0.344079000	-0.675868000
1	-2.782958000	-0.505165000	1.231934000
1	-3.604979000	1.179569000	1.246219000
1	-2.783463000	-0.504003000	-1.232835000
1	-3.605545000	1.180717000	-1.245253000

Succinimide-H...Acetylene

6	2.347446000	0.255478000	-0.000013000
6	1.856341000	-1.204620000	0.000307000

6	0.331180000	-1.117113000	-0.000070000
7	-0.010933000	0.233255000	-0.000296000
6	1.079055000	1.108949000	-0.000048000
1	2.940741000	0.518994000	-0.887621000
1	2.168906000	-1.773795000	0.887937000
1	2.169390000	-1.774398000	-0.886757000
8	-0.465580000	-2.048849000	-0.000199000
1	-0.981253000	0.551624000	-0.000317000
1	2.940947000	0.519369000	0.887334000
8	0.998536000	2.328374000	0.000039000
6	-3.563088000	0.857942000	0.000158000
6	-3.173281000	-0.312370000	0.000090000
1	-2.744626000	-1.303119000	0.000292000
1	-3.947138000	1.862742000	-0.000063000

Succinimide-H...Benzene

6	-3.064367000	0.769706000	-0.000064000
6	-3.063926000	-0.770693000	0.000179000
6	-1.588527000	-1.174182000	-0.000045000
7	-0.837076000	0.000165000	-0.000214000
6	-1.589196000	1.174046000	-0.000044000
1	-3.542997000	1.209355000	0.887184000
1	-3.542422000	-1.210602000	-0.887016000
1	-3.542001000	-1.210278000	0.887765000
8	-1.127582000	-2.308172000	-0.000054000
1	0.182531000	0.000446000	-0.000151000
1	-3.542802000	1.208998000	-0.887603000
8	-1.128939000	2.308328000	0.000054000
6	2.232217000	1.221603000	-0.704308000
6	2.232178000	1.221264000	0.704931000
6	2.238940000	0.000479000	-1.408380000
1	2.207611000	2.168838000	1.249603000
1	2.230340000	0.000757000	-2.502247000
6	2.238833000	-0.000181000	1.408440000
6	2.232536000	-1.220959000	-0.704881000
1	2.230287000	-0.000413000	2.502306000
1	2.208222000	-2.168556000	-1.249518000
6	2.232492000	-1.221290000	0.704364000
1	2.208145000	-2.169143000	1.248557000
1	2.207703000	2.169431000	-1.248533000

Succinimide-Cl complexes

Succinimide-Cl...NH3

6	2.528707000	0.766892000	0.000708000
6	2.525644000	-0.774124000	0.000721000
6	1.056724000	-1.189191000	-0.000163000
7	0.308721000	0.000883000	-0.001488000
6	1.061469000	1.187812000	-0.000091000

1	3.009326000	1.203043000	-0.887155000
1	3.003341000	-1.212128000	0.889269000
1	3.004535000	-1.212258000	-0.887115000
8	0.591784000	-2.315891000	0.000344000
17	-1.410068000	0.004047000	-0.001212000
1	3.008206000	1.202979000	0.889233000
8	0.601186000	2.316487000	0.000326000
7	-4.163870000	0.000036000	0.001312000
1	-4.554139000	0.667364000	0.666885000
1	-4.540373000	-0.914988000	0.249636000
1	-4.552718000	0.237669000	-0.911328000

Succinimide-Cl...OH2

6	2.524607000	0.770798000	-0.013027000
6	2.524632000	-0.770740000	-0.013024000
6	1.057837000	-1.190848000	-0.002110000
7	0.308392000	-0.000005000	0.009960000
6	1.057799000	1.190860000	-0.002115000
1	2.997770000	1.207459000	-0.904575000
1	3.010477000	-1.207167000	0.871824000
1	2.997809000	-1.207388000	-0.904571000
8	0.592616000	-2.316570000	-0.003904000
17	-1.401053000	-0.000034000	0.027714000
1	3.010439000	1.207244000	0.871820000
8	0.592542000	2.316568000	-0.003914000
8	-4.202307000	-0.000022000	0.064286000
1	-4.604683000	0.762475000	-0.372494000
1	-4.604720000	-0.762236000	-0.372955000

Succinimide-Cl...FH

6	-1.153658000	1.900977000	0.000051000
6	-2.339805000	0.915195000	-0.000081000
6	-1.726950000	-0.480383000	-0.000096000
7	-0.321070000	-0.285851000	0.000305000
6	0.101206000	1.041760000	0.000120000
1	-1.123151000	2.548709000	0.888286000
1	-2.981121000	1.005934000	-0.888626000
1	-2.981234000	1.005845000	0.888402000
8	-2.276294000	-1.562586000	-0.000283000
17	0.778169000	-1.588837000	0.000141000
1	-1.122937000	2.548764000	-0.888123000
8	1.265012000	1.422529000	0.000022000
9	3.689363000	0.238149000	-0.000251000
1	2.828284000	0.613748000	-0.000088000

Succinimide-Cl...Acetone

6	-3.808386000	-0.123409000	0.004993000
6	-3.288936000	1.328403000	0.010074000
6	-1.767016000	1.226667000	0.006251000
7	-1.462326000	-0.143607000	-0.000402000
6	-2.568666000	-1.014281000	-0.001512000

1	-4.408916000	-0.368759000	-0.883024000
1	-3.591352000	1.897197000	0.901467000
1	-3.595378000	1.904869000	-0.874987000
8	-0.945506000	2.128680000	0.008453000
17	0.159418000	-0.688166000	-0.005876000
1	-4.404987000	-0.376346000	0.893534000
8	-2.509032000	-2.230212000	-0.006758000
6	3.628260000	-0.077407000	-0.002173000
8	2.873764000	-1.053816000	-0.004104000
6	3.110520000	1.347186000	-0.032856000
6	5.134451000	-0.252915000	0.030592000
1	2.014514000	1.372905000	-0.000815000
1	5.390951000	-1.319218000	-0.001110000
1	3.467133000	1.842454000	-0.951536000
1	3.526437000	1.911702000	0.817861000
1	5.538514000	0.202601000	0.949929000
1	5.594089000	0.273989000	-0.821553000

Succinimide-Cl...Pyridine

6	4.241079000	-0.727030000	-0.001069000
6	4.204654000	0.813417000	-0.000604000
6	2.726414000	1.195305000	0.000001000
7	2.004392000	-0.009334000	0.000379000
6	2.782560000	-1.178487000	-0.000086000
1	4.730954000	-1.153109000	0.886672000
1	4.672777000	1.262170000	-0.888925000
1	4.673578000	1.261733000	0.887524000
8	2.237769000	2.312596000	0.001147000
17	0.280277000	-0.048433000	0.001102000
1	4.729634000	-1.152623000	-0.889794000
8	2.347551000	-2.317709000	-0.000763000
6	-5.157436000	0.056407000	-0.000576000
6	-4.485410000	-1.177826000	0.000477000
6	-3.079599000	-1.182407000	0.000803000
7	-2.336831000	-0.053180000	0.000132000
6	-2.989843000	1.130277000	-0.000880000
6	-4.391723000	1.234815000	-0.001262000
1	-6.250368000	0.098824000	-0.000859000
1	-5.035846000	-2.122509000	0.001032000
1	-2.519882000	-2.123354000	0.001627000
1	-2.358035000	2.024563000	-0.001393000
1	-4.867184000	2.219349000	-0.002079000

Succinimide-Cl...Pyridine-N-Oxide

6	-3.082712000	1.728516000	0.031416000
6	-3.887775000	0.553043000	0.620664000
6	-2.982600000	-0.671480000	0.513907000
7	-1.800424000	-0.230385000	-0.113649000
6	-1.755783000	1.135151000	-0.430960000
1	-2.864467000	2.517144000	0.766601000

1	-4.813399000	0.339959000	0.066107000
1	-4.154670000	0.690806000	1.678408000
8	-3.201504000	-1.811117000	0.880548000
17	-0.473658000	-1.263474000	-0.441494000
1	-3.567844000	2.202448000	-0.834209000
8	-0.818841000	1.703438000	-0.969790000
6	3.276161000	1.599464000	0.870546000
6	2.534455000	1.604517000	-0.323962000
6	2.162850000	0.410143000	-0.939060000
7	2.504379000	-0.810633000	-0.385920000
6	3.229506000	-0.834170000	0.792123000
6	3.619942000	0.349487000	1.417160000
1	3.572607000	2.530443000	1.357927000
1	2.218326000	2.538075000	-0.795533000
1	1.579923000	0.336055000	-1.855318000
1	3.443030000	-1.840057000	1.154357000
1	4.193332000	0.275075000	2.344923000
8	2.124519000	-1.901295000	-0.934743000

Succinimide-Cl...Ethene

6	2.862739000	0.771092000	-0.000362000
6	2.862876000	-0.770777000	-0.000352000
6	1.396358000	-1.192161000	0.000200000
7	0.647450000	-0.000041000	0.000207000
6	1.396143000	1.192203000	-0.000146000
1	3.342180000	1.207564000	-0.888652000
1	3.342845000	-1.207157000	0.887699000
1	3.342135000	-1.207141000	-0.888799000
8	0.929959000	-2.316978000	0.000555000
17	-1.065174000	-0.000173000	0.000720000
1	3.342370000	1.207529000	0.887849000
8	0.929544000	2.316943000	-0.000201000
6	-4.111710000	0.001377000	0.675180000
6	-4.109770000	-0.001309000	-0.676511000
1	-4.114659000	-0.932017000	1.244084000
1	-4.113749000	0.937036000	1.240359000
1	-4.111023000	-0.936954000	-1.241711000
1	-4.110119000	0.932105000	-1.245393000

