

Theoretical Investigation of the Origins of Catalysis of a Retro Diels-Alder Reaction by Antibody 10F11

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Supporting Information

S1-S2 Tables of interaction energies for substrates with side chains:

Table S1, Indole + Substrate or TS

Table S2, Benzene + Substrates or TS

Table S3, Indole and benzene + substrate or TS

S3-S34 Cartesian Coordinates of all B3LYP/6-31G* optimized geometries.

Table S1. Interaction energies between indole and both model substrate **11** and model transition state **TS11** (both stereoisomers). These are B3LYP/6-31G* interaction energies (in kcal/mol) on constrained B3LYP/6-31G* (second column) geometries and PM3 interaction energies for PM3 geometries (third column). $\Delta\Delta E$ values indicate the extra stabilization of the transition state relative to the substrate, positive values indicate a catalytic interaction and negative values an anti-catalytic interaction.

Structure	B3LYP//B3LYP	PM3//PM3
<i>R</i> - 11 + indole	-1.3	1.8
<i>R</i> - TS11 + indole	-1.3	2.6
$\Delta\Delta E$ (<i>R</i>)	+0.0	-0.9
<i>S</i> - 11 + indole	-1.4	2.4
<i>S</i> - TS11 + indole	-1.9	2.8
$\Delta\Delta E$ (<i>S</i>)	-0.5	-0.5

Table S2. Interaction energies between benzene and both model substrate **11** and model transition state **TS11** (both stereoisomers). These are B3LYP/6-31G* energies (in kcal/mol) on

constrained B3LYP/6-31G* (second column) and PM3 energies for PM3 geometries (third column). $\Delta\Delta E$ values indicate the extra stabilization of the transition state relative to the substrate, positive values indicate a catalytic interaction and negative values an anti-catalytic interaction.

Structure	B3LYP//B3LYP	PM3//PM3
<i>R</i> - 11 + benzene	1.7	-1.4
<i>R</i> - TS11 + benzene	1.9	-5.0
$\Delta\Delta E$ (<i>R</i>)	+0.2	+3.7
<i>S</i> - 11 + benzene	1.7	-1.6
<i>S</i> - TS11 + benzene	1.3	-0.7
$\Delta\Delta E$ (<i>S</i>)	-0.4	-0.9

Table S3. Interaction energies between both indole and benzene and both model substrate **11** and model transition state **TS11** (both stereoisomers). These are B3LYP/6-31G* energies (in kcal/mol) on constrained B3LYP/6-31G* (second column) and PM3 energies for PM3 geometries (third column). $\Delta\Delta E$ values indicate the extra stabilization of the transition state relative to the substrate, positive values indicate a catalytic interaction and negative values an anti-catalytic interaction.

Structure	B3LYP//B3LYP	PM3//PM3
<i>R</i> - 11 + indole + benzene	0.5	-0.4
<i>R</i> - TS11 + indole + benzene	-0.2	0.4
$\Delta\Delta E$ (<i>R</i>)	-0.7	-0.9
<i>S</i> - 11 + indole + benzene	0.3	1.5
<i>S</i> - TS11 + indole + benzene	-0.7	1.0
$\Delta\Delta E$ (<i>S</i>)	-0.9	+0.5

Cartesian Coordinates of Complexes with B3LYP/6-31G* optimization

11

1	6	1.249484	-0.702790	0.035432
2	6	2.323886	-1.388297	-0.516748
3	6	3.391827	-0.659649	-1.056001
4	6	3.383023	0.735476	-1.024183
5	6	2.306510	1.424946	-0.452060
6	6	1.240846	0.700610	0.067774
7	6	0.005012	-1.287378	0.664934
8	6	-1.216729	-0.701988	-0.015768
9	6	-1.226085	0.702612	0.057612
10	6	-2.305601	1.427057	-0.435888
11	6	-3.373472	0.742164	-1.028138
12	6	-3.364669	-0.652262	-1.101418
13	6	-2.288844	-1.383643	-0.583312
14	6	0.002784	1.228280	0.757615
15	7	-0.010587	-0.802714	2.097594
16	8	0.022773	0.657774	2.116476
17	1	2.335821	-2.475473	-0.532108
18	1	4.233272	-1.185332	-1.499183
19	1	4.218051	1.291126	-1.442408
20	1	2.305111	2.511814	-0.416931
21	1	-2.317739	2.512389	-0.368418
22	1	-4.214642	1.299435	-1.431431
23	1	-4.198518	-1.174417	-1.563023
24	1	-2.288574	-2.470292	-0.632132
25	1	-0.959252	-0.991844	2.438603
26	1	0.007185	-2.380621	0.700877
27	1	0.003376	2.309176	0.912079

TS11

1	6	1.247220	-0.684750	-0.264482
2	6	2.459967	-1.364402	-0.502831
3	6	3.636287	-0.656122	-0.662485
4	6	3.640607	0.751590	-0.549200
5	6	2.471100	1.434856	-0.281469
6	6	1.249124	0.733604	-0.149551
7	6	0.006814	-1.348938	0.013901
8	6	-1.233919	-0.669010	-0.261383
9	6	-1.224982	0.758430	-0.167248
10	6	-2.452135	1.462979	-0.293689
11	6	-3.622140	0.787647	-0.561713
12	6	-3.623143	-0.624450	-0.680340

13	6	-2.456522	-1.340995	-0.513196
14	6	0.007231	1.380181	0.138366
15	7	-0.169974	-0.853507	1.966277
16	8	0.213340	0.329074	2.117733
17	1	2.456217	-2.449682	-0.568685
18	1	4.564220	-1.182556	-0.868143
19	1	4.572655	1.297283	-0.668597
20	1	2.474103	2.517563	-0.183325
21	1	-2.448380	2.546020	-0.198146
22	1	-4.551746	1.336663	-0.683254
23	1	-4.552224	-1.143840	-0.898660
24	1	-2.458460	-2.425724	-0.590118
25	1	-1.222174	-0.889317	2.009099
26	1	-0.001021	-2.436321	0.013235
27	1	0.016858	2.448160	0.342711

R-11 + indole

6	1.255208	-0.439674	-1.484434
6	1.55052	-1.791816	-1.360278
6	2.157277	-2.249013	-0.183653
6	2.475448	-1.357345	0.841805
6	2.179414	0.003754	0.713429
6	1.570984	0.45579	-0.451759
6	0.636246	0.264503	-2.669868
6	-0.564037	1.070944	-2.213625
6	-0.215522	1.993723	-1.211809
6	-1.149484	2.91171	-0.744447
6	-2.44905	2.889313	-1.264760
6	-2.797626	1.969079	-2.256636
6	-1.850029	1.061322	-2.745793
6	1.241617	1.880564	-0.837958
7	1.671998	1.25651	-3.150279
8	2.028274	2.155279	-2.053723
1	1.321423	-2.482838	-2.168582
1	2.399793	-3.303595	-0.077133
1	2.938833	-1.722520	1.752810
1	2.426982	0.697812	1.512376
1	-0.875318	3.635102	0.019662
1	-3.189689	3.594554	-0.897241
1	-3.808226	1.961594	-2.656533
1	-2.117462	0.357682	-3.531274
1	1.170207	1.890867	-3.781009
1	0.423668	-0.40251	-3.510445
1	1.577565	2.627039	-0.115699
6	0.350379	-1.930212	3.849686

6	-0.566736	-1.147302	3.068360
6	0.54528	-3.110413	3.181200
6	-0.887530	-1.917913	1.915868
6	-1.14816	0.125008	3.213506
7	-0.207473	-3.114163	2.021633
6	-1.745199	-1.448444	0.915822
6	-2.001326	0.59358	2.223312
6	-2.293116	-0.182826	1.081776
1	0.791994	-1.658192	4.798886
1	1.155397	-3.964962	3.440152
1	-0.928086	0.732818	4.087918
1	-0.161912	-3.817905	1.302175
1	-1.967735	-2.046514	0.036078
1	-2.451513	1.577722	2.322032
1	-2.951132	0.219174	0.317660

