

## Supplementary Information

### CO<sub>2</sub>-assisted propane aromatization over phosphorous-modified Ga/ZSM-5 catalysts

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#### ■ Propane conversion over HZSM-5

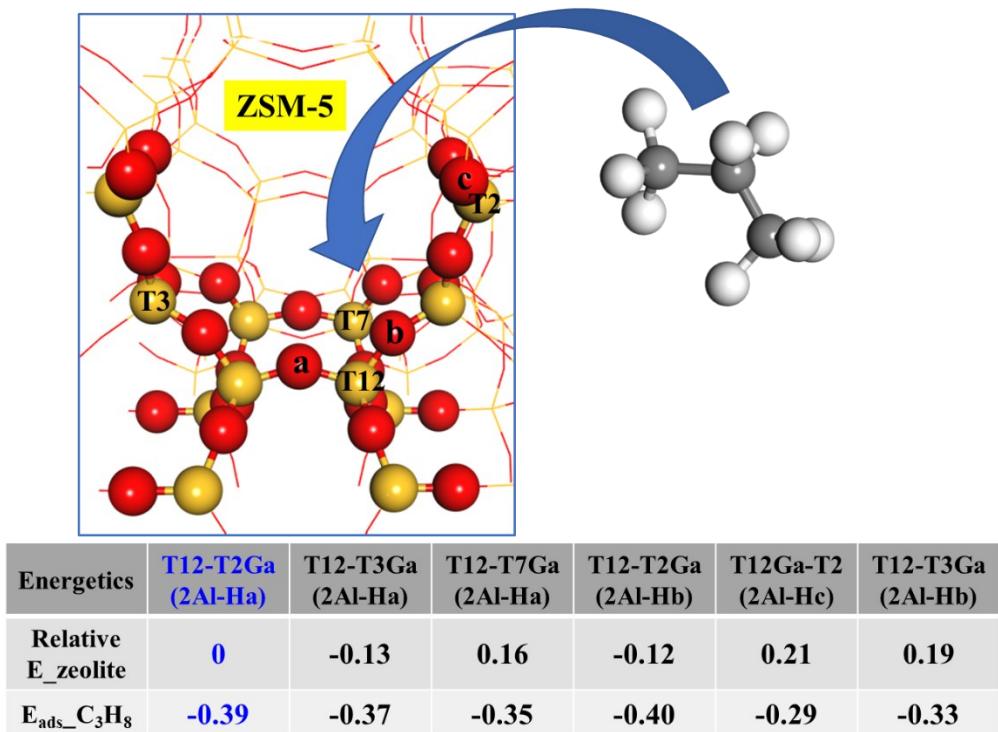
On HZSM-5, the cracking products (41.4% CH<sub>4</sub> and 30.1% C<sub>2</sub>) dominated the products distribution, and only a small amount of propene (10.3%) and liquid aromatics (16.5%) were obtained, as shown in **Table 1**. These results indicated that the C-C bond scission was more facile than C-H bond activation of propane molecule catalyzed by the Brønsted acid site of HZSM-5. To gain insight into the mechanism and kinetics of propane conversion over HZSM-5, DFT studies were performed on propane cracking and dehydrogenation.

As shown in **Figure S7**, the propane molecule was adsorbed above the Brønsted acid site of HZSM-5, and simultaneously interacted with the framework O atom. The H<sub>zeolite</sub>-C and H-O<sub>zeolite</sub> interatomic distances in propane adsorption state were 2.50 and 2.38 Å, respectively, and the adsorption energy was calculated to be -0.65 eV. Catalyzed by the Brønsted acid site, one of the C-C bonds in propane was activated to cleave, resulting in the formation of an ethoxide (C<sub>2</sub>H<sub>5</sub>O) species and a CH<sub>4</sub> molecule. In the transition state, the C-C bond length was elongated to 2.06 from 1.53 Å in the adsorbed state, generating a C<sub>2</sub>H<sub>5</sub> carbonium species; while the H<sub>zeolite</sub>-C distance was calculated to be 1.19 Å, showing the tendency of forming CH<sub>4</sub> molecule. Then, the formed CH<sub>4</sub> desorbed from the zeolite acid site, with the C<sub>2</sub>H<sub>5</sub>O species retained for subsequent dehydrogenation. Finally, an ethylene molecule was produced via H

