Electronic Supplementary Information

Tuning of hyperpolarizability, one- and two-photon absorption of donor-acceptor and donor-acceptor-acceptor-type intramolecular charge Transfer-based sensors

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Table S1: The lowest two excitation energies (in eV) of molecules (1-3) at the CAM-B3LYP/6-31+G(d) and CAM-B3LYP/aug-CC-pVDZ Level of Theory.

Molecule	Medium	Excited State	6-31+G(d)	aug-CC-pVDZ
Molecule **1**	Vacuum	S_1	2.59 (f=2.04)	2.58 (f=2.03)
		S_2	3.96 (f=0.01)	3.95 (f=0.01)
	DCM	S_1	2.47 (f=2.12)	2.46 (f=2.13)
		S_2	3.96 (f=0.02)	3.95 (f=0.02)
	EtOH	S_1	2.51 (f=2.10)	2.50 (f=2.11)
		S_2	3.99 (f=0.02)	3.97 (f=0.02)
	ACN	S_1	2.52 (f=2.09)	2.51 (f=2.10)
		S_2	3.99 (f=0.02)	3.97 (f=0.02)
Molecule **2**	Vacuum	S_1	3.11 (f=0.43)	3.08 (f=0.42)
		S_2	3.20 (f=0.34)	3.18 (f=0.35)
	DCM	S_1	2.81 (f=0.48)	2.80 (f=0.48)
		S_2	3.00 (f=0.52)	2.98 (f=0.52)
	EtOH	S_1	2.78 (f=0.48)	2.77 (f=0.48)
		S_2	3.02 (f=0.50)	3.00 (f=0.50)
	ACN	S_1	2.78 (f=0.48)	2.76 (f=0.48)
		S_2	3.03 (f=0.50)	3.00 (f=0.50)
Molecule **3**	Vacuum	S_1	2.65 (f=0.06)	2.65 (f=0.05)
		S_2	2.80 (f=1.48)	2.78 (f=1.47)
	DCM	S_1	2.68 (f=1.48)	2.66 (f=1.56)
		S_2	2.74 (f=0.24)	2.73 (f=0.15)
	EtOH	S_1	2.69 (f=1.29)	2.67 (f=1.49)
		S_2	2.73 (f=0.38)	2.73 (f=0.19)
	ACN	S_1	2.69 (f=1.23)	2.68 (f=1.45)
		S_2	2.73 (f=0.43)	2.73 (f=0.21)

Table S2: The values of dipole moments (μ), average polarizability (α_{av}) and β_{total} for molecules 1-3 as obtained by using M06-2X/6-31+G(d) Level of Theory.

Molecules	Medium	μ (in Debye)	α_{av} (in a.u.)	β_{tot} (in a.u.)	β_{vec} (in a.u.)	β_{vec}/β_{tot}
Molecule **1**	Vacuum	2.34	467.47	25956.85	-20896.33	-0.81
	DCM	2.12	627.50	97502.42	8597.18	0.09
	EtOH	2.30	644.90	109535.04	30221.51	0.28
	ACN	2.34	649.29	112436.20	32953.05	0.29
Molecule **2**	Vacuum	9.58	271.49	4673.24	-4672.42	-1.00
	DCM	12.73	384.10	18310.23	-18310.25	-1.00
	EtOH	13.17	403.23	21338.76	-21338.76	-1.00
	ACN	13.30	407.61	22133.49	-22133.51	-1.00
Molecule **3**	Vacuum	8.55	569.25	1573.79	490.64	0.31
	DCM	13.36	759.86	9872.37	8209.36	0.83
	EtOH	14.17	789.92	11506.15	9375.69	0.81
	ACN	14.30	794.45	11640.87	9865.13	0.85

Table S3: Computed values of $\mu\beta_{\|}$ (a.u.) of molecules (1-3) in the gas phase and in the solvents studied.

Molecule	Medium	$\mu\beta_{\|}$ (a.u.) CAM-B3LYP/ 6-31+G(d)	$\mu\beta_{\|}$ (a.u.) M06-2X/6-31+G(d)
Molecule **1**	Vacuum	11199.02	11547.44
	DCM	2131.36	4309.82
	EtOH	11768.15	16411.44
	ACN	13730.31	18198.68
Molecule **2**	Vacuum	10250.07	10563.26
	DCM	48136.33	55004.89
	EtOH	58458.02	66328.29
	ACN	60618.58	69481.38
Molecule **3**	Vacuum	1143.80	990.76
	DCM	26287.19	25884.72
	EtOH	31914.94	31360.11
	ACN	33122.28	33291.67

Few state model results for all the three molecules in vacuum phase

The first row and first column represent the labels for the electronic states participated in the few state models. For example, 0 represents the ground state, 1 represents the first excited state, and so on. The values given in *ij*-cell (i^{th} row and j^{th} column) represents the value of δ_{ij}. All these δ_{ij} are evaluated for the brightest TP active state in respective molecules. Thus, the final state in Molecule 1 and 2 is 2nd excited state and that in Molecule 3 is 3rd excited state. Total FSM value is given by

$$\delta_{TP}^{FSM} = \sum_{i,j} \delta_{ij}$$

Table S4: Few state model results for Molecule 1

States/States	0	1	2	3	4
0	3.609	869.403	1.262	-0.251	-5.848
1	869.403	401285.169	1170.507	-102.482	-2324.388
2	1.262	1170.507	7.125	-0.328	-8.774
3	-0.251	-102.482	-0.328	0.028	0.655
4	-5.848	-2324.388	-8.774	0.655	16.274

Table S5: Few state model results for Molecule 2

States/States	0	1	2	3	4
0	15055.893	488.897	-33142.798	31.406	-160.309
1	488.897	142.953	-1076.217	9.239	-5.206
2	-33142.798	-1076.217	72957.817	-69.135	352.892
3	31.406	9.239	-69.135	0.598	-0.334
4	-160.309	-5.206	352.892	-0.334	1.707

Table S6: Few state model results for Molecule 3

States/States	0	1	2	3	4
0	41.554	-9.943	209.546	-43.409	-55.191
1	-9.943	247.743	-2055.133	-1.539	342.839
2	209.546	-2055.133	51980.260	-139.741	-7084.787
3	-43.409	-1.539	-139.741	45.996	43.692
4	-55.191	342.839	-7084.787	43.692	1007.008