Succinimide-Cl...Acetylene

6	2.770427000	0.771167000	-0.000052000
6	2.770571000	-0.770847000	-0.000006000
6	1.304318000	-1.192440000	0.000013000
7	0.555837000	-0.000026000	0.000142000
6	1.304089000	1.192485000	-0.000005000
1	3.249991000	1.207427000	-0.888367000
1	3.250269000	-1.207016000	0.888282000
1	3.250259000	-1.207073000	-0.888271000
8	0.836966000	-2.316796000	-0.000054000
17	-1.153728000	-0.000198000	0.000072000

1	3.250077000	1.207483000	0.888189000
8	0.836570000	2.316785000	-0.000073000
6	-4.254726000	0.616356000	-0.000003000
6	-4.254818000	-0.616268000	-0.000101000
1	-4.252881000	-1.692049000	-0.000185000
1	-4.252643000	1.692137000	0.000085000

Succinimide-Cl...Benzene

6	-3.472744000	1.259102000	0.135642000
6	-3.911802000	-0.217620000	0.199616000
6	-2.637028000	-1.043134000	0.050966000
7	-1.585474000	-0.116700000	-0.078640000
6	-1.957981000	1.240300000	-0.047703000
1	-3.698078000	1.821380000	1.053559000
1	-4.599446000	-0.504019000	-0.609401000
1	-4.384905000	-0.490967000	1.154052000
8	-2.514288000	-2.254617000	0.042067000
17	0.042460000	-0.599316000	-0.271145000
1	-3.911327000	1.808539000	-0.710057000
8	-1.193441000	2.182805000	-0.150561000
6	3.051432000	0.127942000	-1.331478000
6	3.022104000	1.298177000	-0.549967000
6	3.085066000	-1.135733000	-0.707704000
1	2.980501000	2.278315000	-1.033592000
1	3.104807000	-2.045958000	-1.314565000
6	3.033840000	1.206707000	0.854934000
6	3.097242000	-1.226411000	0.698958000
1	3.004567000	2.116720000	1.461375000
1	3.119816000	-2.207207000	1.183311000
6	3.074063000	-0.054389000	1.479283000
1	3.079935000	-0.124834000	2.571140000
1	3.037319000	0.198148000	-2.423215000

Succinimide-Br complexes

Succinimide-Br...NH3

6	2.859718000	0.767657000	0.000195000
6	2.858215000	-0.771701000	0.000786000
6	1.385949000	-1.181944000	0.000098000
7	0.630858000	0.000235000	-0.000330000
6	1.388273000	1.180817000	0.000049000
1	3.337966000	1.205882000	-0.888106000
1	3.334952000	-1.210792000	0.889486000
1	3.336151000	-1.211683000	-0.886819000
8	0.930646000	-2.315071000	-0.000033000
35	-1.254034000	0.001716000	-0.000683000
1	3.337913000	1.206561000	0.888201000
8	0.935344000	2.314931000	0.000227000
7	-3.862115000	-0.001337000	0.001141000
1	-4.240560000	0.647867000	0.690941000
1	-4.233065000	-0.925636000	0.221758000

1	-4.244209000	0.267600000	-0.905568000
---	--------------	-------------	--------------

Succinimide-Br...OH2

6	2.855649000	0.770088000	-0.014997000
6	2.855628000	-0.770131000	-0.015094000
6	1.386387000	-1.186293000	-0.005645000
7	0.632129000	-0.000012000	0.004886000
6	1.386419000	1.186291000	-0.005640000
1	3.328688000	1.208306000	-0.905972000
1	3.339494000	-1.208153000	0.870170000
1	3.328550000	-1.208234000	-0.906188000
8	0.927879000	-2.316206000	-0.007332000
35	-1.228656000	0.000028000	0.023009000
1	3.339424000	1.207976000	0.870386000
8	0.927907000	2.316186000	-0.007359000
8	-3.975155000	0.000005000	0.051168000
1	-4.353871000	0.763347000	-0.406049000
1	-4.353756000	-0.763767000	-0.405427000

Succinimide-Br...FH

6	2.793528000	0.928449000	0.001040000
6	2.910418000	-0.607962000	-0.001938000
6	1.478413000	-1.137243000	-0.000120000
7	0.637493000	-0.007578000	0.001705000
6	1.298093000	1.234458000	0.000041000
1	3.239062000	1.403220000	-0.885327000
1	3.423105000	-1.009711000	0.884200000
1	3.418759000	-1.005998000	-0.892293000
8	1.103865000	-2.296176000	-0.000398000
35	-1.211465000	-0.142206000	0.000653000
1	3.236431000	1.398889000	0.891081000
8	0.752844000	2.324591000	-0.001243000
9	-4.092061000	0.060441000	-0.001119000
1	-4.286351000	0.966333000	-0.003399000

Succinimide-Br...Acetone

6	-3.556675000	-1.243814000	-0.001959000
6	-3.920752000	0.252685000	0.002049000
6	-2.590336000	1.004005000	0.001449000
7	-1.576908000	0.029647000	-0.000997000
6	-2.030440000	-1.297755000	-0.001988000
1	-3.917466000	-1.780136000	-0.891906000
1	-4.487201000	0.563235000	0.892221000
1	-4.490891000	0.567476000	-0.884231000
8	-2.412345000	2.210174000	0.002990000
35	0.242933000	0.446176000	-0.000677000
1	-3.918054000	-1.785449000	0.884474000
8	-1.317160000	-2.289049000	-0.002919000
6	3.680760000	-0.033779000	0.000760000
8	2.840912000	0.873315000	-0.001288000
6	5.161251000	0.284128000	-0.004054000

6	3.292468000	-1.496752000	0.008041000
1	5.315042000	1.370210000	0.008742000
1	2.202364000	-1.615718000	-0.006686000
1	5.630197000	-0.152853000	-0.901058000
1	5.644581000	-0.177736000	0.872416000
1	3.710041000	-1.980672000	0.906484000
1	3.738162000	-1.999882000	-0.865810000

Succinimide-Br...Pyridine

6	-4.235761000	-0.766311000	0.000336000
6	-4.233536000	0.772603000	0.000694000
6	-2.758851000	1.178536000	-0.000315000
7	-2.003526000	0.000152000	-0.000086000
6	-2.762221000	-1.176449000	0.000215000
1	-4.713340000	-1.204972000	-0.888200000
1	-4.709243000	1.212607000	0.889566000
1	-4.710996000	1.213339000	-0.886861000
8	-2.305783000	2.314428000	-0.001275000
35	-0.095450000	-0.003089000	-0.000299000
1	-4.713870000	-1.205669000	0.888232000
8	-2.312088000	-2.313383000	0.001598000
6	5.132640000	0.005159000	0.001116000
6	4.419137000	-1.205817000	-0.000707000
6	3.015331000	-1.164881000	-0.001771000
7	2.325288000	-0.003668000	-0.001121000
6	3.008042000	1.161891000	0.000637000
6	4.411556000	1.211644000	0.001763000
1	6.226157000	0.008582000	0.002007000
1	4.936830000	-2.168524000	-0.001218000
1	2.413855000	-2.079106000	-0.003227000
1	2.400752000	2.072275000	0.001101000
1	4.923208000	2.177573000	0.003118000

Succinimide-Br...Pyridine-N-oxide

6	-3.475855000	1.814949000	0.176350000
6	-4.181398000	0.517287000	0.611692000
6	-3.134790000	-0.588716000	0.474797000
7	-1.962791000	0.019063000	-0.005139000
6	-2.055389000	1.401618000	-0.205062000
1	-3.410404000	2.567424000	0.976083000
1	-5.041222000	0.253088000	-0.021350000
1	-4.526990000	0.534086000	1.655690000
8	-3.266482000	-1.775049000	0.725768000
35	-0.366158000	-0.911591000	-0.345472000
1	-3.939818000	2.295310000	-0.697631000
8	-1.153184000	2.121717000	-0.609440000
6	4.027857000	1.527500000	0.736248000
6	3.181326000	1.662480000	-0.377617000
6	2.496446000	0.560495000	-0.889564000
7	2.636968000	-0.683102000	-0.310459000

6	3.453869000	-0.836513000	0.788660000
6	4.153424000	0.250837000	1.312060000
1	4.567112000	2.385317000	1.142950000
1	3.033194000	2.629148000	-0.864936000
1	1.819661000	0.583818000	-1.742671000
1	3.483302000	-1.854983000	1.176321000
1	4.792911000	0.081478000	2.181964000
8	1.985368000	-1.694210000	-0.775216000

Succinimide-Br...Ethene

6	3.112900000	0.769731000	-0.000266000
6	3.112541000	-0.770687000	0.000007000
6	1.642845000	-1.186921000	-0.000131000
7	0.889244000	0.000072000	-0.000430000
6	1.643392000	1.186661000	0.000088000
1	3.591043000	1.207527000	-0.888762000
1	3.590630000	-1.208745000	0.888400000
1	3.591014000	-1.209106000	-0.887995000
8	1.183752000	-2.316493000	0.000008000
35	-0.981772000	0.000368000	0.000134000
1	3.591714000	1.207963000	0.887638000
8	1.184870000	2.316484000	0.000599000
6	-3.889298000	-0.001069000	0.677146000
6	-3.888565000	0.000605000	-0.677648000
1	-3.895258000	-0.936726000	1.242319000
1	-3.895623000	0.933222000	1.244571000
1	-3.893857000	-0.933663000	-1.245119000
1	-3.894202000	0.936293000	-1.242775000