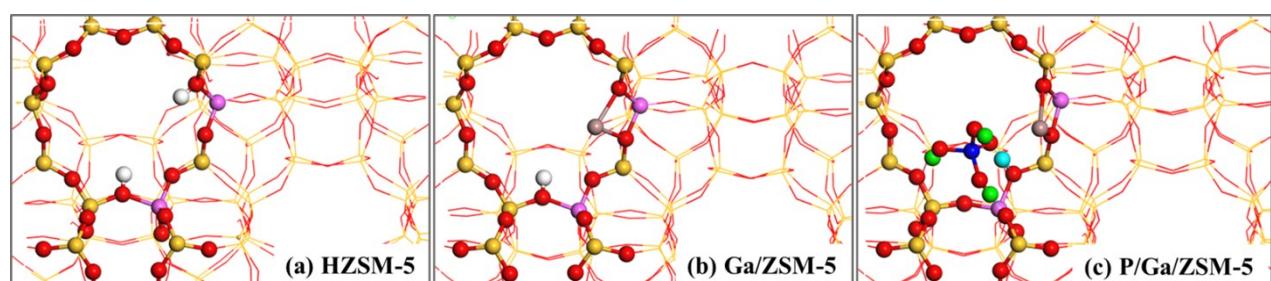
transfer from  $\text{C}_2\text{H}_5\text{O}$  to the framework O of ZSM-5. The C-H and H-O<sub>zeolite</sub> distances were 1.29 and 2.11 Å, respectively, in the transition state configuration. Ethylene adsorbed at the Brønsted acid site through H-π interaction and the calculated H-C distances were 2.33 and 2.18 Å, respectively. The energy diagram of propane cracking to produce methane and ethylene over HZSM-5 was plotted in **Figure S8**, in which the formation of  $\text{CH}_4$  had an activation barrier of 1.62 eV while ethylene formation from the dehydrogenation of  $\text{C}_2\text{H}_5\text{O}$  species needed to overcome a barrier of 1.43 eV. The desorption energy of ethylene was 0.87 eV.

For comparison, the dehydrogenation of propane to propene over HZSM-5 was examined, and the optimized structures of all states involved in the path are illustrated in **Figure S9**. Instead of activating the C-C bond, one of the C-H bonds in propane molecule was activated by the interaction of Brønsted acid site. A  $\text{H}_2$  molecule was produced in the first step from one H of  $\text{C}_3\text{H}_8$  with the Brønsted acid proton, concurrently generating a  $\text{C}_3\text{H}_7\text{O}$  species bound to the ZSM-5 framework. The C-H bond in the transition state of  $\text{H}_2$  formation step was activated to 1.88 from 1.10 Å in the adsorbed state while the H<sub>zeolite</sub>-O<sub>zeolite</sub> distance was elongated to 1.91 Å, and the H-H bond length was optimized to 0.87 Å. Once the  $\text{C}_3\text{H}_7\text{O}$  species was formed, it went through a dehydrogenation step to produce a propane molecule, concerted with the regeneration of the Brønsted acid site of HZSM-5. The C-H and H-O<sub>zeolite</sub> distances were 1.14 and 1.76 Å, respectively in the transition state, with the  $\text{C}_3\text{H}_6\ldots\text{H}$  species moved upward relative to the framework O, as shown in **Figure S9**. In propene adsorption state via the H-π interaction, the H<sub>zeolite</sub>-C distances were calculated to be 1.96 and 2.52 Å, respectively, resulting in an adsorption energy of -1.32 eV. As illustrated in **Figure S8**, the  $\text{H}_2$  formation step had a higher barrier (2.11 eV) than that (0.40 eV) of the dehydrogenation of  $\text{C}_3\text{H}_7\text{O}$  species, indicating that the C-H bond activation of propane by the Brønsted acid site proceeded slowly over HZSM-5.