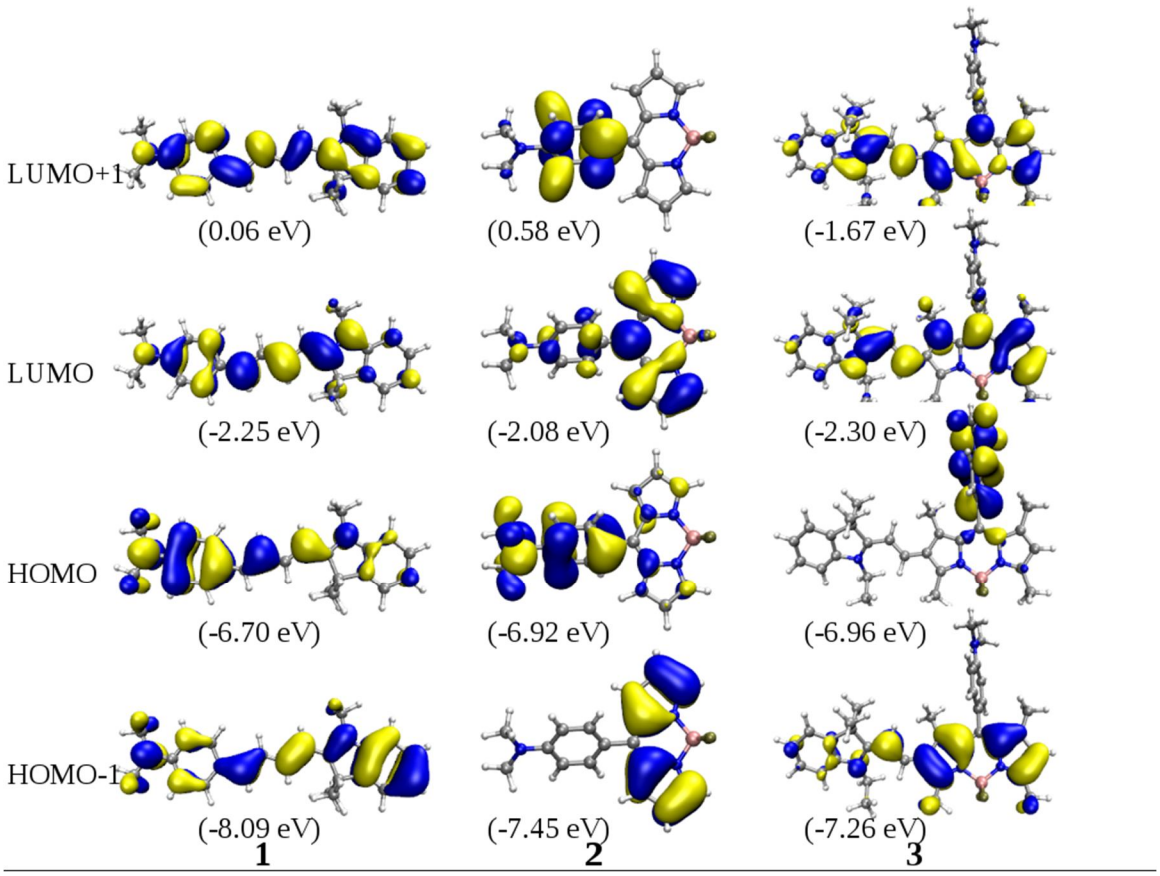

Figure S1: The molecular orbital (MO) pictures involved in the absorption process in ethanol. The HOMO, LUMO and (HOMO-1) to LUMO pictures are shown along with the corresponding energy.

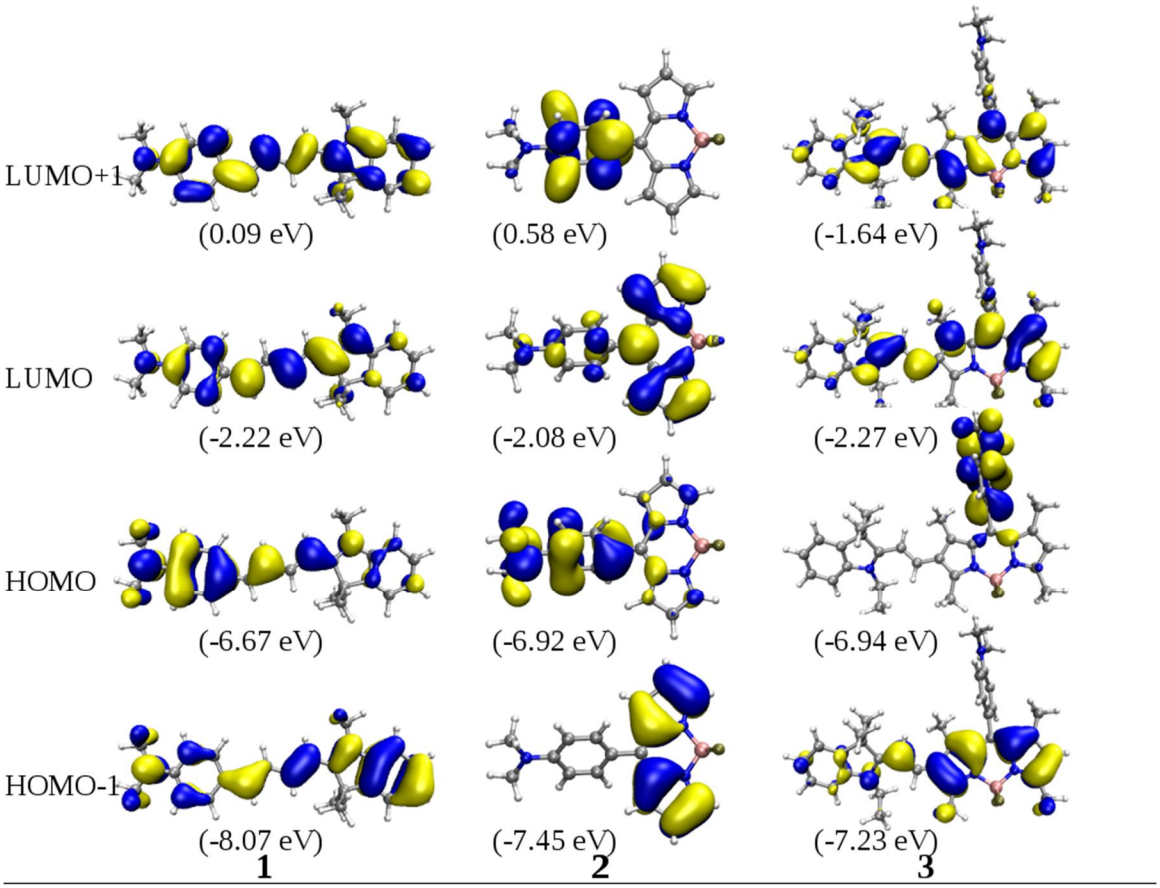

Figure S2: The molecular orbital (MO) pictures involved in the absorption process in acetonitrile. The HOMO, LUMO and (HOMO-1) to LUMO pictures along with the corresponding energy are shown.