Succinimide-Br...Acetylene

6	3.045718000	0.770911000	-0.000190000
6	3.046137000	-0.769816000	0.000218000
6	1.577449000	-1.187810000	0.000017000
7	0.824299000	-0.000067000	-0.000211000
6	1.576801000	1.188097000	-0.000029000
1	3.523908000	1.208504000	-0.888719000
1	3.524549000	-1.207163000	0.888746000
1	3.525039000	-1.207703000	-0.887774000
8	1.117097000	-2.316491000	0.000083000
35	-1.037566000	-0.000513000	-0.000037000
1	3.524362000	1.209079000	0.887802000
8	1.115827000	2.316508000	0.000156000
6	-4.062133000	0.617281000	0.000176000
6	-4.063365000	-0.616240000	-0.000078000
1	-4.071883000	-1.692401000	-0.000306000
1	-4.068275000	1.693459000	0.000412000

Succinimide-Br...Benzene

6	-3.907249000	0.767190000	0.417973000
6	-3.905253000	-0.773358000	0.417043000
6	-2.467997000	-1.188504000	0.109209000

7	-1.733169000	0.000010000	-0.047450000
6	-2.471132000	1.186435000	0.110389000
1	-4.189656000	1.204144000	1.386990000
1	-4.558415000	-1.211621000	-0.351710000
1	-4.186753000	-1.212247000	1.385446000
8	-2.017607000	-2.317185000	0.012018000
35	0.089864000	0.002547000	-0.435961000
1	-4.561722000	1.204724000	-0.350077000
8	-2.023729000	2.316388000	0.014235000
6	2.994765000	0.712833000	-1.027882000
6	3.222607000	1.409539000	0.176463000
6	2.994445000	-0.698635000	-1.036689000
1	3.214492000	2.503320000	0.184638000
1	2.822184000	-1.239783000	-1.971930000
6	3.450382000	0.696597000	1.367551000
6	3.221937000	-1.410438000	0.158870000
1	3.623464000	1.237081000	2.302885000
1	3.213246000	-2.504230000	0.153406000
6	3.450032000	-0.712528000	1.358763000
1	3.622826000	-1.264728000	2.287281000
1	2.822761000	1.265695000	-1.956290000

Succinimide-I complexes

Succinimide-I...NH3

6	3.184511000	0.767618000	0.001188000
6	3.183623000	-0.769974000	0.000916000
6	1.708080000	-1.173832000	0.000134000
7	0.943149000	0.000149000	-0.001065000
6	1.709456000	1.173189000	0.000128000
1	3.661790000	1.208627000	-0.886392000
1	3.659214000	-1.211513000	0.889141000
1	3.660031000	-1.211173000	-0.887046000
8	1.259478000	-2.312041000	0.000406000
53	-1.150342000	0.000674000	-0.000921000
1	3.660280000	1.208222000	0.889786000
8	1.262190000	2.311985000	0.000299000
7	-3.803805000	-0.001024000	0.002702000
1	-4.177612000	0.643135000	0.700201000
1	-4.175677000	-0.927445000	0.214178000
1	-4.182680000	0.278990000	-0.902373000

Succinimide-I...OH2

6	3.173964000	0.769201000	-0.015510000
6	3.173903000	-0.769382000	-0.015258000
6	1.701734000	-1.179581000	-0.007400000
7	0.938834000	-0.000002000	0.000894000
6	1.701830000	1.179523000	-0.007444000
1	3.646233000	1.209069000	-0.906197000
1	3.655270000	-1.209091000	0.870645000
1	3.646399000	-1.209626000	-0.905635000

8	1.249076000	-2.313764000	-0.008377000
53	-1.123428000	0.000072000	0.018013000
1	3.655627000	1.209209000	0.870080000
8	1.249256000	2.313737000	-0.008359000
8	-3.933546000	-0.000269000	0.039821000
1	-4.330866000	0.764942000	-0.399059000
1	-4.329712000	-0.764513000	-0.401782000

Succinimide-I...FH

6	3.151509000	0.850921000	0.000282000
6	3.203904000	-0.687400000	-0.000178000
6	1.748219000	-1.150753000	-0.000010000
7	0.947058000	0.006435000	-0.000209000
6	1.667699000	1.214186000	-0.000018000
1	3.613963000	1.306618000	-0.887557000
1	3.696150000	-1.110591000	0.887712000
1	3.695671000	-1.109985000	-0.888630000
8	1.331349000	-2.296906000	0.000175000
53	-1.103771000	-0.061612000	-0.000029000
1	3.613343000	1.305977000	0.888780000
8	1.174722000	2.330350000	-0.000028000
9	-4.101900000	0.036611000	0.000124000
1	-4.508139000	0.869608000	-0.000027000

Succinimide-I...Acetone

6	4.102560000	-0.307821000	0.006927000
6	3.813783000	1.202986000	-0.004130000
6	2.290064000	1.326701000	-0.008369000
7	1.760296000	0.028495000	-0.000869000
6	2.731868000	-0.985404000	0.008478000
1	4.651376000	-0.644761000	0.898659000
1	4.201368000	1.718890000	-0.894982000
1	4.197481000	1.731165000	0.881191000
8	1.634560000	2.358973000	-0.016829000
53	-0.277731000	-0.342595000	-0.003118000
1	4.655387000	-0.656981000	-0.877600000
8	2.501098000	-2.184871000	0.016376000
6	-3.808546000	0.104451000	0.002294000
8	-2.922359000	-0.760101000	-0.009590000
6	-3.496863000	1.582910000	0.036831000
6	-5.266655000	-0.295572000	-0.015383000
1	-2.418119000	1.761162000	-0.048918000
1	-5.361531000	-1.386846000	0.041311000
1	-3.866858000	2.003801000	0.986854000
1	-4.034822000	2.096978000	-0.775989000
1	-5.732785000	0.073515000	-0.944104000
1	-5.797489000	0.179627000	0.825363000

Succinimide-I...Pyridine

6	4.388082000	-0.768395000	-0.000137000
6	4.387996000	0.768752000	-0.000016000

6	2.910684000	1.170058000	0.000163000
7	2.144087000	0.000055000	0.000012000
6	2.910791000	-1.169847000	-0.000236000
1	4.863846000	-1.210043000	0.888042000
1	4.863710000	1.210476000	-0.888180000
1	4.863945000	1.210338000	0.888089000
8	2.464770000	2.310982000	0.000308000
53	0.029096000	-0.000186000	0.000110000
1	4.864039000	-1.209962000	-0.888242000
8	2.465021000	-2.310812000	-0.000557000
6	-5.273356000	0.000409000	-0.000123000
6	-4.556305000	-1.208304000	0.000360000
6	-3.153373000	-1.165671000	0.000422000
7	-2.468341000	-0.000233000	0.000014000
6	-3.152843000	1.165527000	-0.000449000
6	-4.555758000	1.208800000	-0.000536000
1	-6.366726000	0.000656000	-0.000183000
1	-5.070508000	-2.172696000	0.000692000
1	-2.547947000	-2.076868000	0.000779000
1	-2.547006000	2.076450000	-0.000749000
1	-5.069525000	2.173427000	-0.000924000

Succinimide-I...Pyridine-N-oxide

6	4.410287000	0.444550000	-0.648260000
6	3.823450000	1.804800000	-0.236658000
6	2.364519000	1.522392000	0.126762000
7	2.136393000	0.153098000	-0.049720000
6	3.259580000	-0.553543000	-0.503316000
1	5.237429000	0.108735000	-0.005525000
1	3.837632000	2.553309000	-1.042715000
1	4.315284000	2.249857000	0.640964000
8	1.533391000	2.338416000	0.505179000
53	0.277898000	-0.729726000	0.317624000
1	4.762376000	0.412810000	-1.689913000
8	3.294958000	-1.753205000	-0.736075000
6	-4.432197000	1.519187000	-0.756428000
6	-3.641879000	1.704687000	0.390635000
6	-2.853593000	0.664620000	0.884722000
7	-2.844141000	-0.557858000	0.256161000
6	-3.597096000	-0.761827000	-0.874462000
6	-4.396749000	0.261976000	-1.384215000
1	-5.051061000	2.327783000	-1.150534000
1	-3.620870000	2.661738000	0.917157000
1	-2.210123000	0.722743000	1.762175000
1	-3.499068000	-1.761635000	-1.297676000
1	-4.984815000	0.059537000	-2.282597000
8	-2.100730000	-1.518600000	0.715502000

Succinimide-I...Ethene

6	3.393360000	0.769494000	0.000513000
---	-------------	-------------	-------------

6	3.393469000	-0.769191000	-0.000081000
6	1.920686000	-1.179256000	0.000086000
7	1.157364000	-0.000026000	0.000064000
6	1.920509000	1.179337000	0.000030000
1	3.870690000	1.210082000	-0.887145000
1	3.870670000	-1.209701000	0.887687000
1	3.870106000	-1.208889000	-0.888564000
8	1.468125000	-2.313679000	0.000139000
53	-0.917453000	-0.000072000	-0.000228000
1	3.869731000	1.209248000	0.889113000
8	1.467768000	2.313671000	-0.000232000
6	-3.885338000	0.000274000	0.679188000
6	-3.886082000	-0.000146000	-0.678191000
1	-3.895303000	-0.934865000	1.245304000
1	-3.895491000	0.935764000	1.244722000
1	-3.896758000	-0.935628000	-1.243725000
1	-3.896935000	0.935004000	-1.244273000

Succinimide-I...Acetylene

6	3.337133000	0.769019000	0.000201000
6	3.336784000	-0.770097000	-0.000391000
6	1.865064000	-1.181490000	-0.000152000
7	1.103805000	-0.000035000	0.000003000
6	1.865598000	1.181074000	0.000111000
1	3.814559000	1.208904000	-0.887708000
1	3.814106000	-1.210203000	0.887464000
1	3.813509000	-1.209430000	-0.888958000
8	1.409684000	-2.314059000	-0.000152000
53	-0.957853000	0.000428000	0.000075000
1	3.814151000	1.208137000	0.888715000
8	1.410721000	2.313840000	0.000174000
6	-4.083795000	0.616449000	-0.000910000
6	-4.083524000	-0.617750000	0.000577000
1	-4.101313000	-1.694159000	0.001841000
1	-4.102242000	1.692847000	-0.002161000