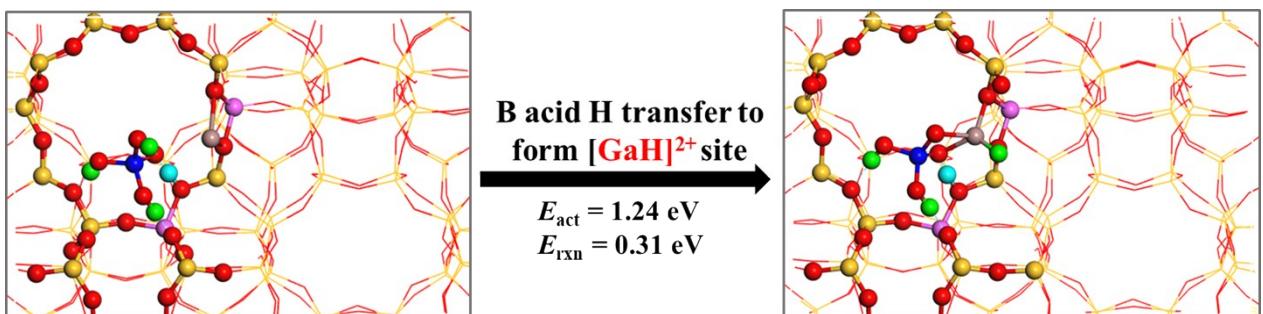
Comparing the energy diagrams between propane cracking and dehydrogenation over HZSM-5, the cracking reaction was found to be kinetically more favorable due to lower barriers, and methane would be the dominate product, as evidenced in **Figure S8**. These DFT calculations are consistent with the experimental results given in **Table 1** in the manuscript.



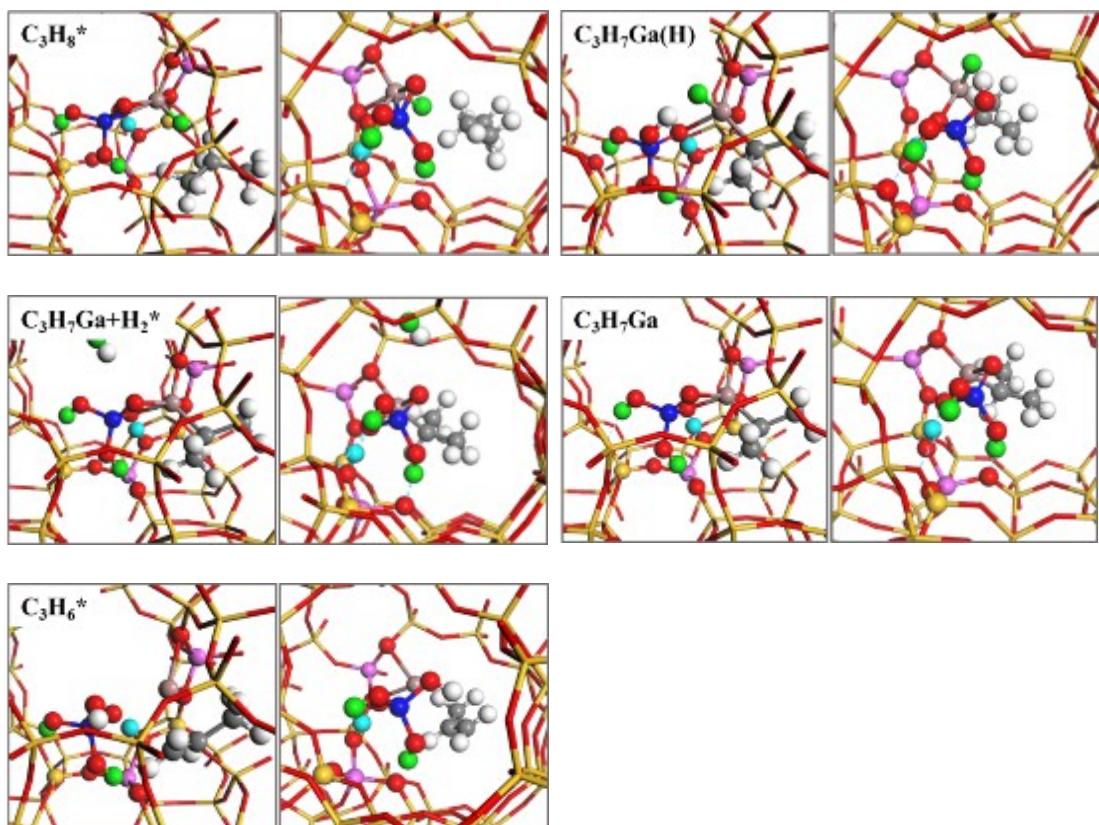
**Figure S1.** Relative stabilities of Ga/ZSM-5 catalysts with different Al substitution T sites and different Ga, H locations. Adsorption energies of C<sub>3</sub>H<sub>8</sub> on these different Ga/ZSM-5 catalysts. T12-T2Ga (2Al-Ha) was the model used in this work. (Yellow: Si, Red: O, Grey: C, White: H).