Optimized Coordinates using CAM-B3LYP/6-31+G(d)

1. Molecule 1/ CAM-B3LYP/6-31G(d)/Gas Phase

1	6	0	-4.913811	-0.634714	-0.000051
2	6	0	-5.081524	0.744042	-0.000068
3	6	0	-6.330365	1.344624	-0.000295
4	6	0	-7.440753	0.500737	-0.000490
5	6	0	-7.292603	-0.884855	-0.000462
6	6	0	-6.022148	-1.463525	-0.000242
7	6	0	-3.436006	-0.964165	0.000233
8	6	0	-2.819461	0.437145	0.000243
9	1	0	-6.463618	2.420463	-0.000337
10	1	0	-8.434882	0.935392	-0.000670
11	1	0	-8.172692	-1.519239	-0.000612
12	1	0	-5.914914	-2.544369	-0.000215
13	7	0	-3.798474	1.350972	0.000141
14	6	0	-3.583584	2.789694	0.000148
15	1	0	-4.545849	3.295814	0.000314
16	1	0	-3.030006	3.091763	0.893093
17	1	0	-3.030253	3.091826	-0.892933
18	6	0	-1.467837	0.809116	0.000227
19	1	0	-1.242273	1.870815	0.000173
20	6	0	-0.390319	-0.058864	0.000189
21	1	0	-0.569366	-1.129785	0.000173
22	6	0	0.954036	0.346093	0.000140
23	1	0	1.169767	1.411166	0.000141
24	6	0	1.975377	-0.576164	0.000090
25	1	0	1.681124	-1.626192	0.000092
26	6	0	3.378183	-0.343002	0.000032
27	6	0	4.263298	-1.444878	-0.000013
28	6	0	3.962127	0.945811	0.000018
29	6	0	5.627568	-1.289204	-0.000069
30	1	0	3.851377	-2.450794	0.000003
31	6	0	5.321706	1.123096	-0.000037
32	1	0	3.328844	1.827108	0.000050
33	6	0	6.208095	0.007649	-0.000087
34	1	0	6.256253	-2.169544	-0.000090
35	1	0	5.717243	2.130137	-0.000050
36	7	0	7.551125	0.179278	-0.000150
37	6	0	8.125617	1.517433	-0.000068
38	1	0	9.211385	1.437996	-0.000057
39	1	0	7.826690	2.080770	-0.891102
40	1	0	7.826667	2.080667	0.891023

41	6	0	8.439876	-0.974322	-0.000232
42	1	0	9.472126	-0.628441	-0.000402
43	1	0	8.289128	-1.594082	0.890734
44	1	0	8.288866	-1.594138	-0.891111
45	6	0	-3.064061	-1.748922	1.273761
46	1	0	-2.000456	-1.994237	1.308890
47	1	0	-3.316501	-1.184362	2.175467
48	1	0	-3.625625	-2.686911	1.295724
49	6	0	-3.063562	-1.749075	-1.273049
50	1	0	-3.315756	-1.184678	-2.174926
51	1	0	-1.999912	-1.994271	-1.307774
52	1	0	-3.625018	-2.687127	-1.295057

2. Molecule 2/ CAM-B3LYP/6-31G(d)/Gas Phase

1	6	0	0.900827	-0.008070	-0.007664
2	6	0	-0.570300	-0.002888	-0.003587
3	6	0	-1.273586	1.208341	0.106284
4	6	0	-1.282161	-1.209385	-0.109294
5	7	0	-2.671062	-1.231150	-0.080841
6	6	0	-0.835661	-2.535499	-0.311035
7	7	0	-2.662435	1.239215	0.085360
8	6	0	-0.817372	2.531361	0.306428
9	6	0	-1.961555	-3.342120	-0.384054
10	6	0	3.013351	0.822432	-0.879121
11	6	0	3.012096	-0.850704	0.855243
12	9	0	-4.401946	0.080295	-1.133491
13	5	0	-3.605002	0.007175	0.004214
14	6	0	-1.937576	3.345290	0.386094
15	6	0	3.748163	-0.019932	-0.016990
16	6	0	-3.071630	-2.494723	-0.242911
17	6	0	-3.053887	2.505282	0.250381
18	6	0	1.629583	0.829219	-0.861670
19	6	0	1.628214	-0.848629	0.844259
20	9	0	-4.397661	-0.060616	1.145243
21	6	0	5.846277	-0.863882	0.910928
22	7	0	5.121922	-0.031574	-0.027700
23	6	0	5.846927	0.901075	-0.866296
24	1	0	0.195525	-2.842282	-0.410292
25	1	0	-1.995592	-4.411911	-0.534974
26	1	0	0.216290	2.831403	0.400344
27	1	0	3.524695	1.474028	-1.576271
28	1	0	3.522412	-1.500387	1.554900
29	1	0	-1.963796	4.415180	0.537878
30	1	0	-4.126061	-2.736057	-0.264400
31	1	0	1.099509	1.476612	-1.553169
32	1	0	-4.106591	2.753460	0.277691
33	1	0	1.097250	-1.489094	1.541531
34	1	0	6.916206	-0.755557	0.732974
35	1	0	5.592539	-1.923328	0.785150
36	1	0	5.644176	-0.583568	1.954125
37	1	0	6.917306	0.745150	-0.731844
38	1	0	5.620399	1.945652	-0.611947
39	1	0	5.617959	0.749252	-1.928232