Succinimide-I...Benzene

6	4.154365000	-0.619660000	0.449394000
6	4.070495000	0.916309000	0.407666000
6	2.601861000	1.240571000	0.135024000
7	1.919223000	0.017543000	0.022902000
6	2.732548000	-1.116334000	0.188042000
1	4.479814000	-1.015443000	1.422741000
1	4.673077000	1.367329000	-0.394496000
1	4.357584000	1.399046000	1.353343000
8	2.094359000	2.345893000	0.028427000
53	-0.108338000	-0.100709000	-0.353090000
1	4.812424000	-1.046016000	-0.321944000
8	2.351010000	-2.274597000	0.129663000
6	-3.096837000	-0.964354000	-0.753802000

6	-3.406586000	-1.324784000	0.574308000
6	-3.094491000	0.396729000	-1.132980000
1	-3.402813000	-2.378178000	0.868819000
1	-2.871160000	0.675509000	-2.167335000
6	-3.711793000	-0.328341000	1.518611000
6	-3.400035000	1.393271000	-0.182372000
1	-3.948591000	-0.607462000	2.549539000
1	-3.390248000	2.447347000	-0.474148000
6	-3.707957000	1.029645000	1.140719000
1	-3.940729000	1.802590000	1.878987000
1	-2.874349000	-1.738629000	-1.494421000

Saccharin-H complexes

Saccharin-H...NH3

6	2.304278000	1.408627000	-0.047107000
6	1.030590000	0.831027000	0.070144000
6	0.882003000	-0.559112000	-0.018723000
6	1.957424000	-1.434275000	-0.203549000
6	3.233973000	-0.849250000	-0.320481000
6	3.404180000	0.552216000	-0.243081000
6	-0.266359000	1.554297000	0.272692000
7	-1.284408000	0.625928000	0.515228000
16	-0.839758000	-0.997964000	0.165262000
1	2.418962000	2.493895000	0.019568000
1	1.813432000	-2.516505000	-0.257607000
1	4.106848000	-1.490750000	-0.471712000
1	4.408840000	0.974079000	-0.336028000
8	-0.421965000	2.771278000	0.246529000
1	-2.276965000	0.845427000	0.249701000
8	-1.454324000	-1.400702000	-1.132858000
8	-1.039518000	-1.865511000	1.351612000
7	-3.910449000	0.651438000	-0.557842000
1	-3.688680000	-0.138954000	-1.168019000
1	-4.210564000	1.417814000	-1.160419000
1	-4.721824000	0.379151000	-0.003002000

Saccharin-H...OH2

6	2.383091000	1.286775000	0.085677000
6	1.072910000	0.804402000	-0.057411000
6	0.823722000	-0.572748000	0.007155000
6	1.830558000	-1.526485000	0.189682000
6	3.143685000	-1.036433000	0.333369000
6	3.415282000	0.350189000	0.282025000
6	-0.162894000	1.622633000	-0.266750000
7	-1.239829000	0.767262000	-0.548111000
16	-0.918154000	-0.892633000	-0.208495000
1	2.576481000	2.361776000	0.037848000
1	1.608518000	-2.596244000	0.222798000
1	3.965861000	-1.741566000	0.484880000

1	4.446184000	0.696934000	0.395113000
8	-0.238563000	2.844392000	-0.221634000
1	-2.197007000	1.065993000	-0.305515000
8	-1.573690000	-1.259915000	1.083222000
8	-1.161509000	-1.735516000	-1.400642000
8	-3.802098000	0.508292000	0.611327000
1	-3.385622000	-0.198446000	1.133707000
1	-4.476390000	0.894823000	1.183211000

Saccharin-H...FH

6	1.506912000	-1.990353000	0.000779000
6	0.581749000	-0.935536000	0.000773000
6	1.028401000	0.393265000	0.000682000
6	2.382613000	0.741445000	-0.000947000
6	3.308868000	-0.320782000	-0.001037000
6	2.876801000	-1.666373000	-0.000161000
6	-0.903842000	-1.057588000	0.000626000
7	-1.468218000	0.194533000	0.000659000
16	-0.350855000	1.528962000	0.000186000
1	1.155907000	-3.025600000	0.000981000
1	2.706450000	1.785393000	-0.001574000
1	4.379516000	-0.098112000	-0.002123000
1	3.621354000	-2.467013000	-0.000181000
8	-1.533293000	-2.126267000	0.000270000
1	-2.483242000	0.328401000	-0.000557000
8	-0.458928000	2.256975000	1.284974000
8	-0.459344000	2.256544000	-1.284838000
1	-3.150461000	-1.732754000	-0.000622000
9	-3.934980000	-1.188657000	-0.001227000

Saccharin-H...Acetone

6	3.299699000	1.091973000	-0.243767000
6	1.965172000	0.740988000	0.012052000
6	1.578110000	-0.604698000	-0.016825000
6	2.467899000	-1.653013000	-0.274048000
6	3.806235000	-1.295134000	-0.530967000
6	4.215476000	0.058182000	-0.515783000
6	0.837578000	1.677950000	0.316895000
7	-0.296105000	0.932351000	0.673691000
16	-0.163307000	-0.751643000	0.340991000
1	3.600042000	2.143008000	-0.223379000
1	2.140146000	-2.695800000	-0.278763000
1	4.539942000	-2.077825000	-0.743640000
1	5.262161000	0.301842000	-0.718045000
8	0.886774000	2.901211000	0.286457000
1	-1.239999000	1.335447000	0.535536000
8	-0.954314000	-1.089530000	-0.876132000
8	-0.385874000	-1.542991000	1.576511000
6	-3.515037000	0.285731000	-0.272530000
8	-2.927260000	1.372218000	-0.203359000

6	-4.161646000	-0.170861000	-1.557598000
6	-3.610621000	-0.645611000	0.914496000
1	-4.225952000	0.661577000	-2.269457000
1	-2.965280000	-0.307322000	1.735445000
1	-5.156786000	-0.602965000	-1.369186000
1	-3.523578000	-0.966821000	-1.977998000
1	-3.338214000	-1.669815000	0.618882000
1	-4.658639000	-0.661806000	1.259548000

Saccharin-H...Pyridine

6	-3.299717000	1.744196000	-0.369964000
6	-2.199638000	0.936932000	-0.042278000
6	-2.333235000	-0.457347000	-0.028994000
6	-3.535668000	-1.113450000	-0.312218000
6	-4.637360000	-0.298750000	-0.641588000
6	-4.520341000	1.109953000	-0.669687000
6	-0.815980000	1.399455000	0.302002000
7	-0.044391000	0.310625000	0.710666000
16	-0.777992000	-1.212443000	0.425528000
1	-3.192877000	2.832259000	-0.382432000
1	-3.614701000	-2.203318000	-0.283149000
1	-5.598539000	-0.764622000	-0.877123000
1	-5.395165000	1.713493000	-0.927524000
8	-0.413028000	2.559211000	0.251587000
1	1.012502000	0.349247000	0.591512000
8	-0.119645000	-1.867463000	-0.741612000
8	-0.914481000	-1.976905000	1.689769000
6	5.353158000	-0.000337000	-0.620185000
6	4.951566000	1.095569000	0.162673000
6	3.605874000	1.191187000	0.552736000
7	2.679502000	0.270373000	0.206126000
6	3.064374000	-0.782369000	-0.552330000
6	4.389560000	-0.956142000	-0.984172000
1	6.393563000	-0.105707000	-0.940402000
1	5.664553000	1.865905000	0.467608000
1	3.247528000	2.029196000	1.158362000
1	2.272989000	-1.492703000	-0.812850000
1	4.653899000	-1.823778000	-1.593916000

Saccharin-H...Pyridine-N-oxide

6	2.896766000	-1.609894000	-0.404734000
6	1.903677000	-0.625636000	-0.526843000
6	1.877630000	0.457307000	0.360166000
6	2.817293000	0.633409000	1.381018000
6	3.813450000	-0.356442000	1.499721000
6	3.851990000	-1.461989000	0.619003000
6	0.795058000	-0.591488000	-1.532774000
7	0.109656000	0.618053000	-1.439014000
16	0.499687000	1.526729000	-0.027523000
1	2.915852000	-2.454955000	-1.098284000

1	2.779142000	1.494717000	2.053079000
1	4.570205000	-0.265897000	2.284276000
1	4.640072000	-2.211106000	0.736593000
8	0.525500000	-1.492748000	-2.326153000
1	-0.905133000	0.674500000	-1.746416000
8	-0.592415000	1.370669000	0.975519000
8	0.961355000	2.886794000	-0.391581000
6	-2.875208000	-1.424890000	1.870792000
6	-2.224427000	-2.001367000	0.768157000
6	-2.148853000	-1.319617000	-0.448667000
7	-2.696327000	-0.064555000	-0.575418000
6	-3.346279000	0.516862000	0.484444000
6	-3.446813000	-0.151175000	1.703441000
1	-2.937422000	-1.948797000	2.826767000
1	-1.768509000	-2.992611000	0.831463000
1	-1.674562000	-1.698565000	-1.355127000
1	-3.722987000	1.518085000	0.278415000
1	-3.964828000	0.349347000	2.524929000
8	-2.557667000	0.590617000	-1.687368000