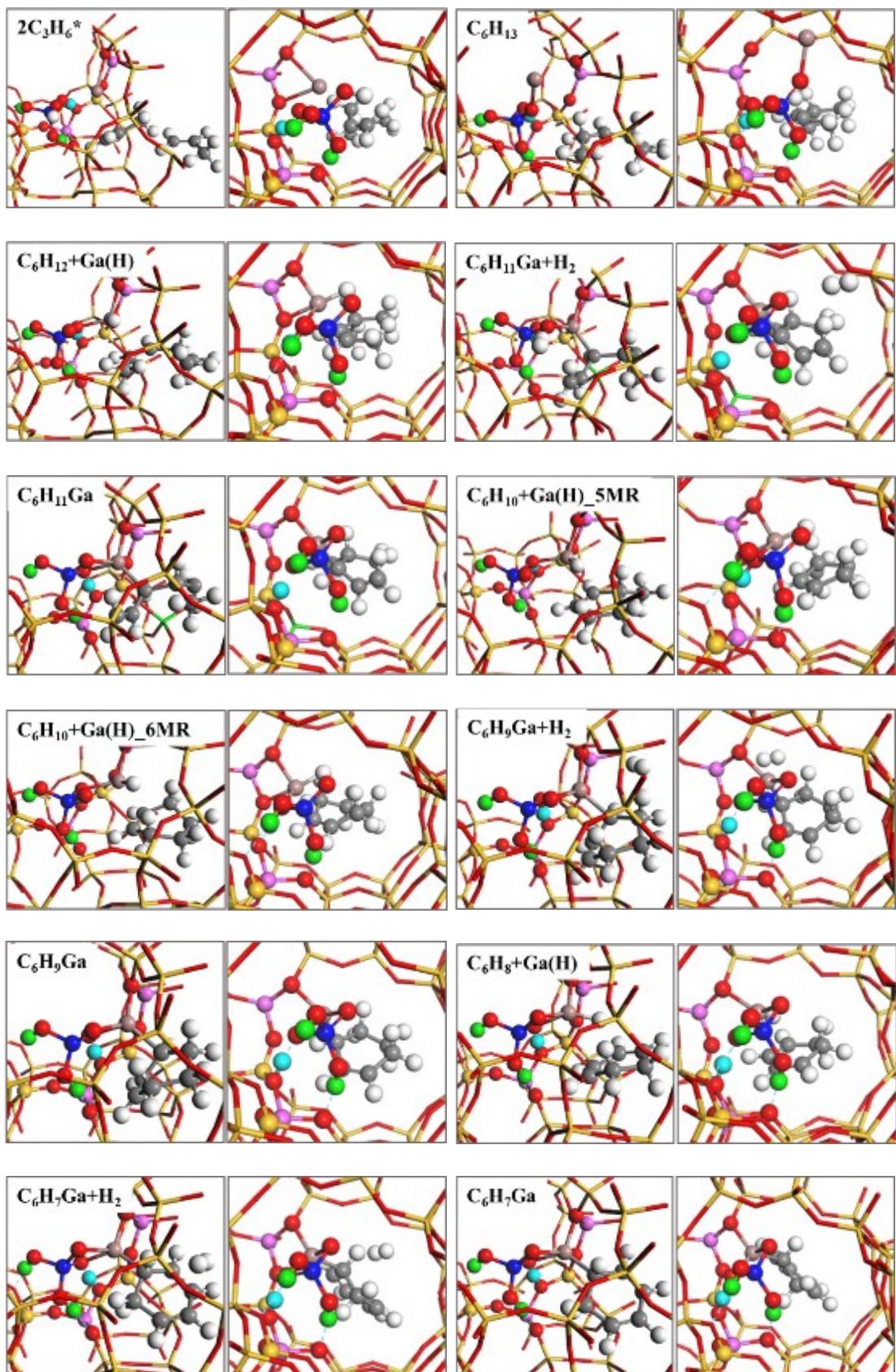
**Figure S2.** Optimized structures of (a) HZSM-5, (b) Ga/ZSM-5 and (c) P/Ga/ZSM-5 (Yellow: Si, Pink: Al, Brown: Ga, Red: O, White: H, Bright green: H of H<sub>3</sub>PO<sub>4</sub>, Bright blue: H of ZSM-5, Dark blue: P).