R-TS11 + indole

6	1.790640	0.623409	0.204711
6	2.643831	1.339764	-0.660158
6	3.051718	0.779776	-1.858204
6	2.639796	-0.524170	-2.210734
6	1.817899	-1.250292	-1.371607
6	1.378455	-0.692248	-0.148046
6	1.419823	1.083163	1.511719
6	0.209438	0.589243	2.117942
6	-0.200994	-0.731841	1.758429
6	-1.287337	-1.326846	2.453416
6	-1.972270	-0.620771	3.417061
6	-1.582365	0.700694	3.749577
6	-0.499846	1.287291	3.127866
6	0.570774	-1.409740	0.788839
7	2.497880	-0.236976	2.599615
8	2.440029	-1.357368	2.041174
1	2.979770	2.333297	-0.372271
1	3.707781	1.336305	-2.522865
1	2.970472	-0.956328	-3.151415
1	1.498042	-2.252045	-1.642985
1	-1.583181	-2.340453	2.195562
1	-2.816829	-1.074900	3.927948
1	-2.135517	1.248788	4.507588
1	-0.186473	2.293448	3.396574
1	1.871939	-0.235552	3.447135
1	1.788473	2.054202	1.834102
1	0.351725	-2.454709	0.584851
6	-1.216141	-1.070052	-3.454141

6	-1.868951	-0.492098	-2.311285
6	-0.301855	-0.154909	-3.901266
6	-1.282556	0.788549	-2.108277
6	-2.881828	-0.918209	-1.433590
7	-0.351652	0.978617	-3.111362
6	-1.656838	1.623544	-1.050608
6	-3.258243	-0.090456	-0.383775
6	-2.643249	1.163659	-0.186645
1	-1.424631	-2.031774	-3.903367
1	0.387244	-0.209870	-4.732429
1	-3.359417	-1.885015	-1.573956
1	0.355405	1.697874	-3.104534
1	-1.187281	2.592684	-0.903835
1	-4.032775	-0.414104	0.305937
1	-2.947985	1.780845	0.653457

S-11 + indole

6	1.170660	0.413154	-2.228025
6	0.907349	-0.351751	-3.357365
6	-0.244455	-0.083337	-4.108403
6	-1.104920	0.951525	-3.735883
6	-0.829653	1.729857	-2.604613
6	0.302924	1.448891	-1.850309
6	2.371661	0.324466	-1.312380
6	1.908529	0.178760	0.122318
6	1.054703	1.229444	0.499709
6	0.594940	1.327780	1.808828
6	0.988239	0.365917	2.744850
6	1.837148	-0.677672	2.370467
6	2.313206	-0.770116	1.057139
6	0.823274	2.191018	-0.640043
7	3.068651	1.662771	-1.416312
8	2.137471	2.726104	-1.038729
1	1.588716	-1.143839	-3.659059
1	-0.463132	-0.677948	-4.991388
1	-1.990862	1.158371	-4.330401
1	-1.493639	2.542764	-2.320911
1	-0.063217	2.141875	2.101755
1	0.616402	0.422379	3.763054
1	2.142643	-1.415416	3.108266
1	2.989644	-1.572913	0.770289
1	3.730455	1.684999	-0.633107
1	3.098050	-0.433710	-1.619450
1	0.236348	3.071151	-0.370421
6	-2.360625	-1.140184	3.451657

6	-2.415093	-1.027476	2.020159
6	-1.412125	-2.084189	3.746910
6	-1.454675	-1.938575	1.498427
6	-3.166086	-0.249831	1.120509
7	-0.868384	-2.574012	2.574022
6	-1.221484	-2.077423	0.126300
6	-2.936470	-0.384629	-0.242161
6	-1.968850	-1.285401	-0.735788
1	-2.963247	-0.600135	4.169416
1	-1.079098	-2.461621	4.704085
1	-3.912644	0.449361	1.489661
1	-0.103441	-3.226764	2.514915
1	-0.475175	-2.770800	-0.252378
1	-3.505722	0.216257	-0.946161
1	-1.802898	-1.355527	-1.806122

S-TS11 + indole

6	0.633646	2.276865	0.113619
6	1.364448	3.273966	-0.566099
6	0.805061	3.936562	-1.642852
6	-0.519357	3.651819	-2.043233
6	-1.264644	2.704960	-1.369105
6	-0.698234	1.986205	-0.290309
6	1.095041	1.630351	1.307927
6	0.586491	0.324799	1.642491
6	-0.735812	0.009644	1.198406
6	-1.322869	-1.220474	1.599398
6	-0.619940	-2.105312	2.385499
6	0.696766	-1.798789	2.809072
6	1.283947	-0.600038	2.459716
6	-1.416063	0.993300	0.444780
7	-0.198150	2.457617	2.623894
8	-1.327402	2.531639	2.085162
1	2.374032	3.509355	-0.237682
1	1.379568	4.688184	-2.177394
1	-0.953400	4.187607	-2.883180
1	-2.286961	2.490050	-1.669589
1	-2.328623	-1.457471	1.264531
1	-1.069674	-3.051423	2.671816
1	1.240202	-2.508150	3.428731
1	2.288592	-0.355668	2.797697
1	-0.192003	1.661516	3.313981
6	-1.104032	-3.703248	-1.041212
6	-0.524025	-2.529745	-1.632778
6	-0.155766	-4.252270	-0.219539

6	0.792740	-2.411573	-1.106474
6	-0.976078	-1.559546	-2.545346
7	0.994340	-3.486645	-0.264124
6	1.641865	-1.352131	-1.444619
6	-0.135345	-0.508231	-2.885469
6	1.157367	-0.398037	-2.330890
1	2.075200	1.904855	1.691107
1	-2.465198	0.835259	0.207902
1	-2.091431	-4.103949	-1.227305
1	-0.198117	-5.139060	0.397806
1	-1.972450	-1.631762	-2.974890
1	2.639759	-1.271997	-1.021359
1	-0.478106	0.253454	-3.579841
1	1.784050	0.445577	-2.604549
1	1.789206	-3.600748	0.344641

R-11 + benzene

1	6	.239333	.917758	-.243071
2	6	-.783764	1.481133	-.996001
3	6	-.721757	2.845741	-1.307831
4	6	.340601	3.630256	-.855243
5	6	1.359300	3.063526	-.079134
6	6	1.305955	1.706543	.215178
7	6	.377979	-.524431	.190997
8	6	1.725877	-1.049453	-.262847
9	6	2.782353	-.268129	.238860
10	6	4.103265	-.631820	.001134
11	6	4.369192	-1.773915	-.764018
12	6	3.320835	-2.549940	-1.262666
13	6	1.990638	-2.197125	-1.003698
14	6	2.271272	.896711	1.051476
15	7	.399599	-.513559	1.703803
16	8	1.480949	.351707	2.169973
17	1	-1.619733	.874864	-1.333487
18	1	-1.509746	3.296604	-1.905211
19	1	.375683	4.688100	-1.101868
20	1	2.180882	3.676267	.284530
21	1	-.467170	-1.149300	-.108333
22	1	4.919839	-.033496	.398629
23	1	5.397703	-2.058204	-.969321
24	1	3.537754	-3.434330	-1.855878
25	1	1.175406	-2.807584	-1.385703
26	1	3.054857	1.488338	1.529140
27	1	.745251	-1.439812	1.976529
28	6	-3.193096	-.775855	1.266281

29	6	-3.319529	-1.979467	.567134
30	6	-3.892297	.354290	.834841
31	6	-4.135154	-2.051091	-.565287
32	6	-4.710238	.283217	-.295142
33	6	-4.827534	-.918161	-.998608
34	1	-2.531786	-.709722	2.125274
35	1	-2.784029	-2.862997	.906604
36	1	-3.791142	1.291223	1.375752
37	1	-4.231989	-2.987862	-1.108373
38	1	-5.254031	1.163338	-.629101
39	1	-5.461920	-.972894	-1.879699

R-TS11 + benzene

1	6	.375815	.547500	-.263199
2	6	-1.017582	.761380	-.400029
3	6	-1.510318	2.035706	-.582959
4	6	-.633931	3.148200	-.600567
5	6	.721966	2.971097	-.433116
6	6	1.259666	1.668157	-.274684
7	6	.943970	-.726830	.007087
8	6	2.327095	-.978724	-.246540
9	6	3.210100	.149092	-.287324
10	6	4.605992	-.074805	-.440774
11	6	5.097648	-1.349921	-.599350
12	6	4.219677	-2.464803	-.578230
13	6	2.867863	-2.285878	-.388097
14	6	2.646756	1.424694	-.074325
15	1	-1.693077	-.089236	-.366336
16	1	-2.579131	2.186678	-.704896
17	1	-1.037873	4.147377	-.740420
18	1	1.396229	3.823973	-.433186
19	1	.276132	-1.577969	.115413
20	1	5.276119	.781396	-.449720
21	1	6.163085	-1.509631	-.739880
22	1	4.621923	-3.465787	-.708641
23	1	2.195235	-3.139938	-.361730
24	1	3.312922	2.279378	.018224
25	6	-4.569776	-.029583	1.154186
26	6	-4.054180	-1.326643	1.215300
27	6	-5.227253	.406697	.001297
28	6	-4.196148	-2.186466	.123240
29	6	-5.367377	-.452692	-1.091431
30	6	-4.851602	-1.749107	-1.030589
31	1	-4.458037	.639309	2.003266
32	1	-3.543304	-1.665603	2.112661