Saccharin-H...Ethene

6	-2.683927000	1.287736000	0.030027000
6	-1.366396000	0.811337000	-0.050540000
6	-1.115723000	-0.566532000	0.004513000
6	-2.127882000	-1.524124000	0.126609000
6	-3.448912000	-1.040178000	0.205999000
6	-3.722178000	0.346007000	0.159163000
6	-0.127015000	1.638929000	-0.190274000
7	0.959091000	0.783176000	-0.402597000
16	0.638142000	-0.886875000	-0.092157000
1	-2.877980000	2.362845000	-0.012249000
1	-1.904389000	-2.593615000	0.159960000
1	-4.275249000	-1.749697000	0.305225000
1	-4.758629000	0.688720000	0.222829000
8	-0.059422000	2.861956000	-0.154884000
1	1.920846000	1.095869000	-0.238417000
8	1.196429000	-1.268758000	1.231690000
8	0.979483000	-1.698406000	-1.285209000
6	4.056898000	0.535655000	0.851013000
6	4.140602000	-0.030009000	-0.374698000
1	4.579874000	1.467791000	1.082394000
1	3.468590000	0.066774000	1.644749000
1	4.731620000	0.426502000	-1.173273000
1	3.626693000	-0.968688000	-0.602173000

Saccharin-H...Acetylene

6	1.999846000	1.855275000	0.006853000
6	0.952092000	0.923802000	0.069894000
6	1.225198000	-0.447350000	-0.026878000
6	2.518376000	-0.959500000	-0.174494000

6	3.567074000	-0.020451000	-0.237640000
6	3.310773000	1.366939000	-0.148768000
6	-0.502955000	1.229858000	0.229026000
7	-1.200532000	0.034674000	0.412698000
16	-0.285952000	-1.395735000	0.068875000
1	1.784456000	2.924494000	0.081701000
1	2.705268000	-2.034503000	-0.239565000
1	4.595720000	-0.372233000	-0.357056000
1	4.147332000	2.069251000	-0.200146000
8	-1.013052000	2.347616000	0.225434000
1	-2.209451000	0.015379000	0.224095000
8	-0.688855000	-1.929964000	-1.256548000
8	-0.281968000	-2.286184000	1.253188000
6	-4.042588000	1.309808000	-0.188506000
6	-4.618917000	0.227481000	-0.323141000
1	-5.158621000	-0.695206000	-0.445949000
1	-3.468130000	2.214947000	-0.068632000

Saccharin-H···Benzene

6	3.222542000	1.564915000	-0.038414000
6	1.991059000	0.892921000	-0.015352000
6	1.956759000	-0.507696000	-0.008193000
6	3.109194000	-1.299925000	-0.031525000
6	4.343718000	-0.620685000	-0.055078000
6	4.398887000	0.791795000	-0.057576000
6	0.632185000	1.520018000	0.007076000
7	-0.324990000	0.514422000	-0.107385000
16	0.271018000	-1.097008000	0.045729000
1	3.246444000	2.657943000	-0.043599000
1	3.053874000	-2.391640000	-0.030751000
1	5.273279000	-1.196743000	-0.071391000
1	5.372944000	1.288508000	-0.076320000
8	0.384502000	2.719252000	0.087596000
1	-1.309095000	0.707832000	0.103660000
8	-0.059350000	-1.885129000	-1.167075000
8	-0.063338000	-1.647167000	1.384788000
6	-3.511847000	1.515451000	-0.112645000
6	-3.377592000	0.898483000	1.149561000
6	-3.422346000	0.740962000	-1.287518000
1	-3.438274000	1.501348000	2.060234000
1	-3.516318000	1.221029000	-2.265713000
6	-3.146876000	-0.489677000	1.235046000
6	-3.186881000	-0.645104000	-1.201421000
1	-3.015796000	-0.966096000	2.210181000
1	-3.087104000	-1.242788000	-2.111360000
6	-3.046261000	-1.259541000	0.058842000
1	-2.837478000	-2.330360000	0.124212000
1	-3.673591000	2.594997000	-0.178415000

Saccharin-Cl complexes

Saccharin-Cl...NH3

6	-2.514850000	1.743339000	0.020905000
6	-1.389461000	0.906281000	-0.041180000
6	-1.548980000	-0.484936000	0.028917000
6	-2.797013000	-1.107551000	0.137502000
6	-3.922485000	-0.262110000	0.198296000
6	-3.782163000	1.143425000	0.142422000
6	0.029722000	1.355141000	-0.176594000
7	0.811994000	0.225647000	-0.518279000
16	0.036558000	-1.299192000	-0.029557000
1	-2.389134000	2.828115000	-0.032247000
1	-2.892069000	-2.195724000	0.177350000
1	-4.919643000	-0.701719000	0.290944000
1	-4.675535000	1.772095000	0.192289000
8	0.448307000	2.498410000	-0.069736000
17	2.519588000	0.298052000	-0.176459000
8	0.502892000	-1.679752000	1.324934000
8	0.116318000	-2.259821000	-1.152302000
7	5.167097000	0.415503000	0.351922000
1	5.451708000	1.355171000	0.628545000
1	5.761611000	0.145889000	-0.431831000
1	5.402749000	-0.203938000	1.127379000

Saccharin-Cl...OH2

6	-2.508837000	1.746351000	0.027279000
6	-1.384942000	0.907425000	-0.039577000
6	-1.546305000	-0.483685000	0.035517000
6	-2.794709000	-1.104096000	0.153025000
6	-3.918188000	-0.256535000	0.218865000
6	-3.776077000	1.148651000	0.158536000
6	0.032418000	1.354965000	-0.185768000
7	0.806500000	0.222337000	-0.550602000
16	0.035176000	-1.303637000	-0.029519000
1	-2.382083000	2.830762000	-0.030335000
1	-2.891377000	-2.191995000	0.195886000
1	-4.915393000	-0.694321000	0.318944000
1	-4.668134000	1.778795000	0.212188000
8	0.459080000	2.493415000	-0.071596000
17	2.505597000	0.294112000	-0.224645000
8	0.522399000	-1.660212000	1.323627000
8	0.102014000	-2.276751000	-1.140956000
8	5.233156000	0.408227000	0.325750000
1	5.447245000	1.244911000	0.760097000
1	5.452905000	-0.262104000	0.986838000

Saccharin-Cl...FH

6	-2.842980000	-1.071741000	-0.361801000
6	-1.514627000	-0.697540000	-0.102482000
6	-1.197881000	0.655236000	0.093736000
6	-2.150195000	1.679753000	0.072555000

6	-3.480277000	1.295385000	-0.187847000
6	-3.819999000	-0.059942000	-0.403912000
6	-0.347958000	-1.622637000	-0.009787000
7	0.721279000	-0.903492000	0.614422000
16	0.547863000	0.852472000	0.362217000
1	-3.091701000	-2.125038000	-0.516492000
1	-1.874288000	2.723429000	0.243373000
1	-4.261441000	2.059754000	-0.224129000
1	-4.862043000	-0.323769000	-0.603924000
8	-0.299595000	-2.793922000	-0.338707000
17	2.322041000	-1.475541000	0.295353000
8	1.230129000	1.226693000	-0.909750000
8	0.862231000	1.564058000	1.615408000
1	3.022198000	1.385616000	-1.064421000
9	3.951023000	1.444821000	-1.165578000

Saccharin-Cl...Acetone

6	3.637510000	1.391495000	-0.499397000
6	2.416482000	0.797628000	-0.141551000
6	2.324462000	-0.597533000	-0.031307000
6	3.410605000	-1.455277000	-0.236274000
6	4.632633000	-0.852655000	-0.594435000
6	4.743078000	0.550724000	-0.725323000
6	1.141169000	1.522050000	0.141587000
7	0.260634000	0.613292000	0.791886000
16	0.663658000	-1.080382000	0.397788000
1	3.708150000	2.478988000	-0.587294000
1	3.312791000	-2.538537000	-0.128253000
1	5.508954000	-1.481914000	-0.773818000
1	5.706099000	0.987156000	-1.004346000
8	0.897298000	2.695978000	-0.085554000
17	-1.441398000	0.927168000	0.650091000
8	-0.114874000	-1.497740000	-0.794468000
8	0.630464000	-1.887210000	1.636919000
6	-4.645392000	-0.014797000	-0.354944000
8	-4.117916000	0.936881000	0.227399000
6	-6.136916000	-0.031993000	-0.629020000
6	-3.855716000	-1.219483000	-0.826930000
1	-6.623347000	0.815258000	-0.129596000
1	-2.775342000	-1.050385000	-0.744771000
1	-6.577266000	-0.983145000	-0.288621000
1	-6.304326000	0.032767000	-1.717349000
1	-4.125758000	-1.464783000	-1.866640000
1	-4.136405000	-2.088421000	-0.207471000

Saccharin-Cl...Pyridine

6	3.968930000	1.606572000	-0.496749000
6	2.822828000	0.871846000	-0.153466000
6	2.896547000	-0.523368000	-0.036527000
6	4.080172000	-1.245561000	-0.223052000

6	5.226861000	-0.502413000	-0.566366000
6	5.170663000	0.903637000	-0.702436000
6	1.464115000	1.438032000	0.107373000
7	0.681055000	0.431021000	0.724089000
16	1.296756000	-1.198348000	0.369759000
1	3.909664000	2.694314000	-0.589973000
1	4.110832000	-2.332494000	-0.111802000
1	6.174667000	-1.022975000	-0.730271000
1	6.078612000	1.451280000	-0.969956000
8	1.094737000	2.581328000	-0.115805000
17	-1.057911000	0.555328000	0.566340000
8	0.609600000	-1.734503000	-0.830712000
8	1.339190000	-1.983890000	1.623197000
6	-6.181762000	-0.392936000	-0.672656000
6	-5.054599000	-1.156336000	-1.021428000
6	-3.787241000	-0.728315000	-0.590465000
7	-3.597576000	0.388219000	0.148545000
6	-4.685335000	1.118158000	0.480623000
6	-5.991135000	0.768929000	0.094420000
1	-7.183535000	-0.695516000	-0.990736000
1	-5.149941000	-2.068238000	-1.616889000
1	-2.883311000	-1.293747000	-0.841358000
1	-4.497925000	2.015790000	1.078300000
1	-6.835494000	1.396934000	0.391248000