3. Molecule 3/ CAM-B3LYP/6-31G(d)/Gas Phase

1	6	0	-6.313919	1.243693	0.301716
2	6	0	-6.411382	-0.009719	-0.286009
3	6	0	-7.624579	-0.592170	-0.615693
4	6	0	-8.776587	0.141891	-0.332968
5	6	0	-8.699539	1.402904	0.255508
6	6	0	-7.462693	1.965094	0.576999
7	6	0	-4.856990	1.571303	0.517798
8	6	0	-4.175018	0.311770	-0.017933
9	1	0	-7.696918	-1.574662	-1.068622
10	1	0	-9.746343	-0.280461	-0.574661
11	1	0	-9.610787	1.952580	0.466690
12	1	0	-7.411526	2.949242	1.033521
13	7	0	-5.099436	-0.533406	-0.478785
14	6	0	-4.892909	-1.793981	-1.192222
15	1	0	-5.640989	-1.827742	-1.988374
16	1	0	-3.917882	-1.743211	-1.679579
17	6	0	-2.771294	0.184698	0.001132
18	1	0	-2.256916	1.111119	0.216507
19	6	0	-2.020532	-0.968958	-0.104354
20	1	0	-2.555175	-1.910437	-0.143635
21	6	0	2.993969	-0.397748	-0.029545
22	6	0	3.300798	1.054207	-0.075794
23	6	0	3.121633	1.862108	1.048840
24	6	0	3.778031	1.653208	-1.242074
25	6	0	3.418025	3.215127	1.020399
26	1	0	2.755961	1.423059	1.973550
27	6	0	4.060545	3.008969	-1.294741
28	1	0	3.925064	1.050098	-2.134306
29	6	0	3.891970	3.833042	-0.159434
30	1	0	3.282032	3.794148	1.924937
31	1	0	4.422026	3.426247	-2.225894
32	7	0	4.175336	5.173847	-0.200363
33	6	0	4.737519	5.759312	-1.402558
34	1	0	4.886141	6.826982	-1.244103
35	1	0	5.708308	5.315614	-1.661757
36	1	0	4.063565	5.640142	-2.259233
37	6	0	4.073720	5.973432	1.005232
38	1	0	4.336263	7.005027	0.772873
39	1	0	3.051812	5.971114	1.403263
40	1	0	4.752350	5.619373	1.793033
41	6	0	-4.432417	2.808920	-0.296174
42	1	0	-3.369473	3.028642	-0.162070
43	1	0	-4.630661	2.675599	-1.363291
44	1	0	-4.999139	3.678799	0.047195
45	6	0	-4.529793	1.767998	2.009220

46	1	0	-4.816187	0.893897	2.600543
47	1	0	-3.462161	1.952398	2.157372
48	1	0	-5.080147	2.631744	2.392731
49	6	0	0.016106	-2.383065	0.023878
50	6	0	-0.617314	-1.110506	-0.088557
51	6	0	0.428559	-0.129467	-0.168078
52	6	0	1.623257	-0.833309	-0.058438
53	7	0	1.330681	-2.203943	0.043991
54	6	0	4.017188	-1.310278	0.063956
55	6	0	5.452970	-1.134140	0.187838
56	6	0	5.983282	-2.395001	0.275092
57	6	0	4.923085	-3.338975	0.221312
58	7	0	3.767017	-2.694749	0.101250
59	1	0	7.029707	-2.648633	0.382058
60	5	0	2.373042	-3.359199	0.074422
61	6	0	5.030362	-4.819706	0.306891
62	1	0	4.620722	-5.173889	1.258684
63	1	0	4.454240	-5.299256	-0.488809
64	1	0	6.074367	-5.129430	0.235597
65	6	0	6.249137	0.128745	0.244159
66	1	0	6.269119	0.638312	-0.723103
67	1	0	5.837638	0.837875	0.966725
68	1	0	7.279242	-0.100559	0.527801
69	6	0	0.206685	1.329570	-0.418663
70	1	0	-0.081119	1.860446	0.497435
71	1	0	1.095362	1.820255	-0.807627
72	1	0	-0.596846	1.464430	-1.149223
73	6	0	-0.601496	-3.735899	0.141413
74	1	0	-0.554611	-4.087724	1.177234
75	1	0	-1.646449	-3.732655	-0.173733
76	1	0	-0.058275	-4.458843	-0.469970
77	6	0	-5.020242	-3.019314	-0.292775
78	1	0	-4.291982	-3.005808	0.523230
79	1	0	-6.015747	-3.080095	0.154706
80	1	0	-4.858656	-3.926102	-0.882779
81	9	0	2.235602	-4.141190	-1.070804
82	9	0	2.183605	-4.130633	1.216149

4. Molecule 1/ CAM-B3LYP/6-31G(d)/Dichloromethane

1	6	0	-4.918910	-0.630701	-0.000047
2	6	0	-5.075684	0.749735	-0.000061
3	6	0	-6.319643	1.361029	-0.000076
4	6	0	-7.436741	0.525221	-0.000075
5	6	0	-7.299393	-0.862454	-0.000056
6	6	0	-6.033115	-1.451937	-0.000041
7	6	0	-3.444441	-0.969429	-0.000043
8	6	0	-2.821755	0.427053	-0.000043
9	1	0	-6.441589	2.437811	-0.000088
10	1	0	-8.427430	0.968035	-0.000089
11	1	0	-8.184539	-1.490177	-0.000058
12	1	0	-5.932415	-2.533266	-0.000031
13	7	0	-3.789317	1.346476	-0.000030
14	6	0	-3.564765	2.786397	0.000024
15	1	0	-4.523727	3.297671	0.000446
16	1	0	-3.009280	3.080515	0.893286
17	1	0	-3.009928	3.080706	-0.893583
18	6	0	-1.463151	0.792838	-0.000017
19	1	0	-1.233853	1.853271	-0.000116
20	6	0	-0.397471	-0.079486	0.000118
21	1	0	-0.573142	-1.150685	0.000253
22	6	0	0.954089	0.329553	0.000082
23	1	0	1.164713	1.395689	-0.000044
24	6	0	1.968595	-0.590189	0.000173
25	1	0	1.676746	-1.640380	0.000282
26	6	0	3.379739	-0.350541	0.000121
27	6	0	4.266558	-1.447267	0.000196
28	6	0	3.957401	0.938278	-0.000011
29	6	0	5.634000	-1.286095	0.000135
30	1	0	3.858665	-2.454776	0.000306
31	6	0	5.319794	1.121113	-0.000071
32	1	0	3.321719	1.817991	-0.000073
33	6	0	6.209813	0.010997	-0.000009
34	1	0	6.264883	-2.165245	0.000211
35	1	0	5.710006	2.130451	-0.000184
36	7	0	7.555699	0.188209	-0.000089
37	6	0	8.122838	1.527946	-0.000053
38	1	0	9.208975	1.452946	0.000023
39	1	0	7.820420	2.091429	-0.890159
40	1	0	7.820298	2.091425	0.890013
41	6	0	8.446529	-0.961661	-0.000076
42	1	0	9.477515	-0.612118	-0.000360
43	1	0	8.297404	-1.583825	0.889841
44	1	0	8.297026	-1.584104	-0.889729
45	6	0	-3.074976	-1.757290	1.272005

46	1	0	-2.014247	-2.013961	1.296560
47	1	0	-3.314985	-1.187564	2.173705
48	1	0	-3.647337	-2.688611	1.293967
49	6	0	-3.074976	-1.757371	-1.272043
50	1	0	-3.314769	-1.187599	-2.173772
51	1	0	-2.014302	-2.014275	-1.296484
52	1	0	-3.647518	-2.688579	-1.294073