33	1	-5.633380	1.414132	-.044019
34	1	-3.798446	-3.197027	.171971
35	1	-5.878925	-.112863	-1.988222
36	1	-4.961763	-2.418295	-1.879978
37	7	1.548132	-.222624	2.064746
38	8	2.007956	.931260	2.025903
39	1	2.351426	-.910040	2.075656

S-11 + benzene

1	6	1.670151	-1.073758	-.352378
2	6	2.009616	-2.141098	-1.173864
3	6	3.352646	-2.527749	-1.268771
4	6	4.334186	-1.859679	-.535231
5	6	3.988327	-.793988	.305149
6	6	2.657789	-.401582	.385170
7	6	.294346	-.495825	-.107220
8	6	.323471	.990870	-.404652
9	6	1.298450	1.656013	.360101
10	6	1.426405	3.039087	.291884
11	6	.588032	3.759848	-.566937
12	6	-.379732	3.099892	-1.327249
13	6	-.525496	1.710107	-1.240362
14	6	2.060389	.694699	1.238792
15	7	.035505	-.650854	1.375392
16	8	1.084746	.038348	2.127610
17	1	1.243765	-2.668070	-1.737966
18	1	3.630478	-3.355046	-1.916353
19	1	5.372852	-2.169604	-.613523
20	1	4.751663	-.279720	.884432
21	1	-.507944	-1.031273	-.621610
22	1	2.171780	3.554025	.893660
23	1	.690477	4.839264	-.640230
24	1	-1.026131	3.668961	-1.990367
25	1	-1.292707	1.198371	-1.816134
26	1	2.772697	1.172651	1.914478
27	1	-.783653	-.064924	1.567585
28	6	-3.637400	-.291835	1.351639
29	6	-3.558332	-1.671577	1.141503
30	6	-3.992625	.557294	.299977
31	6	-3.838713	-2.201849	-.120226
32	6	-4.276142	.025506	-.960530
33	6	-4.200114	-1.353956	-1.170204
34	1	-3.430241	.119652	2.336525
35	1	-3.275210	-2.329857	1.958028
36	1	-4.052150	1.629922	.463878

37	1	-3.778881	-3.274690	-.283527
38	1	-4.561001	.684551	-1.776774
39	1	-4.423815	-1.767544	-2.150276

S-TS11 + benzene

1	6	2.166453	-.823811	-.520813
2	6	2.763923	-2.036693	-.922715
3	6	4.120052	-2.238369	-.745818
4	6	4.912087	-1.247367	-.125293
5	6	4.341787	-.066782	.307664
6	6	2.962556	.175903	.105197
7	6	.754599	-.577552	-.575804
8	6	.277376	.780462	-.649921
9	6	1.088826	1.787407	-.038369
10	6	.587822	3.114208	.045923
11	6	-.634404	3.435279	-.502248
12	6	-1.422898	2.440297	-1.130891
13	6	-.985779	1.133776	-1.186936
14	6	2.309601	1.370978	.540550
15	1	2.147262	-2.805534	-1.381940
16	1	4.579882	-3.165151	-1.077791
17	1	5.975643	-1.420016	.015574
18	1	4.947581	.692829	.795473
19	1	.112873	-1.359853	-.973104
20	1	1.192889	3.874993	.533090
21	1	-.999302	4.457677	-.454442
22	1	-2.384491	2.707974	-1.559800
23	1	-1.603777	.363389	-1.640170
24	1	2.882127	2.087982	1.124208
25	6	-2.933109	-1.667761	.872401
26	6	-3.522743	-2.285864	-.233903
27	6	-3.431873	-.446999	1.335675
28	6	-4.609258	-1.685124	-.874216
29	6	-4.519419	.153031	.696498
30	6	-5.108227	-.466002	-.408344
31	1	-2.084225	-2.131021	1.368439
32	1	-3.138245	-3.237154	-.593029
33	1	-2.979551	.031492	2.200683
34	1	-5.069565	-2.168053	-1.732456
35	1	-4.908140	1.100575	1.060410
36	1	-5.955841	-.000635	-.904965
37	7	.367264	-.583742	1.409758
38	8	1.309356	-.012014	2.006614
39	1	-.465055	.058719	1.366789

R-11 + indole + benzene

1	6	.687873	-.049642	.638587
2	6	1.007766	-1.344769	.246814
3	6	.282924	-2.412967	.791479
4	6	-.730580	-2.183096	1.723752
5	6	-1.043879	-.879121	2.121056
6	6	-.329382	.181772	1.576376
7	6	1.349435	1.235490	.196029
8	6	.295747	2.203068	-.308013
9	6	-.682265	2.458242	.669018
10	6	-1.667852	3.413581	.447157
11	6	-1.690289	4.101319	-.772111
12	6	-.722194	3.844587	-1.746140
13	6	.285504	2.900281	-1.512700
14	6	-.438382	1.650854	1.919447
15	7	1.938056	1.855349	1.444416
16	8	.885352	2.036126	2.440956
17	1	1.815149	-1.524726	-.457948
18	1	.526836	-3.431930	.499839
19	1	-1.291381	-3.017890	2.132167
20	1	-1.831230	-.700110	2.848699
21	1	2.177868	1.078929	-.499623
22	1	-2.415313	3.620522	1.209260
23	1	-2.463427	4.841539	-.960145
24	1	-.746414	4.385475	-2.688599
25	1	1.049402	2.714083	-2.264528
26	1	-1.130996	1.868481	2.734771
27	1	2.151608	2.825989	1.191139
28	6	4.806565	-.160739	.500421
29	6	5.108810	.336019	-.770521
30	6	4.752896	-1.540842	.711438
31	6	5.346998	-.543677	-1.829852
32	6	4.993627	-2.421276	-.345807
33	6	5.285242	-1.922813	-1.618056
34	1	4.585222	.521900	1.315594
35	1	5.160866	1.409703	-.935031
36	1	4.514185	-1.927399	1.698454
37	1	5.581704	-.155485	-2.817830
38	1	4.952603	-3.494870	-.179426
39	1	5.471066	-2.607964	-2.441417
40	6	-4.126509	-2.944985	.344938
41	6	-3.952739	-1.634518	-.218270
42	6	-3.170207	-3.753727	-.210946
43	6	-2.850885	-1.715424	-1.114998
44	6	-4.603800	-.398187	-.058014

45	7	-2.408063	-3.022555	-1.103084
46	6	-2.381022	-.606817	-1.826486
47	6	-4.141007	.704164	-.764136
48	6	-3.035801	.603185	-1.635602
49	1	-4.881917	-3.251625	1.055854
50	1	-2.970778	-4.805104	-.054762
51	1	-5.454786	-.308404	.612996
52	1	-1.563507	-3.347550	-1.546105
53	1	-1.528177	-.685170	-2.495486
54	1	-4.632695	1.665764	-.643564
55	1	-2.688221	1.487506	-2.160441

R-TS11 + indole + benzene

1	6	-.396691	-.588610	.670910
2	6	-1.693720	-.036743	.623269
3	6	-2.022488	1.038296	1.431150
4	6	-1.069403	1.576089	2.323714
5	6	.203395	1.043914	2.394381
6	6	.562568	-.051489	1.574064
7	6	-.017703	-1.779563	-.033319
8	6	1.371941	-2.014590	-.333832
9	6	2.330463	-1.469835	.575991
10	6	3.699348	-1.814227	.419626
11	6	4.104487	-2.615750	-.624105
12	6	3.155084	-3.132246	-1.540917
13	6	1.812810	-2.854105	-1.387894
14	6	1.838699	-.691873	1.647544
15	1	-2.435628	-.467316	-.044172
16	1	-3.025091	1.455301	1.388703
17	1	-1.340100	2.417055	2.957028
18	1	.938322	1.457479	3.078830
19	1	-.761043	-2.251975	-.671286
20	1	4.424190	-1.415865	1.124899
21	1	5.156672	-2.855875	-.749783
22	1	3.489229	-3.759267	-2.363256
23	1	1.080487	-3.265728	-2.078653
24	1	2.533668	-.367854	2.418037
25	6	-5.591996	-.674761	.530865
26	6	-5.182297	-1.603629	-.429242
27	6	-5.902412	.632843	.149088
28	6	-5.083896	-1.224373	-1.770471
29	6	-5.802003	1.012279	-1.191982
30	6	-5.392987	.083831	-2.151755
31	1	-5.669038	-.970410	1.573672
32	1	-4.942951	-2.621237	-.131949