Saccharin-Cl...Pyridine-N-oxide

6	-4.241760000	0.809060000	-0.241167000
6	-2.859483000	0.577806000	-0.158183000
6	-2.379612000	-0.728643000	0.017592000
6	-3.215338000	-1.847615000	0.096111000
6	-4.601282000	-1.608405000	0.010721000
6	-5.106176000	-0.298147000	-0.152782000
6	-1.790594000	1.618427000	-0.244003000
7	-0.555970000	0.946988000	-0.458150000
16	-0.602270000	-0.727089000	0.147107000
1	-4.615617000	1.827382000	-0.377448000
1	-2.812098000	-2.855910000	0.220438000
1	-5.296252000	-2.450473000	0.073748000
1	-6.187266000	-0.146027000	-0.214473000
8	-1.935129000	2.829164000	-0.204058000
17	0.905979000	1.777833000	-0.028571000
8	-0.165996000	-0.758713000	1.565449000
8	0.033766000	-1.618552000	-0.848717000
6	3.580798000	-2.090415000	-0.472230000
6	4.191910000	-1.103552000	-1.265976000
6	4.185093000	0.234512000	-0.872527000
7	3.585907000	0.623333000	0.311039000
6	2.980592000	-0.334383000	1.103103000
6	2.970622000	-1.676212000	0.723780000

1	3.567603000	-3.137061000	-0.781925000
1	4.676939000	-1.357839000	-2.212067000
1	4.620690000	1.060752000	-1.434759000
1	2.517473000	0.064835000	2.004460000
1	2.457545000	-2.385673000	1.377041000
8	3.543293000	1.858532000	0.642342000

Saccharin-Cl...Ethene

6	-2.746964000	1.780064000	0.035762000
6	-1.640307000	0.919228000	-0.041592000
6	-1.828062000	-0.468586000	0.035513000
6	-3.087289000	-1.064403000	0.165018000
6	-4.193200000	-0.194940000	0.241331000
6	-4.024240000	1.207263000	0.179206000
6	-0.216562000	1.339820000	-0.201612000
7	0.532330000	0.191351000	-0.577797000
16	-0.264059000	-1.320224000	-0.043195000
1	-2.599650000	2.861812000	-0.023137000
1	-3.204793000	-2.150191000	0.209277000
1	-5.197766000	-0.613099000	0.351156000
1	-4.903211000	1.854747000	0.241421000
8	0.234249000	2.468817000	-0.090925000
17	2.237399000	0.232285000	-0.244978000
8	-0.226807000	-2.295621000	-1.154079000
8	0.231081000	-1.682502000	1.305227000
6	5.320682000	0.358559000	-0.336613000
6	5.038597000	0.247075000	0.981192000
1	5.477968000	-0.525582000	-0.959886000
1	5.403450000	1.336406000	-0.818134000
1	4.958049000	-0.730385000	1.463845000
1	4.884683000	1.131549000	1.604771000

Saccharin-Cl...Acetylene

6	-2.692273000	1.758744000	0.088807000
6	-1.574435000	0.915246000	-0.015282000
6	-1.743140000	-0.476506000	0.028506000
6	-2.993564000	-1.092455000	0.149251000
6	-4.110595000	-0.240250000	0.252751000
6	-3.960874000	1.165255000	0.224529000
6	-0.157710000	1.359412000	-0.171400000
7	0.604738000	0.230610000	-0.581962000
16	-0.169135000	-1.305644000	-0.079951000
1	-2.559851000	2.843509000	0.055972000
1	-3.096204000	-2.180493000	0.167029000
1	-5.108824000	-0.674609000	0.357288000
1	-4.848117000	1.798996000	0.307269000
8	0.279066000	2.490695000	-0.034469000
17	2.305845000	0.283557000	-0.251238000
8	0.340352000	-1.693556000	1.255987000
8	-0.126130000	-2.252581000	-1.214686000

6	5.417973000	0.742936000	-0.015565000
6	5.201829000	-0.175232000	0.778125000
1	5.007916000	-0.976775000	1.469123000
1	5.609149000	1.545578000	-0.705668000

Saccharin-Cl...Benzene

6	3.958390000	1.111509000	-0.052456000
6	2.610648000	0.717488000	-0.049716000
6	2.281257000	-0.644652000	0.001448000
6	3.239655000	-1.663512000	0.027592000
6	4.589911000	-1.261416000	0.024554000
6	4.943135000	0.107043000	-0.012644000
6	1.432915000	1.633324000	-0.095795000
7	0.291250000	0.850066000	-0.428195000
16	0.513003000	-0.866571000	0.039343000
1	4.214545000	2.173661000	-0.091511000
1	2.953222000	-2.718034000	0.052903000
1	5.376169000	-2.021053000	0.052653000
1	6.000380000	0.386161000	-0.013763000
8	1.433010000	2.843245000	0.060736000
17	-1.249758000	1.489420000	0.025214000
8	0.051928000	-1.730982000	-1.069389000
8	0.016539000	-1.068882000	1.420447000
6	-4.064588000	0.038386000	-1.323092000
6	-4.516479000	0.797512000	-0.225604000
6	-3.304580000	-1.126586000	-1.107011000
1	-5.103649000	1.705883000	-0.392619000
1	-2.935764000	-1.708161000	-1.956860000
6	-4.214016000	0.385261000	1.088120000
6	-3.002477000	-1.537702000	0.205708000
1	-4.565380000	0.974879000	1.940612000
1	-2.403422000	-2.436764000	0.370884000
6	-3.460425000	-0.785125000	1.302950000
1	-3.212627000	-1.098969000	2.321140000
1	-4.296276000	0.360701000	-2.342862000

Saccharin-Br complexes

Saccharin-Br...NH3

6	2.855395000	1.763694000	0.025250000
6	1.749065000	0.901907000	-0.034774000
6	1.939437000	-0.484960000	0.027591000
6	3.200745000	-1.080485000	0.131444000
6	4.308128000	-0.210739000	0.189750000
6	4.136645000	1.191466000	0.138994000
6	0.315588000	1.315886000	-0.160682000
7	-0.456377000	0.173674000	-0.433151000
16	0.365917000	-1.325933000	-0.036346000
1	2.705026000	2.845637000	-0.021730000
1	3.319969000	-2.166426000	0.167809000
1	5.315224000	-0.628557000	0.276405000

1	5.016331000	1.839450000	0.186818000
8	-0.112924000	2.461658000	-0.088472000
35	-2.333111000	0.215724000	-0.085165000
8	-0.050040000	-1.789424000	1.311133000
8	0.286471000	-2.247503000	-1.193998000
7	-4.828142000	0.275432000	0.363703000
1	-5.073012000	-0.353202000	1.128744000
1	-5.372236000	-0.006809000	-0.451501000
1	-5.133554000	1.212295000	0.627156000

Saccharin-Br...OH2

6	2.873690000	1.739722000	-0.031229000
6	1.755735000	0.892759000	0.027487000
6	1.928546000	-0.497267000	-0.028758000
6	3.182716000	-1.109418000	-0.123374000
6	4.301064000	-0.254096000	-0.180620000
6	4.147512000	1.150454000	-0.137235000
6	0.331011000	1.330494000	0.147149000
7	-0.449545000	0.195023000	0.460927000
16	0.349158000	-1.324146000	0.024071000
1	2.737392000	2.823677000	0.011374000
1	3.288250000	-2.196914000	-0.154067000
1	5.302941000	-0.685293000	-0.261075000
1	5.035548000	1.786854000	-0.184152000
8	-0.090592000	2.473748000	0.047705000
35	-2.294069000	0.255269000	0.114115000
8	-0.085181000	-1.746014000	-1.329729000
8	0.256626000	-2.260767000	1.166608000
8	-4.967503000	0.280804000	-0.365075000
1	-5.135810000	0.113941000	-1.302936000
1	-5.404072000	-0.453545000	0.088625000

Saccharin-Br...FH

6	2.893951000	1.715249000	0.064900000
6	1.766000000	0.882999000	-0.014278000
6	1.920434000	-0.509680000	0.037117000
6	3.165395000	-1.138420000	0.145014000
6	4.293312000	-0.297635000	0.223035000
6	4.158298000	1.109063000	0.185674000
6	0.350488000	1.341189000	-0.151793000
7	-0.436471000	0.216472000	-0.505864000
16	0.333984000	-1.319378000	-0.040947000
1	2.772357000	2.801074000	0.025895000
1	3.256722000	-2.227312000	0.170532000
1	5.288362000	-0.742029000	0.315112000
1	5.053570000	1.733747000	0.248739000
8	-0.062621000	2.485138000	-0.039653000
35	-2.275123000	0.300621000	-0.165735000
8	-0.136598000	-1.721746000	1.306178000
8	0.250445000	-2.258908000	-1.180527000

1	-5.160963000	-0.506958000	1.141253000
9	-5.062916000	0.151336000	0.496599000

Saccharin-Br...Acetone

6	3.293347000	2.100577000	-0.043979000
6	2.375147000	1.039355000	-0.076377000
6	2.820291000	-0.276142000	0.113932000
6	4.163631000	-0.606716000	0.320165000
6	5.081083000	0.462509000	0.350440000
6	4.650749000	1.797121000	0.172449000
6	0.901161000	1.159548000	-0.298369000
7	0.383567000	-0.129074000	-0.529547000
16	1.445056000	-1.412842000	0.061097000
1	2.944449000	3.126251000	-0.190870000
1	4.483876000	-1.643121000	0.454619000
1	6.142239000	0.254923000	0.514994000
1	5.387683000	2.604579000	0.201485000
8	0.253061000	2.198814000	-0.325106000
35	-1.465626000	-0.394921000	-0.282210000
8	1.027149000	-1.817106000	1.425036000
8	1.614740000	-2.426635000	-1.003897000
6	-4.773880000	0.346261000	0.208430000
8	-4.027696000	-0.619768000	0.009982000
6	-6.266042000	0.146548000	0.364812000
6	-4.255626000	1.764163000	0.310777000
1	-6.506255000	-0.923727000	0.375326000
1	-3.189857000	1.816155000	0.057404000
1	-6.786665000	0.638045000	-0.474008000
1	-6.617042000	0.627876000	1.291908000
1	-4.405655000	2.122446000	1.343300000
1	-4.838918000	2.426016000	-0.349307000