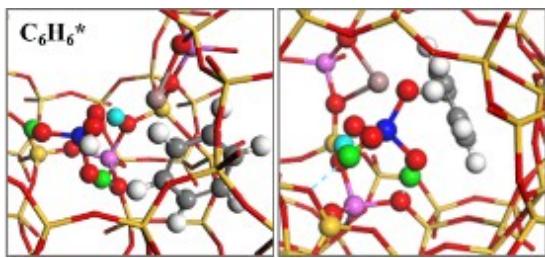


**Figure S3.** Transfer of the Brønsted acid proton to form new  $[\text{GaH}]^{2+}$  active site for propane dehydrogenation to propene over P/Ga/ZSM-5 (Yellow: Si, Pink: Al, Brown: Ga, Red: O, Bright green: H of  $\text{H}_3\text{PO}_4$ , Bright blue: H of ZSM-5, Dark blue: P).

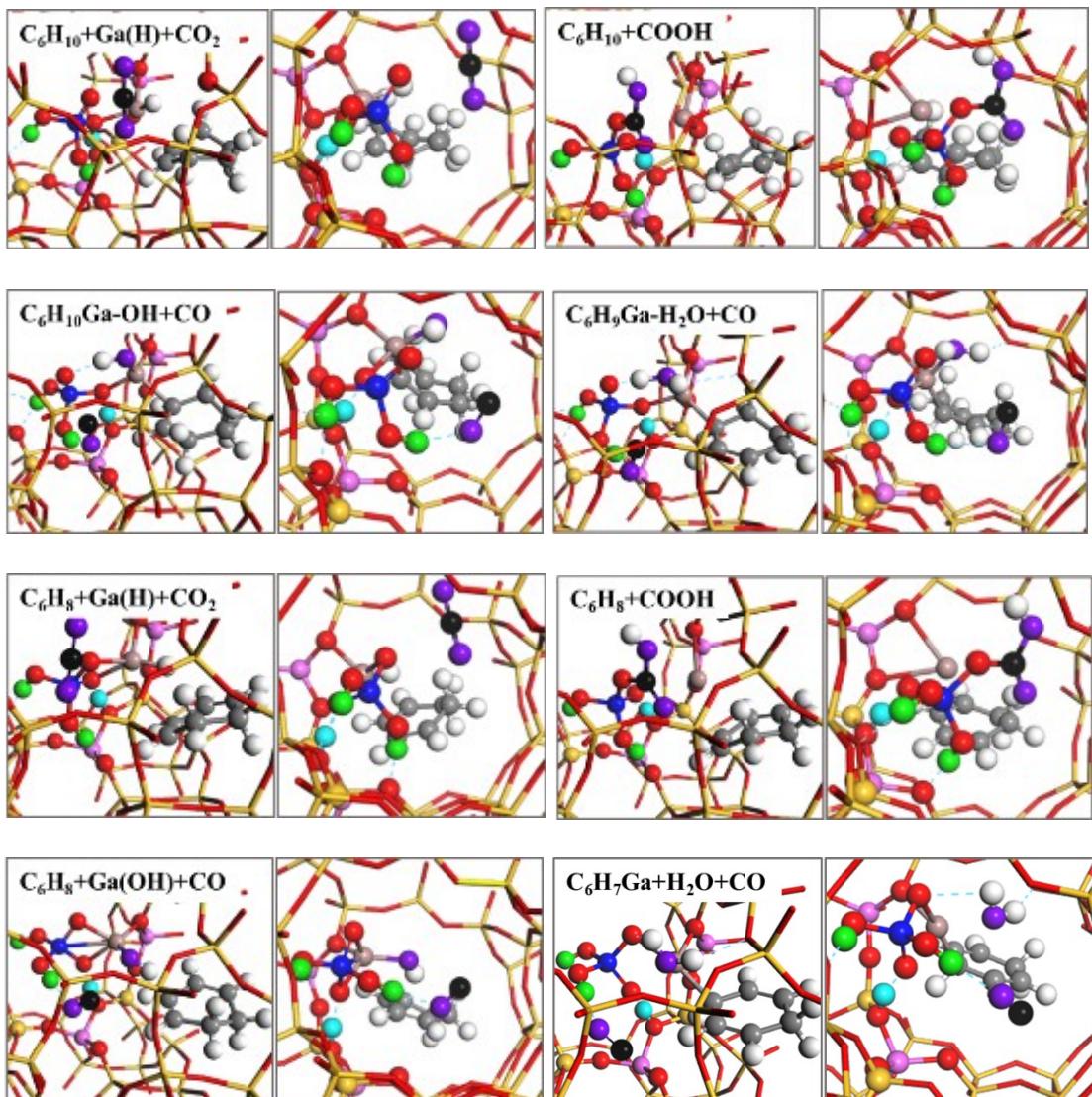


**Figure S4.** Optimized structures of reactant, intermediates, and product associated with propane dehydrogenation to propene over P/Ga/ZSM-5 (Yellow: Si, Pink: Al, Brown: Ga, Red: O, Grey: C, White: H, Bright green: H of  $\text{H}_3\text{PO}_4$ , Bright blue: H of ZSM-5, Dark blue: P).