33	1	-6.228252	1.353479	.894967
34	1	-4.770100	-1.948286	-2.518253
35	1	-6.046295	2.029017	-1.488854
36	1	-5.318194	.377853	-3.195504
37	6	2.095508	3.699258	.679461
38	6	2.566347	2.746145	-.288734
39	6	.742498	3.811488	.508860
40	6	1.424879	2.299862	-1.011727
41	6	3.826084	2.216986	-.621660
42	7	.331724	2.992130	-.526285
43	6	1.507229	1.330471	-2.016067
44	6	3.912522	1.256809	-1.621627
45	6	2.762295	.807778	-2.303628
46	1	2.695376	4.254952	1.387712
47	1	.023071	4.418192	1.040562
48	1	4.718660	2.552177	-.098654
49	1	-.627570	2.721015	-.683978
50	1	.620794	.990648	-2.545170
51	1	4.879953	.835337	-1.880475
52	1	2.860556	.043503	-3.068956
53	7	.124085	-3.020540	1.558033
54	8	.643902	-2.392097	2.510214
55	1	.838044	-3.672067	1.138811

S-11 + indole + benzene

1	6	.499620	2.090377	-.344204
2	6	.472577	2.868345	-1.494999
3	6	-.421775	3.944316	-1.569616
4	6	-1.260645	4.241155	-.493427
5	6	-1.221940	3.463691	.670675
6	6	-.347793	2.385428	.734563
7	6	1.416524	.926823	-.036758
8	6	.591050	-.274361	.377831
9	6	-.249923	.020899	1.464775
10	6	-1.018991	-.978233	2.052608
11	6	-.948475	-2.280137	1.546840
12	6	-.111979	-2.574347	.468170
13	6	.673713	-1.573607	-.115794
14	6	-.100978	1.457386	1.902108
15	7	2.220138	1.349553	1.173479
16	8	1.310217	1.654356	2.279477
17	1	1.140758	2.649567	-2.324664
18	1	-.455127	4.556734	-2.466866
19	1	-1.944206	5.083731	-.557228
20	1	-1.868142	3.700395	1.512483

21	1	2.138176	.712439	-.829673
22	1	-1.666416	-.751025	2.895818
23	1	-1.561583	-3.061291	1.985485
24	1	-.057931	-3.592521	.089940
25	1	1.348520	-1.806478	-.936365
26	1	-.666075	1.712594	2.800798
27	1	2.673925	.492050	1.505035
28	6	5.029800	-1.014443	.890936
29	6	5.527488	.016611	.088828
30	6	4.568961	-2.196770	.305361
31	6	5.566884	-.136782	-1.299164
32	6	4.612980	-2.350694	-1.082636
33	6	5.112593	-1.321217	-1.884652
34	1	5.008550	-.898807	1.971798
35	1	5.878292	.938020	.544968
36	1	4.180950	-2.997176	.929626
37	1	5.954690	.664380	-1.922819
38	1	4.263467	-3.273789	-1.538290
39	1	5.149561	-1.442661	-2.964273
40	6	-4.511878	-2.550323	.364155
41	6	-4.187545	-1.228440	-.096935
42	6	-3.735784	-3.428065	-.346628
43	6	-3.186609	-1.375829	-1.097334
44	6	-4.627866	.066362	.231472
45	7	-2.944460	-2.727227	-1.237632
46	6	-2.612677	-.280578	-1.750925
47	6	-4.060394	1.155804	-.415688
48	6	-3.056868	.985739	-1.393171
49	1	-5.243725	-2.815128	1.115372
50	1	-3.685732	-4.507453	-.302140
51	1	-5.398227	.209837	.985436
52	1	-2.213964	-3.126436	-1.804889
53	1	-1.838187	-.413314	-2.501680
54	1	-4.387626	2.161214	-.164847
55	1	-2.621854	1.859329	-1.868118

S-TS11 + indole + benzene

1	6	-.415405	2.208947	-.366577
2	6	-.531539	3.293249	-1.261577
3	6	-1.555824	4.210582	-1.117015
4	6	-2.467750	4.094603	-.044395
5	6	-2.350610	3.060988	.863649
6	6	-1.335253	2.087870	.710720
7	6	.684478	1.288674	-.375238
8	6	.503942	-.029882	.176327

9	6	-.455415	-.167874	1.227677
10	6	-.580044	-1.421367	1.884642
11	6	.199279	-2.489519	1.500916
12	6	1.134134	-2.354772	.445556
13	6	1.297011	-1.144237	-.195807
14	6	-1.162883	.993767	1.613667
15	1	.188750	3.394227	-2.070011
16	1	-1.654886	5.031640	-1.821878
17	1	-3.261516	4.828399	.067468
18	1	-3.046291	2.974522	1.694417
19	1	1.456273	1.417368	-1.130050
20	1	-1.305265	-1.526197	2.686530
21	1	.086286	-3.448102	1.999199
22	1	1.744064	-3.206727	.155111
23	1	2.036802	-1.029872	-.983714
24	1	-1.797876	.948373	2.494874
25	6	4.659352	.885623	.053361
26	6	5.089869	.779460	-1.272068
27	6	4.755536	-.217217	.906742
28	6	5.617768	-.425418	-1.742367
29	6	5.285816	-1.421406	.437532
30	6	5.717075	-1.525687	-.886917
31	1	4.241770	1.820543	.417598
32	1	5.018004	1.637279	-1.935954
33	1	4.425623	-.135581	1.939212
34	1	5.955599	-.505817	-2.772482
35	1	5.364341	-2.276431	1.104054
36	1	6.132208	-2.461834	-1.251705
37	6	-3.428783	-3.242158	.560420
38	6	-3.509905	-1.977682	-.116319
39	6	-2.446259	-3.968751	-.057617
40	6	-2.522089	-1.995220	-1.140302
41	6	-4.303910	-.826705	.036255
42	7	-1.906571	-3.230276	-1.094252
43	6	-2.296099	-.900325	-1.981773
44	6	-4.083494	.261204	-.797878
45	6	-3.080074	.230570	-1.789543
46	1	-4.044645	-3.578886	1.383509
47	1	-2.083203	-4.966128	.148982
48	1	-5.076314	-.789844	.800816
49	1	-1.071424	-3.474899	-1.602683
50	1	-1.527306	-.928314	-2.749560
51	1	-4.682245	1.159961	-.681222
52	1	-2.921588	1.104882	-2.413759
53	7	1.581378	1.860674	1.345492
54	8	.696609	2.118688	2.196198

55 1 2.012782 .925261 1.560549

R-11 with *N*-formylethanolamine

1	6	-0.945983	-1.558806	-0.121618
2	6	-0.869729	-2.929773	0.088473
3	6	-0.005913	-3.416915	1.077764
4	6	0.774730	-2.538195	1.830078
5	6	0.710229	-1.156133	1.609122
6	6	-0.155667	-0.676304	0.631796
7	6	-1.834631	-0.829161	-1.104637
8	6	-2.663507	0.195885	-0.354447
9	6	-1.853715	1.093359	0.364115
10	6	-2.420415	2.154262	1.061029
11	6	-3.812463	2.305478	1.055581
12	6	-4.617321	1.416114	0.341062
13	6	-4.044484	0.360524	-0.379350
14	6	-0.388959	0.759436	0.214965
15	7	-0.912025	-0.066861	-2.029491
16	8	-0.080141	0.835674	-1.224201
17	1	-1.475749	-3.613781	-0.500783
18	1	0.057042	-4.486736	1.257484
19	1	1.449314	-2.924101	2.588859
20	1	1.353051	-0.487716	2.173588
21	1	-1.792687	2.852803	1.608990
22	1	-4.268066	3.121411	1.609704
23	1	-5.696504	1.542823	0.343242
24	1	-4.673000	-0.326105	-0.941927
25	1	-1.509649	0.603746	-2.524079
26	1	-2.426084	-1.496882	-1.737380
27	1	0.288080	1.477713	0.680295
28	6	3.759621	1.105320	1.355556
29	8	3.748934	0.165346	2.141155
30	1	3.938994	2.150129	1.682534
31	7	3.575380	1.012792	0.019605
32	6	3.261099	-0.233821	-0.669338
33	6	3.213001	0.041307	-2.175200
34	8	2.470156	1.214176	-2.470472
35	1	3.453220	1.854415	-0.532500
36	1	4.021984	-0.986867	-0.433614
37	1	2.300528	-0.626640	-0.327057
38	1	4.222684	0.221876	-2.560878
39	1	2.808753	-0.843075	-2.689504
40	1	1.557660	1.068420	-2.149321