5. Molecule 2/ CAM-B3LYP/6-31G(d)/Dichloromethane

1	6	0	0.902935	-0.000146	-0.000164
2	6	0	-0.561118	-0.000052	-0.000087
3	6	0	-1.275599	1.210002	0.104736
4	6	0	-1.275759	-1.210021	-0.104806
5	7	0	-2.666379	-1.232952	-0.074775
6	6	0	-0.831028	-2.532750	-0.313241
7	7	0	-2.666221	1.233096	0.074911
8	6	0	-0.830688	2.532678	0.313137
9	6	0	-1.957991	-3.343169	-0.386497
10	6	0	3.015958	0.881049	-0.825954
11	6	0	3.015912	-0.881570	0.825505
12	9	0	-4.407490	0.064318	-1.137685
13	5	0	-3.587834	0.000128	0.000093
14	6	0	-1.957544	3.343236	0.386487
15	6	0	3.754170	-0.000286	-0.000234
16	6	0	-3.067111	-2.501675	-0.241261
17	6	0	-3.066783	2.501865	0.241438
18	6	0	1.634257	0.884148	-0.809455
19	6	0	1.634210	-0.884537	0.809064
20	9	0	-4.407445	-0.063957	1.137904
21	6	0	5.849369	-0.933134	0.839737
22	7	0	5.119689	-0.000369	-0.000328
23	6	0	5.849333	0.933682	-0.838986
24	1	0	0.198820	-2.841878	-0.416616
25	1	0	-1.989321	-4.412661	-0.540284
26	1	0	0.199209	2.841684	0.416385
27	1	0	3.527007	1.563571	-1.492808
28	1	0	3.526920	-1.564219	1.492255
29	1	0	-1.988729	4.412735	0.540251
30	1	0	-4.120046	-2.749655	-0.263606
31	1	0	1.107308	1.560315	-1.474912
32	1	0	-4.119686	2.749967	0.263929
33	1	0	1.107226	-1.560666	1.474531
34	1	0	6.917947	-0.794699	0.680854
35	1	0	5.602210	-1.973367	0.595518
36	1	0	5.639957	-0.769509	1.904207
37	1	0	6.917910	0.795336	-0.680008
38	1	0	5.601785	1.973567	-0.593615
39	1	0	5.640296	0.771243	-1.903694

6. Molecule 3/ CAM-B3LYP/6-31G(d)/Dichloromethane

1	6	0	-6.296952	1.187678	0.406956
2	6	0	-6.391153	0.014114	-0.328074
3	6	0	-7.599477	-0.520595	-0.744810
4	6	0	-8.753266	0.179140	-0.391248
5	6	0	-8.680720	1.360737	0.346455
6	6	0	-7.447731	1.876853	0.751000
7	6	0	-4.841854	1.479694	0.674379
8	6	0	-4.165149	0.290673	-0.000757
9	1	0	-7.665225	-1.439464	-1.315871
10	1	0	-9.720436	-0.206856	-0.696121
11	1	0	-9.593612	1.885339	0.609088
12	1	0	-7.400995	2.799668	1.321153
13	7	0	-5.077378	-0.488243	-0.564786
14	6	0	-4.863178	-1.663555	-1.414780
15	1	0	-5.575714	-1.583953	-2.238794
16	1	0	-3.866413	-1.579426	-1.848105
17	6	0	-2.751037	0.153026	0.012420
18	1	0	-2.233544	1.063525	0.283161
19	6	0	-2.020790	-0.992832	-0.149234
20	1	0	-2.555827	-1.930694	-0.246211
21	6	0	2.987889	-0.389127	-0.031951
22	6	0	3.275838	1.064866	-0.093873
23	6	0	3.026860	1.893003	1.002426
24	6	0	3.802988	1.646339	-1.247587
25	6	0	3.300598	3.250669	0.958037
26	1	0	2.622741	1.467867	1.917187
27	6	0	4.061488	3.006304	-1.317400
28	1	0	4.008771	1.026873	-2.116347
29	6	0	3.814280	3.852737	-0.213247
30	1	0	3.109545	3.845181	1.842329
31	1	0	4.463794	3.408616	-2.238325
32	7	0	4.058404	5.203127	-0.277328
33	6	0	4.745182	5.754645	-1.431133
34	1	0	4.840093	6.832809	-1.305919
35	1	0	5.752127	5.332181	-1.557284
36	1	0	4.179651	5.575753	-2.351778
37	6	0	3.949965	6.011332	0.923395
38	1	0	4.162272	7.050226	0.672483
39	1	0	2.937170	5.970352	1.337959
40	1	0	4.655631	5.694241	1.704448
41	6	0	-4.401965	2.801475	0.014246
42	1	0	-3.339013	2.994123	0.181773
43	1	0	-4.592793	2.793839	-1.062273
44	1	0	-4.966156	3.626968	0.456387
45	6	0	-4.519909	1.492641	2.180324

46	1	0	-4.814494	0.554532	2.658576
47	1	0	-3.451453	1.650648	2.349906
48	1	0	-5.065434	2.309074	2.661043
49	6	0	0.031652	-2.393083	0.016664
50	6	0	-0.602415	-1.130756	-0.119476
51	6	0	0.426586	-0.149054	-0.205298
52	6	0	1.635700	-0.841860	-0.067442
53	7	0	1.351967	-2.212613	0.053468
54	6	0	4.030463	-1.290153	0.084541
55	6	0	5.451499	-1.094342	0.226425
56	6	0	6.001755	-2.352690	0.334697
57	6	0	4.961471	-3.306090	0.278401
58	7	0	3.793147	-2.674819	0.134388
59	1	0	7.050533	-2.588147	0.458869
60	5	0	2.407240	-3.341679	0.116866
61	6	0	5.091709	-4.785411	0.384366
62	1	0	4.665107	-5.141877	1.327389
63	1	0	4.555830	-5.287385	-0.425395
64	1	0	6.144110	-5.072129	0.347861
65	6	0	6.235891	0.176730	0.284454
66	1	0	6.292768	0.661984	-0.693858
67	1	0	5.790557	0.899317	0.972688
68	1	0	7.255078	-0.039328	0.614583
69	6	0	0.198868	1.300589	-0.497680
70	1	0	-0.031109	1.868712	0.411496
71	1	0	1.067707	1.765735	-0.958141
72	1	0	-0.647154	1.413148	-1.181453
73	6	0	-0.615998	-3.731327	0.143206
74	1	0	-0.968695	-3.891124	1.168145
75	1	0	-1.479085	-3.812565	-0.522310
76	1	0	0.078088	-4.533250	-0.102370
77	6	0	-5.053265	-2.979005	-0.668424
78	1	0	-4.368706	-3.070598	0.179108
79	1	0	-6.072697	-3.075947	-0.286641
80	1	0	-4.865812	-3.809658	-1.354145
81	9	0	2.284802	-4.175316	-1.007464
82	9	0	2.222828	-4.108268	1.276499