Saccharin-Br...Pyridine

6	4.016077000	1.810807000	0.261801000
6	2.941789000	0.928494000	0.068740000
6	3.163845000	-0.454510000	0.072696000
6	4.428716000	-1.026112000	0.244466000
6	5.504622000	-0.136102000	0.436270000
6	5.299876000	1.262566000	0.445656000
6	1.508500000	1.311889000	-0.146655000
7	0.781806000	0.171606000	-0.510315000
16	1.618785000	-1.319146000	-0.169237000
1	3.840288000	2.889959000	0.260792000
1	4.573698000	-2.109497000	0.233048000
1	6.512956000	-0.534948000	0.579947000
1	6.155574000	1.926720000	0.596966000
8	1.052257000	2.448341000	-0.060614000
35	-1.148214000	0.150198000	-0.267900000
8	1.125161000	-1.901094000	1.105976000
8	1.654473000	-2.159158000	-1.391237000

6	-6.237590000	0.039447000	0.382563000
6	-5.456865000	-1.110606000	0.591213000
6	-4.068735000	-1.032517000	0.397616000
7	-3.462904000	0.112647000	0.016534000
6	-4.205071000	1.222520000	-0.185393000
6	-5.598149000	1.227277000	-0.012231000
1	-7.321227000	0.010905000	0.525532000
1	-5.910779000	-2.055845000	0.899455000
1	-3.412500000	-1.895031000	0.547146000
1	-3.655745000	2.117984000	-0.490619000
1	-6.164857000	2.145753000	-0.184956000

Saccharin-Br...Pyridine-N-oxide

6	-3.269924000	2.402888000	0.102127000
6	-2.567586000	1.190815000	0.014815000
6	-3.267820000	-0.012565000	-0.145360000
6	-4.661353000	-0.079209000	-0.244244000
6	-5.361543000	1.140805000	-0.157347000
6	-4.674524000	2.364015000	0.015017000
6	-1.081452000	1.026452000	0.081192000
7	-0.761238000	-0.289155000	-0.285321000
16	-2.130973000	-1.389612000	-0.192476000
1	-2.722606000	3.340737000	0.229488000
1	-5.180375000	-1.031749000	-0.378779000
1	-6.453305000	1.139428000	-0.223229000
1	-5.246745000	3.293764000	0.079507000
8	-0.270156000	1.903076000	0.363782000
35	0.937516000	-0.971340000	0.232629000
8	-2.238966000	-2.139085000	-1.465369000
8	-2.107570000	-2.112429000	1.102129000
6	5.034208000	1.944805000	-0.704108000
6	4.124075000	2.026284000	0.363683000
6	3.534453000	0.874422000	0.884840000
7	3.836315000	-0.362434000	0.359600000
6	4.715687000	-0.466782000	-0.693729000
6	5.322373000	0.671276000	-1.225617000
1	5.499429000	2.841546000	-1.118262000
1	3.851679000	2.987436000	0.806060000
1	2.816957000	0.850885000	1.704236000
1	4.868921000	-1.488671000	-1.041056000
1	6.017620000	0.543537000	-2.058945000
8	3.269920000	-1.424604000	0.833334000

Saccharin-Br...Ethene

6	-3.048933000	1.786846000	0.034516000
6	-1.953522000	0.911462000	-0.033547000
6	-2.159758000	-0.473184000	0.040288000
6	-3.427009000	-1.052740000	0.162053000
6	-4.522575000	-0.169082000	0.229032000
6	-4.335013000	1.230735000	0.167936000

6	-0.520307000	1.311217000	-0.181963000
7	0.227446000	0.154824000	-0.499414000
16	-0.601840000	-1.339590000	-0.034188000
1	-2.886596000	2.866570000	-0.022023000
1	-3.559072000	-2.136890000	0.205731000
1	-5.533378000	-0.574190000	0.330712000
1	-5.206126000	1.889520000	0.222688000
8	-0.069054000	2.445132000	-0.100242000
35	2.088798000	0.181152000	-0.149053000
8	-0.555644000	-2.287723000	-1.169974000
8	-0.151865000	-1.760381000	1.314890000
6	5.008041000	0.200383000	-0.312841000
6	4.754710000	0.239114000	1.019088000
1	5.125302000	-0.750229000	-0.839541000
1	5.115551000	1.118840000	-0.895696000
1	4.660651000	-0.678975000	1.604837000
1	4.651767000	1.189988000	1.548295000

Saccharin-Br...Acetylene

6	-2.994583000	1.780536000	0.088856000
6	-1.895779000	0.911639000	-0.004702000
6	-2.096867000	-0.475455000	0.029416000
6	-3.362057000	-1.063032000	0.133763000
6	-4.460749000	-0.185735000	0.226516000
6	-4.278414000	1.215965000	0.206236000
6	-0.465245000	1.322401000	-0.140761000
7	0.285332000	0.177403000	-0.501079000
16	-0.537792000	-1.336121000	-0.067789000
1	-2.836339000	2.862038000	0.063447000
1	-3.490049000	-2.148470000	0.145784000
1	-5.469977000	-0.597403000	0.316608000
1	-5.151915000	1.869638000	0.280327000
8	-0.016010000	2.452813000	-0.021661000
35	2.133450000	0.198001000	-0.148910000
8	-0.081147000	-1.783631000	1.269973000
8	-0.489913000	-2.255378000	-1.226210000
6	5.161477000	0.574992000	-0.085249000
6	4.964578000	-0.164710000	0.882465000
1	4.801556000	-0.811423000	1.727259000
1	5.345701000	1.221644000	-0.925465000

Saccharin-Br...Benzene

6	4.085963000	1.396580000	0.177867000
6	2.848772000	0.750153000	0.028004000
6	2.790010000	-0.650646000	0.011384000
6	3.922025000	-1.465454000	0.117446000
6	5.160818000	-0.810676000	0.266492000
6	5.240345000	0.600403000	0.298293000
6	1.521951000	1.423046000	-0.121779000
7	0.587107000	0.451445000	-0.550067000

16	1.100955000	-1.201198000	-0.151053000
1	4.130594000	2.488908000	0.191855000
1	3.847452000	-2.555550000	0.088825000
1	6.074221000	-1.404900000	0.359954000
1	6.217011000	1.078139000	0.415406000
8	1.285070000	2.611732000	0.037677000
35	-1.240341000	0.782014000	-0.233503000
8	0.914993000	-2.060643000	-1.341592000
8	0.532443000	-1.597248000	1.159963000
6	-4.246708000	1.052025000	-0.322911000
6	-3.988335000	0.897009000	1.056640000
6	-4.402018000	-0.085831000	-1.142233000
1	-3.873855000	1.779433000	1.693468000
1	-4.597369000	0.033998000	-2.211872000
6	-3.883803000	-0.394472000	1.612907000
6	-4.290425000	-1.372276000	-0.585200000
1	-3.673597000	-0.514504000	2.679540000
1	-4.398367000	-2.254600000	-1.222756000
6	-4.030113000	-1.526406000	0.791437000
1	-3.934173000	-2.528109000	1.220146000
1	-4.335947000	2.054291000	-0.753085000

Saccharin-I complexes

Saccharin-I...NH3

6	3.197235000	1.786442000	0.023157000
6	2.105846000	0.905607000	-0.025961000
6	2.321410000	-0.477218000	0.023279000
6	3.593517000	-1.051631000	0.109671000
6	4.686614000	-0.162978000	0.157303000
6	4.490130000	1.236132000	0.115511000
6	0.660436000	1.291830000	-0.126260000
7	-0.112671000	0.141457000	-0.285573000
16	0.757897000	-1.340065000	-0.040048000
1	3.026881000	2.865793000	-0.013591000
1	3.732053000	-2.135469000	0.140122000
1	5.701955000	-0.563618000	0.227979000
1	5.359089000	1.899121000	0.154501000
8	0.225867000	2.440864000	-0.100042000
53	-2.206731000	0.163424000	-0.033009000
8	0.409585000	-1.918158000	1.284034000
8	0.655317000	-2.186071000	-1.255074000
7	-4.775243000	0.185442000	0.265302000
1	-5.107495000	1.103823000	0.561355000
1	-5.066986000	-0.489594000	0.972897000
1	-5.256985000	-0.050976000	-0.602644000

Saccharin-I...OH2

6	3.168741000	1.803303000	0.026042000
6	2.083876000	0.914191000	-0.024405000
6	2.309915000	-0.467409000	0.027613000

6	3.586525000	-1.031819000	0.115475000
6	4.672299000	-0.134633000	0.164380000
6	4.465227000	1.262902000	0.121565000
6	0.640027000	1.295221000	-0.129045000
7	-0.117306000	0.133756000	-0.335671000
16	0.760609000	-1.352175000	-0.029152000
1	2.990539000	2.881264000	-0.012998000
1	3.733480000	-2.114498000	0.146382000
1	5.690408000	-0.527549000	0.237200000
1	5.328837000	1.932608000	0.161713000
8	0.190284000	2.434730000	-0.080458000
53	-2.168491000	0.141823000	-0.055410000
8	0.393475000	-1.882678000	1.307451000
8	0.675298000	-2.225592000	-1.222988000
8	-4.908267000	0.170614000	0.294340000
1	-5.173854000	0.303809000	1.215311000
1	-5.353971000	0.879146000	-0.191240000