R-TS11 with *N*-formylethanolamine

1	6	1.119231	-1.201778	0.800038
2	6	1.880308	-2.115334	0.042355
3	6	2.681980	-1.664762	-0.991230
4	6	2.724023	-0.291803	-1.319340
5	6	1.972838	0.617101	-0.599844
6	6	1.160677	0.182303	0.472794
7	6	0.161528	-1.595756	1.794474
8	6	-0.196603	-0.666904	2.838927
9	6	-0.133847	0.723691	2.515722
10	6	-0.606681	1.673723	3.458854
11	6	-1.066097	1.263367	4.691232
12	6	-1.105665	-0.114332	5.017369
13	6	-0.698637	-1.063971	4.102378
14	6	0.322353	1.065898	1.220833
15	7	-1.534210	-1.134444	0.794396
16	8	-1.358948	-0.028515	0.200693
17	1	1.830439	-3.175072	0.279932
18	1	3.273698	-2.371116	-1.566458
19	1	3.323907	0.045707	-2.158694
20	1	1.991419	1.672502	-0.858929
21	1	-0.579569	2.729617	3.201699
22	1	-1.401395	1.996645	5.419098
23	1	-1.464236	-0.423382	5.995290
24	1	-0.741640	-2.122313	4.347768
25	1	-2.127550	-0.967905	1.643959
26	1	0.050317	-2.657233	2.002539
27	1	0.253628	2.103489	0.902179
28	6	0.720651	1.610217	-4.425640
29	8	1.663187	0.878232	-4.696288
30	1	0.708495	2.688114	-4.688214
31	7	-0.414939	1.226573	-3.796679
32	6	-0.658541	-0.128761	-3.321436
33	6	-2.163133	-0.323243	-3.133726
34	8	-2.713476	0.684217	-2.293661
35	1	-1.098498	1.919772	-3.516840
36	1	-0.254860	-0.834416	-4.054652
37	1	-0.142514	-0.305266	-2.369766
38	1	-2.680111	-0.231991	-4.095128
39	1	-2.354118	-1.331452	-2.737496
40	1	-2.355795	0.529975	-1.398815

S-11 with *N*-formylethanolamine

1	6	-1.148366	-1.357041	-2.034742
2	6	-1.905200	-1.975554	-3.021275

3	6	-3.053030	-1.331749	-3.501239
4	6	-3.421293	-0.079659	-3.007134
5	6	-2.646887	0.551197	-2.025381
6	6	-1.518231	-0.096845	-1.539755
7	6	0.114519	-1.872155	-1.379641
8	6	-0.067893	-1.872254	0.125440
9	6	-0.419976	-0.601455	0.612586
10	6	-0.589483	-0.385632	1.977292
11	6	-0.414650	-1.462110	2.856176
12	6	-0.061485	-2.724157	2.374898
13	6	0.123810	-2.934906	1.002816
14	6	-0.531058	0.402458	-0.509162
15	7	1.195226	-0.864001	-1.701131
16	8	0.769995	0.448161	-1.200213
17	1	-1.614054	-2.946807	-3.413722
18	1	-3.658824	-1.811002	-4.265323
19	1	-4.312235	0.411568	-3.388482
20	1	-2.927520	1.531492	-1.647912
21	1	-0.831206	0.596132	2.370834
22	1	-0.546904	-1.303851	3.922448
23	1	0.071809	-3.549938	3.068647
24	1	0.402428	-3.917522	0.628608
25	1	1.967685	-1.087552	-1.064302
26	1	0.455204	-2.829979	-1.782862
27	1	-0.703818	1.428433	-0.179586
28	6	0.616829	3.063359	2.743809
29	8	0.345883	2.303236	3.664948
30	1	0.102254	4.035870	2.604331
31	7	1.561181	2.844615	1.800657
32	6	2.340794	1.616538	1.714676
33	6	3.365109	1.765754	0.584699
34	8	2.799504	2.341794	-0.581152
35	1	1.624674	3.457578	0.995470
36	1	2.843331	1.430013	2.670912
37	1	1.682839	0.763772	1.526039
38	1	4.166680	2.446356	0.892288
39	1	3.824831	0.785478	0.383096
40	1	2.133872	1.715413	-0.930194

S-TS11 with *N*-formylethanolamine

1	6	-2.815820	0.230823	-1.008205
2	6	-4.060561	0.697556	-1.477178
3	6	-4.878350	1.446093	-0.650553
4	6	-4.456851	1.783524	0.653908
5	6	-3.225062	1.368187	1.120463

6	6	-2.388984	0.570131	0.305454
7	6	-1.867512	-0.465884	-1.830657
8	6	-0.903054	-1.339948	-1.210081
9	6	-0.486738	-1.004838	0.116070
10	6	0.558299	-1.754114	0.718669
11	6	1.125442	-2.821009	0.055764
12	6	0.692856	-3.164471	-1.248650
13	6	-0.287599	-2.426416	-1.879321
14	6	-1.096382	0.120919	0.719871
15	7	-0.465352	0.983337	-1.979622
16	8	-0.366453	1.552714	-0.855681
17	1	-4.373494	0.453898	-2.489317
18	1	-5.847237	1.784278	-1.007010
19	1	-5.104988	2.379508	1.290335
20	1	-2.892543	1.637574	2.119581
21	1	0.899089	-1.480871	1.713421
22	1	1.912256	-3.399170	0.531091
23	1	1.144323	-4.012064	-1.756524
24	1	-0.609719	-2.680593	-2.886192
25	1	0.360587	0.350918	-2.122562
26	1	-2.138470	-0.664460	-2.864769
27	1	-0.703891	0.480510	1.668337
28	6	4.364575	-0.665433	2.436896
29	8	5.243303	-1.281838	1.854094
30	1	4.204369	-0.743317	3.531667
31	7	3.477856	0.179789	1.852852
32	6	3.493676	0.520857	0.438852
33	6	3.032238	1.970029	0.272559
34	8	1.787112	2.191939	0.919505
35	1	2.782821	0.656901	2.413975
36	1	4.511466	0.377994	0.062940
37	1	2.833368	-0.154301	-0.124214
38	1	3.757234	2.641275	0.746733
39	1	2.986618	2.225913	-0.796343
40	1	1.077970	1.905562	0.309733

Cartesian Coordinates of Complexes with PM3 optimization

11

6		-0.676172	0.105973	-1.225511
	6	-1.097778	-0.422812	-2.432934
	6	-2.247688	-1.215336	-2.449669
	6	-2.957940	-1.462885	-1.281256
	6	-2.538037	-0.924775	-0.062782
	6	-1.395682	-0.144430	-0.042499

6	0.531019	0.983436	-0.996046
6	1.368887	0.284735	0.049923
6	0.651439	0.036169	1.235167
6	1.258382	-0.592933	2.307570
6	2.594508	-0.981654	2.186503
6	3.302080	-0.738092	1.015662
6	2.693333	-0.098661	-0.066586
6	-0.777231	0.527167	1.160410
7	-0.015342	2.254431	-0.383485
8	-0.734824	1.977824	0.902587
1	-0.542458	-0.221951	-3.354752
1	-2.593367	-1.642687	-3.396745
1	-3.858824	-2.084461	-1.313891
1	-3.101267	-1.112643	0.856968
1	1.085946	1.231333	-1.927321
1	0.700686	-0.782280	3.230613
1	3.087819	-1.483681	3.025520
1	4.348727	-1.050709	0.937543
1	3.250038	0.092481	-0.989873
1	-1.356196	0.451126	2.100856
1	0.710165	2.864440	-0.092937

TS11

6	1.077263	0.715123	-0.597829
6	2.139919	1.437264	-1.206743
6	3.299774	1.653520	-0.517008
6	3.445575	1.190641	0.816266
6	2.432448	0.513380	1.433399
6	1.225503	0.241515	0.727921
6	-0.189058	0.534704	-1.221051
6	-0.984029	-0.574985	-0.824027
6	-0.830330	-1.052527	0.502661
6	-1.694515	-2.084077	0.974696
6	-2.626720	-2.629277	0.140980
6	-2.766279	-2.162967	-1.194000
6	-1.978313	-1.152809	-1.664510
6	0.130611	-0.427651	1.322176
1	2.010620	1.807611	-2.229604
1	4.130466	2.194885	-0.981499
1	4.383490	1.391049	1.344524
1	2.529186	0.165779	2.467794
1	-0.350441	0.972877	-2.218992
1	-1.585536	-2.428819	2.008963
1	-3.282357	-3.434470	0.488480
1	-3.519720	-2.627883	-1.838333