7. Molecule 1/ CAM-B3LYP/6-31G(d)/Ethanol

1	6	0	-4.916856	-0.633148	-0.000033
2	6	0	-5.076692	0.747074	-0.000066
3	6	0	-6.321971	1.355846	-0.000251
4	6	0	-7.437340	0.517642	-0.000387
5	6	0	-7.296995	-0.869860	-0.000341
6	6	0	-6.029369	-1.456851	-0.000164
7	6	0	-3.441453	-0.968144	0.000180
8	6	0	-2.822994	0.430039	0.000161
9	1	0	-6.445860	2.432369	-0.000305
10	1	0	-8.428949	0.958488	-0.000534
11	1	0	-8.180774	-1.499596	-0.000446
12	1	0	-5.926761	-2.538014	-0.000129
13	7	0	-3.792018	1.346689	0.000091
14	6	0	-3.571041	2.787526	0.000091
15	1	0	-4.531314	3.296144	0.000476
16	1	0	-3.016362	3.082401	0.893379
17	1	0	-3.016974	3.082515	-0.893545
18	6	0	-1.464270	0.799287	0.000132
19	1	0	-1.236982	1.860124	0.000035
20	6	0	-0.399746	-0.072551	0.000152
21	1	0	-0.575380	-1.143577	0.000205
22	6	0	0.953472	0.336452	0.000096
23	1	0	1.164128	1.402612	0.000050
24	6	0	1.965720	-0.584152	0.000096
25	1	0	1.673041	-1.634079	0.000141
26	6	0	3.378832	-0.346169	0.000040
27	6	0	4.263174	-1.444248	0.000032
28	6	0	3.958718	0.941183	-0.000006
29	6	0	5.631497	-1.285587	-0.000024
30	1	0	3.853341	-2.450960	0.000083
31	6	0	5.322115	1.121617	-0.000058
32	1	0	3.324469	1.821952	-0.000004
33	6	0	6.209984	0.010094	-0.000079
34	1	0	6.260365	-2.166213	0.000002
35	1	0	5.713994	2.130385	-0.000108
36	7	0	7.556894	0.184189	-0.000150
37	6	0	8.127102	1.522509	0.000103
38	1	0	9.213054	1.444945	0.000297
39	1	0	7.825999	2.087265	-0.889691
40	1	0	7.825675	2.087045	0.889923
41	6	0	8.444292	-0.968229	-0.000303
42	1	0	9.476306	-0.621748	-0.000699
43	1	0	8.293188	-1.590262	0.889430
44	1	0	8.292591	-1.590431	-0.889807
45	6	0	-3.070511	-1.754199	1.273186

46	1	0	-2.009348	-2.008791	1.299180
47	1	0	-3.312116	-1.183379	2.173785
48	1	0	-3.641189	-2.686465	1.295883
49	6	0	-3.070159	-1.754386	-1.272602
50	1	0	-3.311522	-1.183704	-2.173354
51	1	0	-2.008984	-2.008968	-1.298260
52	1	0	-3.640820	-2.686662	-1.295315

8. Molecule 2/ CAM-B3LYP/6-31G(d)/Ethanol

1	6	0	0.903185	0.000034	0.000032
2	6	0	-0.559649	0.000020	-0.000001
3	6	0	-1.275245	-1.210397	-0.103502
4	6	0	-1.275293	1.210416	0.103461
5	7	0	-2.666163	1.232825	0.071601
6	6	0	-0.831747	2.532809	0.314012
7	7	0	-2.666115	-1.232855	-0.071722
8	6	0	-0.831640	-2.532765	-0.314087
9	6	0	-1.959375	3.343190	0.386290
10	6	0	3.016405	-0.887819	0.819340
11	6	0	3.016440	0.887875	-0.819205
12	9	0	-4.408246	-0.060581	1.137904
13	5	0	-3.585622	-0.000040	0.000044
14	6	0	-1.959236	-3.343178	-0.386486
15	6	0	3.755209	0.000060	0.000111
16	6	0	-3.067740	2.502049	0.238873
17	6	0	-3.067638	-2.502089	-0.239039
18	6	0	1.635084	-0.890998	0.802405
19	6	0	1.635117	0.891045	-0.802334
20	9	0	-4.408532	0.060458	-1.137604
21	6	0	5.849826	0.939105	-0.833211
22	7	0	5.119542	0.000128	0.000147
23	6	0	5.849938	-0.939188	0.833034
24	1	0	0.197491	2.843095	0.419683
25	1	0	-1.990920	4.412574	0.540812
26	1	0	0.197616	-2.843003	-0.419734
27	1	0	3.527004	-1.575678	1.481095
28	1	0	3.527075	1.575678	-1.480997
29	1	0	-1.990737	-4.412552	-0.541087
30	1	0	-4.120614	2.750491	0.260449
31	1	0	1.108759	-1.572311	1.463025
32	1	0	-4.120502	-2.750570	-0.260665
33	1	0	1.108822	1.572318	-1.463018
34	1	0	6.918172	0.799536	-0.674465
35	1	0	5.601924	1.977287	-0.581857
36	1	0	5.640901	0.782430	-1.898678
37	1	0	6.918273	-0.799151	0.674635
38	1	0	5.602425	-1.977306	0.580995
39	1	0	5.640743	-0.783233	1.898545