Saccharin-l...FH

6	3.204412000	1.760801000	0.050662000
6	2.102341000	0.893808000	-0.014018000
6	2.300427000	-0.492638000	0.032963000
6	3.564858000	-1.082935000	0.127627000
6	4.667532000	-0.207699000	0.190689000
6	4.488731000	1.193974000	0.154405000
6	0.669461000	1.306906000	-0.129964000
7	-0.104177000	0.159064000	-0.384071000
16	0.737104000	-1.349509000	-0.035708000
1	3.048233000	2.842297000	0.015484000
1	3.690111000	-2.168451000	0.153252000
1	5.676909000	-0.621249000	0.269886000
1	5.365079000	1.846039000	0.205711000
8	0.236540000	2.449805000	-0.061081000
53	-2.141839000	0.205221000	-0.083743000
8	0.333977000	-1.847024000	1.302675000
8	0.649406000	-2.236444000	-1.218286000
1	-5.417723000	-0.542284000	0.933467000
9	-5.072837000	0.120181000	0.384420000

Saccharin-l...Acetone

6	-4.076353000	-1.534184000	-0.368747000
6	-2.908931000	-0.789754000	-0.139071000
6	-2.976393000	0.606727000	-0.053650000
6	-4.170652000	1.324709000	-0.172545000
6	-5.340295000	0.572387000	-0.401557000
6	-5.292578000	-0.836918000	-0.499188000
6	-1.528279000	-1.345832000	0.030043000
7	-0.665910000	-0.310334000	0.412217000
16	-1.347488000	1.283990000	0.221656000
1	-4.021566000	-2.624010000	-0.436718000

1	-4.194398000	2.414612000	-0.093164000
1	-6.299032000	1.088487000	-0.505331000
1	-6.217988000	-1.391804000	-0.677395000
8	-1.205301000	-2.520718000	-0.108990000
53	1.402686000	-0.505774000	0.260191000
8	-1.271662000	2.012391000	1.511068000
8	-0.810878000	1.916449000	-1.011292000
6	4.781261000	0.186464000	-0.324314000
8	4.007432000	-0.693674000	0.078746000
6	4.300203000	1.542542000	-0.782901000
6	6.269405000	-0.071348000	-0.363023000
1	3.211740000	1.554089000	-0.916794000
1	6.503648000	-1.027457000	0.120670000
1	4.808166000	1.830639000	-1.716467000
1	4.578225000	2.286700000	-0.016921000
1	6.809344000	0.753745000	0.128592000
1	6.599633000	-0.094842000	-1.415153000

Saccharin-I...Pyridine

6	-4.267936000	1.812940000	-0.260687000
6	-3.195442000	0.923691000	-0.092416000
6	-3.432583000	-0.455139000	-0.041432000
6	-4.709428000	-1.016950000	-0.139469000
6	-5.784001000	-0.120092000	-0.307108000
6	-5.565114000	1.275042000	-0.367325000
6	-1.746948000	1.293246000	0.042003000
7	-0.996731000	0.150886000	0.305982000
16	-1.884238000	-1.325056000	0.167475000
1	-4.080407000	2.889303000	-0.302171000
1	-4.865062000	-2.097794000	-0.090051000
1	-6.802183000	-0.510885000	-0.391603000
1	-6.419936000	1.944755000	-0.498090000
8	-1.296109000	2.434725000	-0.045973000
53	1.134092000	0.125394000	0.140746000
8	-1.496119000	-2.036661000	-1.079665000
8	-1.849996000	-2.058307000	1.458659000
6	6.350590000	0.023862000	-0.271859000
6	5.579119000	-1.101965000	-0.607197000
6	4.183632000	-1.032670000	-0.480019000
7	3.560351000	0.084893000	-0.043269000
6	4.294209000	1.172951000	0.281372000
6	5.693529000	1.181199000	0.179683000
1	7.439947000	0.000030000	-0.361037000
1	6.045446000	-2.024018000	-0.962951000
1	3.534750000	-1.877503000	-0.727840000
1	3.731890000	2.045026000	0.626877000
1	6.251187000	2.080909000	0.451312000

Saccharin-I...Pyridine-N-oxide

6	-3.834792000	2.173011000	-0.461388000
---	--------------	-------------	--------------

6	-2.970337000	1.083488000	-0.274162000
6	-3.392782000	-0.022770000	0.473122000
6	-4.662501000	-0.116796000	1.051448000
6	-5.528116000	0.978957000	0.858932000
6	-5.118628000	2.107987000	0.113656000
6	-1.574012000	0.958441000	-0.806526000
7	-1.095039000	-0.325140000	-0.545064000
16	-2.081528000	-1.234320000	0.558999000
1	-3.503163000	3.036198000	-1.044769000
1	-4.967363000	-0.996586000	1.624080000
1	-6.531774000	0.953764000	1.293110000
1	-5.813902000	2.941904000	-0.018317000
8	-0.959568000	1.839930000	-1.404239000
53	0.955599000	-0.780081000	-0.711658000
8	-2.484269000	-2.515775000	-0.070077000
8	-1.455177000	-1.243715000	1.906798000
6	4.943325000	1.955463000	1.440435000
6	4.955741000	0.629807000	1.907442000
6	4.426368000	-0.399192000	1.126909000
7	3.900845000	-0.126256000	-0.109549000
6	3.862921000	1.159467000	-0.586646000
6	4.383837000	2.206018000	0.176029000
1	5.351255000	2.767816000	2.045357000
1	5.369730000	0.376516000	2.886223000
1	4.381173000	-1.451541000	1.407725000
1	3.406244000	1.259996000	-1.571252000
1	4.338333000	3.217241000	-0.234860000
8	3.404063000	-1.097365000	-0.825807000

Saccharin-l-Ethene

6	3.366601000	1.802151000	0.038376000
6	2.282179000	0.913157000	-0.023160000
6	2.507029000	-0.468453000	0.035151000
6	3.782178000	-1.033074000	0.140877000
6	4.867574000	-0.135996000	0.201207000
6	4.661615000	1.261534000	0.151810000
6	0.838963000	1.292829000	-0.147544000
7	0.082204000	0.131645000	-0.357966000
16	0.956047000	-1.350213000	-0.042677000
1	3.189327000	2.880084000	-0.005677000
1	3.928470000	-2.115703000	0.176379000
1	5.884589000	-0.528955000	0.287951000
1	5.524974000	1.930981000	0.200953000
8	0.388807000	2.432959000	-0.109015000
53	-1.988724000	0.144253000	-0.075767000
8	0.570846000	-1.884284000	1.288203000
8	0.885915000	-2.224648000	-1.237532000
6	-4.757672000	0.137119000	0.962872000
6	-4.935084000	0.173466000	-0.384925000

1	-4.701761000	-0.812943000	1.500682000
1	-4.695380000	1.057150000	1.549907000
1	-5.025979000	-0.746455000	-0.968392000
1	-5.018899000	1.123717000	-0.918786000

Saccharin-I...Acetylene

6	3.313554000	1.799133000	0.057356000
6	2.227313000	0.912875000	-0.012504000
6	2.449734000	-0.469849000	0.031016000
6	3.724125000	-1.037801000	0.128313000
6	4.811058000	-0.143373000	0.196913000
6	4.607569000	1.254993000	0.163326000
6	0.786491000	1.299178000	-0.130974000
7	0.030868000	0.139714000	-0.374284000
16	0.900068000	-1.351772000	-0.048928000
1	3.138254000	2.877785000	0.024881000
1	3.868508000	-2.121005000	0.151668000
1	5.827409000	-0.539146000	0.278063000
1	5.472122000	1.922339000	0.218749000
8	0.335710000	2.436563000	-0.069020000
53	-2.019698000	0.149920000	-0.080128000
8	0.507737000	-1.876577000	1.282664000
8	0.829850000	-2.226042000	-1.242701000
6	-4.967552000	0.031996000	0.927176000
6	-5.137386000	0.282860000	-0.269861000
1	-5.309869000	0.501385000	-1.309880000
1	-4.845429000	-0.188400000	1.974008000

Saccharin-I...Benzene

6	3.926036000	1.937257000	0.163023000
6	2.910934000	0.977950000	0.023556000
6	3.196908000	-0.377528000	0.233497000
6	4.470377000	-0.848342000	0.569168000
6	5.486076000	0.118974000	0.706948000
6	5.216430000	1.492113000	0.507610000
6	1.485578000	1.254258000	-0.340923000
7	0.838838000	0.031382000	-0.580367000
16	1.723691000	-1.362009000	0.014665000
1	3.701038000	2.994618000	-0.000197000
1	4.666477000	-1.913198000	0.718683000
1	6.498194000	-0.199415000	0.972409000
1	6.026491000	2.217845000	0.621915000
8	0.971925000	2.361214000	-0.454749000
53	-1.235876000	-0.068380000	-0.580366000
8	1.163309000	-1.791196000	1.320419000
8	1.881268000	-2.344240000	-1.083452000
6	-4.253669000	-1.073776000	1.119047000
6	-4.196095000	-0.923584000	-0.282552000
6	-4.369673000	0.060587000	1.941531000
1	-4.122626000	-1.805373000	-0.926450000

1	-4.408775000	-0.055518000	3.028542000
6	-4.255171000	0.366965000	-0.857165000
6	-4.427542000	1.347676000	1.369125000
1	-4.233855000	0.481957000	-1.945244000
1	-4.511669000	2.228107000	2.012793000
6	-4.371397000	1.502696000	-0.027075000
1	-4.409638000	2.501535000	-0.471112000
1	-4.199871000	-2.071657000	1.563490000