1	-2.084667	-0.779285	-2.688994
1	0.147023	-0.641471	2.398588
7	-1.218342	1.768705	0.007909
8	-0.972442	1.526884	1.162276
1	-2.161209	1.572594	-0.262069

R-11 + indole

6	0.561984	1.987060	0.133104
6	1.774621	2.085364	-0.527256
6	2.884198	1.432654	0.014030
6	2.774207	0.701341	1.191196
6	1.550442	0.593833	1.854870
6	0.451049	1.247392	1.324779
6	-0.738498	2.638994	-0.269275
6	-1.769324	1.537139	-0.361412
6	-1.889676	0.813540	0.839637
6	-2.820564	-0.203267	0.959048
6	-3.630552	-0.501028	-0.139344
6	-3.505853	0.208498	-1.327970
6	-2.572324	1.240395	-1.448649
6	-0.940706	1.304647	1.909385
7	-1.108550	3.520447	0.903445
8	-1.263412	2.720336	2.163082
1	1.862757	2.670424	-1.448382
1	3.854761	1.515059	-0.487296
1	3.655511	0.197303	1.603077
1	1.463228	0.014225	2.779608
1	-0.660205	3.260549	-1.188139
1	-2.917346	-0.762698	1.895311
1	-4.368266	-1.306833	-0.062085
1	-4.145673	-0.041944	-2.180803
1	-2.476932	1.803382	-2.382852
1	-1.059501	0.831028	2.903016
1	-2.008973	3.920780	0.794284
6	2.470742	-3.169033	0.469636
6	1.242858	-2.911763	-0.243423
6	3.453101	-2.390700	-0.088182
6	1.526245	-1.945217	-1.242533
6	-0.056045	-3.408215	-0.103961
7	2.923430	-1.683719	-1.206239
6	0.528587	-1.442071	-2.084162
6	-1.038794	-2.907201	-0.937149
6	-0.752927	-1.927780	-1.904978
1	2.575995	-3.868447	1.295086
1	4.504683	-2.315042	0.189487

1	-0.278519	-4.168172	0.650710
1	3.274543	-0.789459	-1.450311
1	0.751927	-0.683914	-2.840487
1	-2.068912	-3.266187	-0.840382
1	-1.572569	-1.537326	-2.519291

R-TS11 + indole

6	-0.023632	1.735234	-0.228367
6	1.069584	2.510780	-0.702143
6	2.169004	2.692529	0.089200
6	2.222301	2.136577	1.393155
6	1.177939	1.403662	1.881584
6	0.026049	1.182135	1.073613
6	-1.228177	1.568912	-0.967538
6	-2.032217	0.427253	-0.699858
6	-1.993539	-0.108494	0.612922
6	-2.893523	-1.158721	0.961527
6	-3.746798	-1.666548	0.025904
6	-3.768089	-1.143820	-1.295203
6	-2.944917	-0.114629	-1.649912
6	-1.108449	0.477031	1.539689
1	1.012230	2.950731	-1.703656
1	3.021196	3.278737	-0.269667
1	3.117124	2.302846	2.001742
1	1.207769	0.974002	2.888838
1	-1.310873	2.056177	-1.952099
1	-2.873670	-1.549637	1.984870
1	-4.429242	-2.484420	0.279302
1	-4.460237	-1.579791	-2.023048
1	-2.961385	0.302793	-2.662720
1	-1.176820	0.205539	2.600871
6	3.272938	-1.527501	1.112724
6	2.151030	-1.943239	0.311903
6	4.076782	-0.730522	0.331071
6	2.298566	-1.351396	-0.970566
6	1.040823	-2.752133	0.579954
7	3.460662	-0.544992	-0.931299
6	1.347188	-1.538895	-1.982162
6	0.108622	-2.936070	-0.421682
6	0.253895	-2.327022	-1.683016
1	3.439590	-1.809601	2.148945
1	5.015627	-0.242809	0.593384
1	0.923280	-3.216266	1.563463
1	3.956971	-0.277090	-1.741899
1	1.464455	-1.071922	-2.964342

1	-0.773725	-3.557477	-0.236307
1	-0.520873	-2.489039	-2.439734
7	-2.376199	2.726637	0.230064
8	-2.225765	2.424008	1.386767
1	-3.288823	2.532909	-0.130224

S-11 + indole

6	-1.188468	1.651580	-1.324662
6	-1.460782	1.246425	-2.619686
6	-2.549123	0.398849	-2.839332
6	-3.349172	-0.019510	-1.782680
6	-3.079370	0.392971	-0.475761
6	-1.994775	1.223109	-0.254096
6	-0.084010	2.582067	-0.882416
6	0.711976	1.838649	0.164574
6	-0.087840	1.397320	1.235219
6	0.472022	0.699380	2.291281
6	1.846384	0.452845	2.276425
6	2.635807	0.887651	1.218478
6	2.072950	1.588397	0.149599
6	-1.540142	1.787247	1.070836
7	-0.790313	3.730997	-0.196657
8	-1.594174	3.257325	0.977959
1	-0.838759	1.586731	-3.453710
1	-2.775754	0.066036	-3.857647
1	-4.201482	-0.679752	-1.974225
1	-3.711633	0.067594	0.356591
1	0.530315	2.974713	-1.722097
1	-0.151208	0.350166	3.120942
1	2.302920	-0.102611	3.102789
1	3.711491	0.683333	1.222575
1	2.693016	1.931005	-0.685041
1	-2.193096	1.560163	1.935483
1	-0.148464	4.357324	0.226094
6	1.750984	-3.263241	1.861759
6	0.886231	-2.949027	0.752417
6	3.028641	-2.891578	1.519210
6	1.688726	-2.365052	-0.262163
6	-0.488953	-3.103744	0.548911
7	3.007234	-2.255354	0.249120
6	1.140558	-1.927035	-1.473972
6	-1.024520	-2.668517	-0.647533
6	-0.221522	-2.081090	-1.643020
1	1.428319	-3.718814	2.794400
1	3.946055	-2.986080	2.100339

1	-1.113813	-3.553020	1.326261
1	3.798894	-2.230422	-0.341776
1	1.764931	-1.471700	-2.248168
1	-2.100438	-2.763532	-0.830474
1	-0.699952	-1.725398	-2.563586

S-TS11 + indole

6	-1.905182	0.876717	-0.523924
6	-2.911801	0.712526	-1.515000
6	-3.895725	-0.219302	-1.338964
6	-3.942067	-1.008927	-0.160873
6	-2.998455	-0.859984	0.815381
6	-1.940111	0.078350	0.644906
6	-0.926201	1.907607	-0.583158
6	0.296919	1.718041	0.116556
6	0.274747	0.891597	1.268875
6	1.463148	0.745873	2.044074
6	2.606592	1.388795	1.667757
6	2.628651	2.210831	0.509122
6	1.502658	2.385853	-0.242464
6	-0.951515	0.297812	1.631378
1	-2.879964	1.341455	-2.411370
1	-4.667831	-0.363842	-2.101781
1	-4.751679	-1.737054	-0.045619
1	-3.032755	-1.455843	1.734098
1	-0.945699	2.600861	-1.439177
1	1.436436	0.106594	2.933600
1	3.526708	1.275526	2.250598
1	3.563498	2.711519	0.235989
1	1.506274	3.027216	-1.130846
1	-1.050494	-0.183397	2.612852
6	2.837967	-2.320903	0.669680
6	1.694261	-2.344087	-0.209672
6	3.734549	-1.409518	0.171169
6	1.933058	-1.401166	-1.242780
6	0.499348	-3.069054	-0.192236
7	3.242407	-0.880799	-1.055649
6	0.983105	-1.143143	-2.237087
6	-0.436513	-2.809930	-1.176145
6	-0.204746	-1.847490	-2.175139
1	2.952345	-2.936301	1.558298
1	4.707945	-1.121555	0.568726
1	0.317709	-3.814508	0.587414
1	3.469968	0.038944	-1.341968
1	1.168322	-0.403184	-3.021152

1	-1.386720	-3.354034	-1.178637
1	-0.985190	-1.659426	-2.920031
7	-1.668325	3.015677	0.938013
8	-1.885741	2.326718	1.902047
1	-0.937627	3.686161	1.067342