9. Molecule 3/ CAM-B3LYP/6-31G(d)/Ethanol

1	6	0	-6.299161	1.186248	0.398396
2	6	0	-6.389972	0.009354	-0.331659
3	6	0	-7.596527	-0.529572	-0.748102
4	6	0	-8.752109	0.169878	-0.399750
5	6	0	-8.682998	1.355091	0.332832
6	6	0	-7.451646	1.875075	0.737648
7	6	0	-4.845251	1.481272	0.667933
8	6	0	-4.165855	0.292167	-0.003113
9	1	0	-7.659623	-1.450999	-1.315226
10	1	0	-9.718039	-0.219139	-0.704810
11	1	0	-9.597339	1.879329	0.591283
12	1	0	-7.407182	2.800170	1.304231
13	7	0	-5.074795	-0.491238	-0.563977
14	6	0	-4.857574	-1.674142	-1.403157
15	1	0	-5.569807	-1.603536	-2.228078
16	1	0	-3.860902	-1.592123	-1.836609
17	6	0	-2.749870	0.157813	0.010428
18	1	0	-2.234327	1.071408	0.274330
19	6	0	-2.019752	-0.987015	-0.145469
20	1	0	-2.552729	-1.926010	-0.240697
21	6	0	2.989905	-0.388177	-0.031564
22	6	0	3.278361	1.065271	-0.092440
23	6	0	3.013828	1.895106	0.999171
24	6	0	3.820290	1.645593	-1.240102
25	6	0	3.285724	3.253011	0.955881
26	1	0	2.597735	1.471414	1.909202
27	6	0	4.076465	3.006041	-1.309275
28	1	0	4.038943	1.024995	-2.104892
29	6	0	3.811915	3.854252	-0.210334
30	1	0	3.081338	3.848717	1.836320
31	1	0	4.490247	3.407259	-2.225586
32	7	0	4.050774	5.205700	-0.274351
33	6	0	4.754391	5.757050	-1.418273
34	1	0	4.838049	6.836551	-1.296730
35	1	0	5.766849	5.342079	-1.523932
36	1	0	4.207199	5.569039	-2.347968
37	6	0	3.928428	6.014695	0.924918
38	1	0	4.139676	7.053984	0.674856
39	1	0	2.912077	5.970499	1.330084
40	1	0	4.627790	5.700396	1.712756
41	6	0	-4.405943	2.803278	0.008114
42	1	0	-3.344735	2.999732	0.181891
43	1	0	-4.590318	2.793069	-1.069479
44	1	0	-4.975714	3.626968	0.446372
45	6	0	-4.526585	1.496093	2.174841

46	1	0	-4.821032	0.558009	2.653275
47	1	0	-3.458661	1.655979	2.345815
48	1	0	-5.074431	2.312780	2.652512
49	6	0	0.032013	-2.386579	0.027971
50	6	0	-0.599424	-1.124252	-0.113389
51	6	0	0.429289	-0.145331	-0.204794
52	6	0	1.639326	-0.839370	-0.064004
53	7	0	1.353476	-2.209468	0.062414
54	6	0	4.033617	-1.291238	0.081398
55	6	0	5.453315	-1.097737	0.221947
56	6	0	6.003256	-2.358235	0.323992
57	6	0	4.962911	-3.309349	0.266627
58	7	0	3.794061	-2.675344	0.127319
59	1	0	7.052207	-2.594728	0.444953
60	5	0	2.407425	-3.338136	0.118277
61	6	0	5.091777	-4.789406	0.368606
62	1	0	4.682926	-5.146414	1.319339
63	1	0	4.541169	-5.290375	-0.431735
64	1	0	6.142943	-5.077657	0.313009
65	6	0	6.240297	0.171755	0.285806
66	1	0	6.307501	0.655774	-0.692516
67	1	0	5.790653	0.896017	0.969469
68	1	0	7.256027	-0.046616	0.625085
69	6	0	0.203355	1.302700	-0.505752
70	1	0	-0.022906	1.876983	0.400380
71	1	0	1.071775	1.762569	-0.972572
72	1	0	-0.644900	1.412257	-1.187142
73	6	0	-0.623090	-3.721048	0.157771
74	1	0	-1.032235	-3.850111	1.165854
75	1	0	-1.450415	-3.819065	-0.550165
76	1	0	0.080344	-4.530619	-0.027638
77	6	0	-5.045910	-2.982057	-0.643289
78	1	0	-4.362119	-3.064065	0.205831
79	1	0	-6.065816	-3.076810	-0.262261
80	1	0	-4.855817	-3.818656	-1.320903
81	9	0	2.275361	-4.173542	-1.005802
82	9	0	2.230316	-4.109273	1.278244

10. Molecule 1/ CAM-B3LYP/6-31G(d)/Acetonitrile

1	6	0	4.917110	-0.632312	0.000026
2	6	0	5.075914	0.747922	0.000053
3	6	0	6.320752	1.357532	0.000131
4	6	0	7.436675	0.520035	0.000170
5	6	0	7.297276	-0.867641	0.000134
6	6	0	6.030038	-1.455418	0.000062
7	6	0	3.441964	-0.968428	-0.000039
8	6	0	2.822549	0.429414	-0.000033
9	1	0	6.443911	2.434118	0.000167
10	1	0	8.427985	0.961571	0.000232
11	1	0	8.181516	-1.496731	0.000166
12	1	0	5.927737	-2.536581	0.000039
13	7	0	3.790767	1.346630	-0.000012
14	6	0	3.568890	2.787460	-0.000029
15	1	0	4.528871	3.296493	-0.000401
16	1	0	3.014019	3.081806	-0.893305
17	1	0	3.014605	3.081936	0.893572
18	6	0	1.463476	0.798001	-0.000032
19	1	0	1.235865	1.858722	0.000056
20	6	0	0.399916	-0.074541	-0.000110
21	1	0	0.576691	-1.145298	-0.000206
22	6	0	-0.953851	0.333239	-0.000071
23	1	0	-1.165277	1.399229	0.000019
24	6	0	-1.965554	-0.587597	-0.000130
25	1	0	-1.673036	-1.637530	-0.000216
26	6	0	-3.378834	-0.348831	-0.000083
27	6	0	-4.264296	-1.445952	-0.000137
28	6	0	-3.957473	0.939033	0.000017
29	6	0	-5.632606	-1.285861	-0.000084
30	1	0	-3.855347	-2.453038	-0.000229
31	6	0	-5.320718	1.120800	0.000069
32	1	0	-3.322592	1.819344	0.000059
33	6	0	-6.209658	0.010296	0.000032
34	1	0	-6.262704	-2.165682	-0.000152
35	1	0	-5.711683	2.129954	0.000158
36	7	0	-7.556349	0.186150	0.000107
37	6	0	-8.124632	1.525338	-0.000019
38	1	0	-9.210672	1.449414	-0.000144
39	1	0	-7.822508	2.089551	0.889769
40	1	0	-7.822303	2.089459	-0.889793
41	6	0	-8.445449	-0.964984	0.000152
42	1	0	-9.476947	-0.616996	0.000505
43	1	0	-8.295323	-1.587313	-0.889570
44	1	0	-8.294828	-1.587582	0.889594
45	6	0	3.071673	-1.754798	-1.273104

46	1	0	2.010652	-2.009886	-1.299460
47	1	0	3.313078	-1.183783	-2.173640
48	1	0	3.642779	-2.686822	-1.295903
49	6	0	3.071576	-1.754876	1.272947
50	1	0	3.312862	-1.183893	2.173535
51	1	0	2.010565	-2.010016	1.299184
52	1	0	3.642720	-2.686876	1.295762