R-11 + benzene

6	0.563462	-0.455711	0.810932
6	1.802593	-0.368028	0.202134
6	2.783120	-1.301150	0.543145
6	2.521215	-2.293121	1.478785
6	1.271235	-2.384152	2.096126
6	0.295697	-1.464589	1.754305
6	-0.615236	0.459954	0.583717
6	-1.761610	-0.428357	0.159756
6	-2.035327	-1.438357	1.101544
6	-3.056583	-2.346020	0.883790
6	-3.804349	-2.242857	-0.291512
6	-3.532022	-1.247556	-1.222177
6	-2.504835	-0.326915	-1.002949
6	-1.110777	-1.381895	2.297789
7	-0.946007	1.026005	1.947295
8	-1.279822	-0.059459	2.926486
1	2.011305	0.426622	-0.527042
1	3.768424	-1.245279	0.068821
1	3.302712	-3.014600	1.739292
1	1.067549	-3.163988	2.836867
1	-0.396651	1.296540	-0.122257
1	-3.271831	-3.128916	1.618360
1	-4.613719	-2.956214	-0.479546
1	-4.127090	-1.182814	-2.139205
1	-2.286884	0.456343	-1.736554
1	-1.349419	-2.087485	3.116689
1	-1.781946	1.558900	1.930065
6	1.555288	2.967210	-1.073490
6	0.603544	3.036845	-2.086001
6	2.847768	2.537436	-1.361089
6	0.944704	2.682416	-3.387253
6	3.188282	2.183050	-2.662833
6	2.237045	2.255804	-3.675433
1	1.287503	3.247866	-0.048646
1	-0.413832	3.371100	-1.856996
1	3.597229	2.485681	-0.563899
1	0.196624	2.740090	-4.184519
1	4.205502	1.848064	-2.890414

1 2.505867 1.977685 -4.699684

R-TS11 + benzene

6	0.566788	-0.234520	0.693372	
6		1.583986	0.711800	0.370358
6		2.801855	0.639366	0.979239
6		3.065662	-0.355836	1.959285
6		2.105712	-1.259394	2.307921
6		0.829615	-1.230542	1.668653
6		-0.730025	-0.167541	0.142512
6		-1.560307	-1.307151	0.171477
6		-1.296284	-2.305143	1.146528
6		-2.176892	-3.424702	1.252080
6		-3.236367	-3.544867	0.403530
6		-3.494364	-2.549747	-0.580122
6		-2.690850	-1.454357	-0.688374
6		-0.210770	-2.112763	2.019655
1		1.369744	1.491519	-0.375651
1		3.592187	1.353539	0.724007
1		4.052234	-0.379323	2.433532
1		2.292703	-2.019854	3.074100
1		-0.981981	0.665678	-0.529691
1		-1.974805	-4.179913	2.019831
1		-3.906989	-4.408125	0.466132
1		-4.352673	-2.680365	-1.247359
1		-2.884726	-0.678859	-1.437734
1		-0.083045	-2.784083	2.878963
6		0.929860	3.647078	-1.664764
6		-0.056567	3.303560	-2.583693
6		2.256391	3.301887	-1.906312
6		0.283059	2.614881	-3.743700
6		2.596088	2.615152	-3.067551
6		1.609030	2.270349	-3.985116
1		0.663005	4.188476	-0.751025
1		-1.099750	3.576085	-2.393689
1		3.032158	3.568677	-1.180576
1		-0.493030	2.344490	-4.466984
1		3.639642	2.344263	-3.257990
1		1.875986	1.727878	-4.897888
7		-1.587794	0.456519	2.073311
8		-1.266615	-0.335403	2.907730
1		-2.546898	0.412450	1.797135

S-11 + benzene

6		-1.688572	0.203024	-0.249947
6		-1.838598	0.575492	-1.574322
6		-2.758754	-0.119444	-2.362230
6		-3.509747	-1.159578	-1.827993
6		-3.359978	-1.536298	-0.491401
6		-2.445032	-0.853413	0.290248
6		-0.755816	0.824807	0.760834
6		0.112429	-0.298890	1.276364
6		-0.639054	-1.357154	1.821250
6		-0.004807	-2.472089	2.339321
6		1.391109	-2.526058	2.302014
6		2.131076	-1.482987	1.761193
6		1.493900	-0.354545	1.242218
6		-2.128509	-1.103230	1.746311
7		-1.647244	1.283633	1.893973
8		-2.406343	0.137124	2.492639
1		-1.243466	1.395214	-1.993354
1		-2.889475	0.161607	-3.412408
1		-4.229090	-1.690819	-2.459920
1		-3.954378	-2.352896	-0.069171
1		-0.178950	1.691132	0.362783
1		-0.586101	-3.295427	2.767029
1		1.905249	-3.405148	2.704922
1		3.224140	-1.544233	1.736665
1		2.073682	0.467993	0.801181
1		-2.765254	-1.854551	2.251680
1		-1.119343	1.613296	2.665714
6		2.301462	2.413605	-0.980287
6		1.756807	2.243309	-2.249162
6		3.510243	1.805736	-0.653514
6		2.421040	1.465367	-3.191870
6		4.174061	1.027975	-1.596863
6		3.628756	0.857086	-2.865163
1		1.777904	3.026011	-0.237689
1		0.800297	2.714507	-2.501677
1		3.945440	1.949602	0.341544
1		1.992263	1.330246	-4.190188
1		5.125767	0.550996	-1.341099
1		4.150671	0.243744	-3.606927

S-TS11 + benzene

6		-1.625746	-1.428285	-0.408069
6		-2.639000	-1.502941	-1.402684
6		-3.663206	-2.397421	-1.266257
6		-3.744405	-3.235404	-0.124294

6	-2.796573	-3.169458	0.857152
6	-1.698292	-2.272248	0.726224
6	-0.584674	-0.458972	-0.439180
6	0.626392	-0.748746	0.246882
6	0.554285	-1.599963	1.378822
6	1.726513	-1.817401	2.161488
6	2.908607	-1.241594	1.796934
6	2.981405	-0.399657	0.655373
6	1.870114	-0.146057	-0.095034
6	-0.702522	-2.137358	1.721240
1	-2.578632	-0.837630	-2.270925
1	-4.440331	-2.474420	-2.033746
1	-4.584285	-3.932900	-0.040463
1	-2.859229	-3.800895	1.750212
1	-0.563165	0.264312	-1.270318
1	1.655769	-2.458966	3.046823
1	3.817955	-1.417726	2.380826
1	3.943132	0.052662	0.389410
1	1.916628	0.527954	-0.962688
1	-0.831806	-2.641661	2.687402
6	2.101818	3.657265	-0.244202
6	0.878083	4.227253	-0.579506
6	2.809166	2.922598	-1.190622
6	0.365354	4.069958	-1.863222
6	2.295304	2.763138	-2.473903
6	1.074844	3.339675	-2.811153
1	2.507280	3.783895	0.764922
1	0.319501	4.802398	0.166149
1	3.768684	2.465898	-0.923510
1	-0.596503	4.521409	-2.127443
1	2.853110	2.186081	-3.218692
1	0.672958	3.218256	-3.822283
7	-1.258009	0.639158	1.120710
8	-1.516334	-0.067493	2.061637
1	-0.489123	1.260876	1.270315

R-11 + indole + benzene

6	-0.666981	-0.833563	-1.615931
6	0.601957	-0.650168	-2.135937
6	0.879505	0.536054	-2.817148
6	-0.098369	1.511431	-2.967010
6	-1.378864	1.331410	-2.438778
6	-1.660089	0.150864	-1.772937
6	-1.159585	-2.047922	-0.868297
6	-1.704461	-1.554054	0.452203

6	-2.714588	-0.587900	0.287713
6	-3.366560	-0.058102	1.387233
6	-2.995300	-0.496295	2.660624
6	-1.990027	-1.442382	2.822576
6	-1.333548	-1.982692	1.714514
6	-2.979142	-0.266991	-1.166567
7	-2.325267	-2.560161	-1.685589
8	-3.398388	-1.519733	-1.820437
1	1.373768	-1.420903	-2.008217
1	1.875009	0.690157	-3.247248
1	0.136400	2.438920	-3.500717
1	-2.146479	2.103158	-2.555648
1	-0.390872	-2.848023	-0.767527
1	-4.155791	0.690040	1.259725
1	-3.499459	-0.083117	3.540714
1	-1.706023	-1.767676	3.828968
1	-0.535334	-2.723981	1.838784
1	-3.828120	0.418228	-1.354426
1	-2.801856	-3.297661	-1.225244
6	2.549139	-3.166439	-0.215323
6	2.449949	-2.953098	1.155997
6	3.414445	-2.389595	-0.980077
6	3.207576	-1.955504	1.761057
6	4.176424	-1.396013	-0.373623
6	4.069534	-1.175782	0.995892
1	1.942926	-3.943288	-0.694293
1	1.767068	-3.563553	1.757218
1	3.503210	-2.567388	-2.057611
1	3.124600	-1.781736	2.839130
1	4.861214	-0.788155	-0.973896
1	4.665411	-0.390451	1.473111
6	0.541522	4.279662	-0.306895
6	0.316743	3.331742	0.757903
6	1.577492	3.812468	-1.075044
6	1.252765	2.278290	0.594132
6	-0.601476	3.289579	1.810376
7	2.098698	2.618228	-0.497552
6	1.271132	1.169292	1.446324
6	-0.583818	2.189300	2.647189
6	0.331177	1.138307	2.459365
1	-0.019721	5.199548	-0.449606
1	2.021710	4.257060	-1.965850
1	-1.314031	4.106833	1.954712
1	2.487560	1.909346	-1.070837
1	1.991148	0.351152	1.308425
1	-1.303576	2.119907	3.469686