11. Molecule 2/ CAM-B3LYP/6-31G(d)/Acetonitrile

1	6	0	0.903255	0.000036	0.000018
2	6	0	-0.559324	0.000022	-0.000007
3	6	0	-1.275220	1.210430	0.103726
4	6	0	-1.275179	-1.210412	-0.103710
5	7	0	-2.666077	-1.232773	-0.071723
6	6	0	-0.831716	-2.532807	-0.314059
7	7	0	-2.666120	1.232738	0.071768
8	6	0	-0.831814	2.532830	0.314173
9	6	0	-1.959424	-3.343257	-0.386093
10	6	0	3.016538	0.890417	-0.816692
11	6	0	3.016521	-0.890350	0.816768
12	9	0	-4.408436	0.060973	-1.137720
13	5	0	-3.585288	-0.000029	-0.000047
14	6	0	-1.959555	3.343226	0.386287
15	6	0	3.755268	0.000039	0.000048
16	6	0	-3.067714	-2.502162	-0.238791
17	6	0	-3.067807	2.502120	0.238763
18	6	0	1.635298	0.893447	-0.799897
19	6	0	1.635281	-0.893382	0.799942
20	9	0	-4.408633	-0.061052	1.137479
21	6	0	5.849813	-0.943019	0.828855
22	7	0	5.119357	0.000065	0.000052
23	6	0	5.849742	0.942970	-0.829015
24	1	0	0.197517	-2.843251	-0.419205
25	1	0	-1.990970	-4.412671	-0.540361
26	1	0	0.197404	2.843301	0.419388
27	1	0	3.527537	1.579760	-1.476474
28	1	0	3.527499	-1.579696	1.476558
29	1	0	-1.991146	4.412622	0.540675
30	1	0	-4.120563	-2.750715	-0.260113
31	1	0	1.109126	1.576235	-1.459042
32	1	0	-4.120665	2.750640	0.260027
33	1	0	1.109094	-1.576183	1.459061
34	1	0	6.918103	-0.802237	0.671020
35	1	0	5.602245	-1.979965	0.572107
36	1	0	5.640459	-0.791879	1.895000
37	1	0	6.918046	0.802232	-0.671233
38	1	0	5.602185	1.979962	-0.572457
39	1	0	5.640297	0.791611	-1.895114

12. Molecule 3/ CAM-B3LYP/6-31G(d)/Acetonitrile

1	6	0	-6.292179	1.186809	0.402358
2	6	0	-6.390313	0.008504	-0.324429
3	6	0	-7.600815	-0.530585	-0.729019
4	6	0	-8.752871	0.170169	-0.371639
5	6	0	-8.676440	1.356792	0.357977
6	6	0	-7.441174	1.877010	0.750512
7	6	0	-4.835813	1.480506	0.659466
8	6	0	-4.163424	0.288919	-0.014427
9	1	0	-7.669279	-1.453214	-1.293557
10	1	0	-9.721728	-0.218947	-0.667118
11	1	0	-9.588106	1.882021	0.623780
12	1	0	-7.391025	2.803179	1.314851
13	7	0	-5.077707	-0.494264	-0.566223
14	6	0	-4.869016	-1.681431	-1.401448
15	1	0	-5.589686	-1.615479	-2.219298
16	1	0	-3.876894	-1.601729	-1.845682
17	6	0	-2.747380	0.151976	-0.009045
18	1	0	-2.229356	1.065156	0.251322
19	6	0	-2.019023	-0.993558	-0.166057
20	1	0	-2.552450	-1.932289	-0.260821
21	6	0	2.989021	-0.387310	-0.035421
22	6	0	3.274430	1.066686	-0.094663
23	6	0	2.998032	1.896295	0.994230
24	6	0	3.824324	1.647969	-1.238010
25	6	0	3.267508	3.254808	0.953096
26	1	0	2.573943	1.471860	1.900183
27	6	0	4.077872	3.008979	-1.305441
28	1	0	4.051080	1.027824	-2.101005
29	6	0	3.802952	3.856748	-0.208642
30	1	0	3.053808	3.850471	1.831388
31	1	0	4.497209	3.411180	-2.218786
32	7	0	4.040835	5.208256	-0.270821
33	6	0	4.751828	5.760605	-1.409704
34	1	0	4.836707	6.839699	-1.285583
35	1	0	5.764143	5.344073	-1.510197
36	1	0	4.209946	5.575014	-2.343084
37	6	0	3.903067	6.018410	0.925918
38	1	0	4.114492	7.057911	0.676937
39	1	0	2.882382	5.972072	1.319831
40	1	0	4.594384	5.706852	1.721877
41	6	0	-4.399993	2.800479	-0.006732
42	1	0	-3.337067	2.995601	0.157586
43	1	0	-4.593493	2.788182	-1.082704
44	1	0	-4.964837	3.625928	0.434650
45	6	0	-4.505661	1.497813	2.163850

46	1	0	-4.799306	0.561618	2.646515
47	1	0	-3.436069	1.654700	2.326699
48	1	0	-5.047401	2.317327	2.643625
49	6	0	0.034738	-2.391354	0.012578
50	6	0	-0.598174	-1.130355	-0.133551
51	6	0	0.429158	-0.150135	-0.223073
52	6	0	1.640003	-0.841674	-0.075426
53	7	0	1.356024	-2.212000	0.052127
54	6	0	4.034304	-1.288186	0.084818
55	6	0	5.452324	-1.091502	0.234304
56	6	0	6.004458	-2.350979	0.340727
57	6	0	4.966782	-3.304215	0.277397
58	7	0	3.797295	-2.672691	0.130165
59	1	0	7.053124	-2.585128	0.468640
60	5	0	2.411945	-3.337908	0.117143
61	6	0	5.098412	-4.784002	0.380431
62	1	0	4.672933	-5.143947	1.322655
63	1	0	4.564976	-5.285711	-0.431116
64	1	0	6.151379	-5.068576	0.343916
65	6	0	6.236656	0.179424	0.302714
66	1	0	6.311326	0.662073	-0.675726
67	1	0	5.780379	0.903834	0.981734
68	1	0	7.249959	-0.036876	0.650545
69	6	0	0.202573	1.296845	-0.528526
70	1	0	-0.027641	1.872966	0.375382
71	1	0	1.072303	1.756549	-0.993070
72	1	0	-0.643144	1.403708	-1.213456
73	6	0	-0.618315	-3.726740	0.142827
74	1	0	-1.018140	-3.860299	1.154084
75	1	0	-1.451842	-3.822653	-0.557873
76	1	0	0.083995	-4.535042	-0.052515
77	6	0	-5.049417	-2.984835	-0.631821
78	1	0	-4.357692	-3.060870	0.211351
79	1	0	-6.065757	-3.077765	-0.240915
80	1	0	-4.864940	-3.825464	-1.305977
81	9	0	2.287050	-4.178916	-1.003837
82	9	0	2.230941	-4.104936	1.279581