1	0.285009	0.271579	3.128946
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R-TS11 + indole + benzene

6	0.390828	-0.570186	1.408953
6	-0.930510	-0.576838	1.933238
6	-1.335435	0.425368	2.769669
6	-0.444787	1.465904	3.138687
6	0.833629	1.491292	2.657453
6	1.281381	0.468142	1.773593
6	0.904453	-1.624876	0.603500
6	1.984142	-1.338419	-0.276055
6	2.882294	-0.307754	0.102418
6	4.055712	-0.087384	-0.677959
6	4.282756	-0.834256	-1.796881
6	3.370978	-1.852171	-2.186194
6	2.256936	-2.110881	-1.441418
6	2.607502	0.407658	1.284776
1	-1.617233	-1.385726	1.644892
1	-2.353872	0.432583	3.172278
1	-0.800799	2.251259	3.813397
1	1.529608	2.289614	2.937559
1	0.244488	-2.476664	0.373290
1	4.755654	0.695327	-0.365030
1	5.171895	-0.660866	-2.411902
1	3.580122	-2.427540	-3.093992
1	1.552249	-2.899219	-1.728083
1	3.366231	1.084882	1.697400
6	-3.410104	-2.867827	0.224911
6	-3.148558	-2.894049	-1.141396
6	-4.049807	-1.768929	0.789988
6	-3.519183	-1.817692	-1.941116
6	-4.426140	-0.695142	-0.010804
6	-4.159729	-0.719137	-1.376107
1	-3.113654	-3.712055	0.856325
1	-2.648729	-3.760504	-1.586633
1	-4.256064	-1.748970	1.865572
1	-3.307661	-1.833802	-3.015694
1	-4.937513	0.165877	0.432907
1	-4.454797	0.125823	-2.007723
6	-0.580082	3.763373	0.125468
6	-0.107444	2.886578	-0.917100
6	-1.814817	3.314228	0.526145
6	-1.097690	1.889511	-1.115686
6	1.065824	2.859954	-1.677432
7	-2.197179	2.205524	-0.276607

6	-0.922653	0.847184	-2.033626
6	1.234426	1.830068	-2.583238
6	0.259869	0.828625	-2.747844
1	-0.040689	4.626670	0.506175
1	-2.472177	3.720135	1.295045
1	1.825848	3.635447	-1.545482
1	-2.819891	1.505212	0.047925
1	-1.690189	0.072734	-2.162545
1	2.149319	1.778224	-3.182451
1	0.448133	0.020028	-3.461757
7	2.168452	-2.363979	1.999408
8	2.826487	-1.480725	2.488334
1	2.696160	-3.017546	1.456583

S-11 + indole + benzene

6	-0.000660	2.162863	-0.512447
6	-0.518017	2.888309	-1.571425
6	-1.576260	3.766343	-1.325901
6	-2.091312	3.918222	-0.044029
6	-1.566956	3.191010	1.027029
6	-0.526528	2.311697	0.784202
6	1.154752	1.191002	-0.561186
6	0.640795	-0.116435	-0.005560
6	0.100087	0.022989	1.286243
6	-0.420710	-1.072016	1.953816
6	-0.387341	-2.317592	1.323605
6	0.147818	-2.455339	0.048377
6	0.670023	-1.351489	-0.629289
6	0.182983	1.444468	1.796699
7	2.169928	1.744561	0.414600
8	1.606367	1.827365	1.803246
1	-0.103359	2.778787	-2.578564
1	-1.999507	4.344707	-2.153791
1	-2.917459	4.615252	0.130972
1	-1.969330	3.312967	2.037786
1	1.621045	1.101668	-1.566739
1	-0.848360	-0.961930	2.955621
1	-0.801146	-3.192254	1.836908
1	0.165148	-3.439650	-0.430788
1	1.093551	-1.458294	-1.633135
1	-0.127326	1.589190	2.849448
1	2.945393	1.133685	0.534524
6	5.368905	0.242564	0.522191
6	5.634306	0.416021	-0.832646
6	5.111898	-1.029847	1.022944

6	5.641827	-0.682359	-1.686243
6	5.119375	-2.128127	0.169138
6	5.384211	-1.954345	-1.185385
1	5.368203	1.107041	1.195566
1	5.838391	1.417447	-1.225756
1	4.903421	-1.166048	2.089229
1	5.853155	-0.545957	-2.751697
1	4.917397	-3.129152	0.563636
1	5.392392	-2.818940	-1.856797
6	-4.063165	-2.803808	0.833093
6	-3.986963	-1.493612	0.237841
6	-3.457429	-3.691974	-0.022773
6	-3.303595	-1.625896	-0.999091
6	-4.427426	-0.234209	0.658044
7	-2.903850	-2.981064	-1.120815
6	-3.046516	-0.521206	-1.820450
6	-4.169914	0.851922	-0.155283
6	-3.481814	0.711452	-1.375077
1	-4.527368	-3.028042	1.790002
1	-3.334342	-4.769529	0.086594
1	-4.954805	-0.124471	1.610085
1	-2.744047	-3.405406	-1.998750
1	-2.512521	-0.630634	-2.768824
1	-4.490200	1.852972	0.153452
1	-3.276034	1.609560	-1.970070

S-TS11 + indole + benzene

6	2.104632	-1.272553	-0.490597
6	2.508384	-1.792742	-1.751101
6	3.676532	-1.370053	-2.320392
6	4.509921	-0.435451	-1.652958
6	4.156365	0.066247	-0.432764
6	2.927762	-0.328894	0.170544
6	0.966275	-1.754343	0.213752
6	0.347476	-0.896104	1.163728
6	1.161436	0.071244	1.806563
6	0.593390	0.891661	2.825417
6	-0.721350	0.749820	3.163237
6	-1.536811	-0.212100	2.509812
6	-1.018361	-1.025829	1.544218
6	2.522515	0.132870	1.443847
1	1.868214	-2.528708	-2.249542
1	3.990002	-1.753170	-3.297009
1	5.445284	-0.127209	-2.131433
1	4.799534	0.777846	0.096537

1	0.366269	-2.556685	-0.244529
1	1.230002	1.634614	3.318563
1	-1.169169	1.382333	3.936687
1	-2.591718	-0.296164	2.794165
1	-1.649051	-1.767656	1.032974
1	3.217524	0.728313	2.049606
6	-3.695929	-2.689985	-0.214815
6	-3.274065	-2.583303	-1.536498
6	-4.333101	-1.617147	0.401246
6	-3.482518	-1.401093	-2.239629
6	-4.548639	-0.437660	-0.304492
6	-4.122288	-0.329402	-1.624492
1	-3.529559	-3.619374	0.340095
1	-2.775964	-3.428886	-2.022140
1	-4.662833	-1.700257	1.442404
1	-3.143854	-1.312653	-3.277587
1	-5.060521	0.402596	0.176926
1	-4.290434	0.599095	-2.181070
6	-0.518557	3.668323	0.766804
6	0.000483	2.970728	-0.383365
6	-1.774287	3.176166	1.027053
6	-0.983444	2.033017	-0.791573
6	1.210361	3.053986	-1.079598
7	-2.121554	2.219986	0.034645
6	-0.766108	1.150869	-1.856711
6	1.421149	2.181373	-2.130160
6	0.452954	1.230462	-2.502099
1	0.005349	4.450088	1.310444
1	-2.467418	3.458769	1.819356
1	1.965655	3.788906	-0.786521
1	-2.762690	1.483285	0.209404
1	-1.530324	0.418757	-2.148324
1	2.365826	2.214882	-2.682838
1	0.675673	0.543516	-3.325259
7	1.989092	-2.702990	1.678826
8	2.834436	-1.982116	2.145301
1	1.250894	-2.934928	2.312549