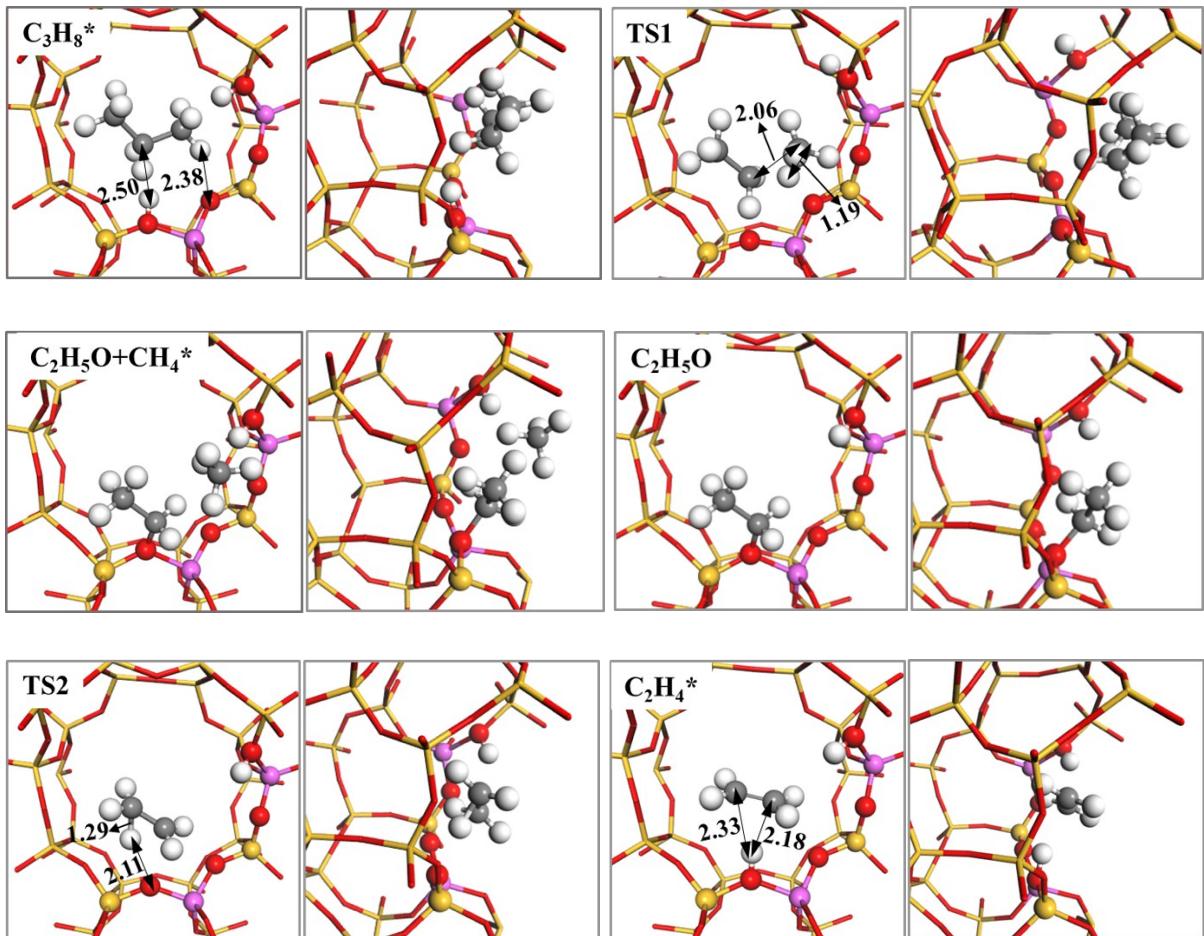




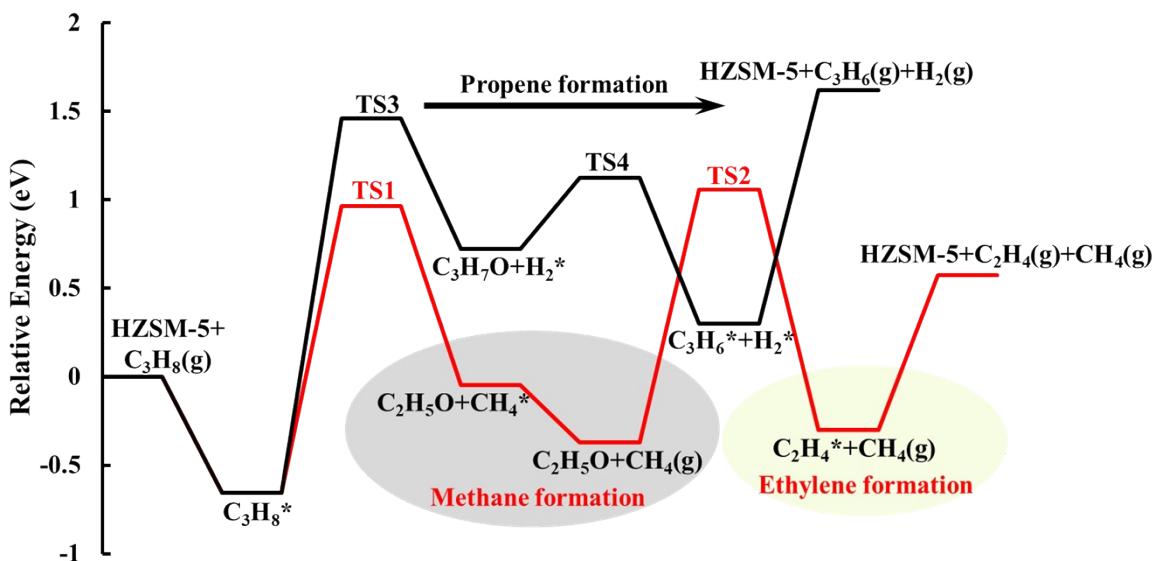
**Figure S5.** Optimized structures of reactant, intermediates, and product associated with propene aromatization to benzene over P/Ga/ZSM-5 (Yellow: Si, Pink: Al, Brown: Ga, Red: O, Grey: C, White: H, Bright green: H of  $\text{H}_3\text{PO}_4$ , Bright blue: H of ZSM-5, Dark blue: P).



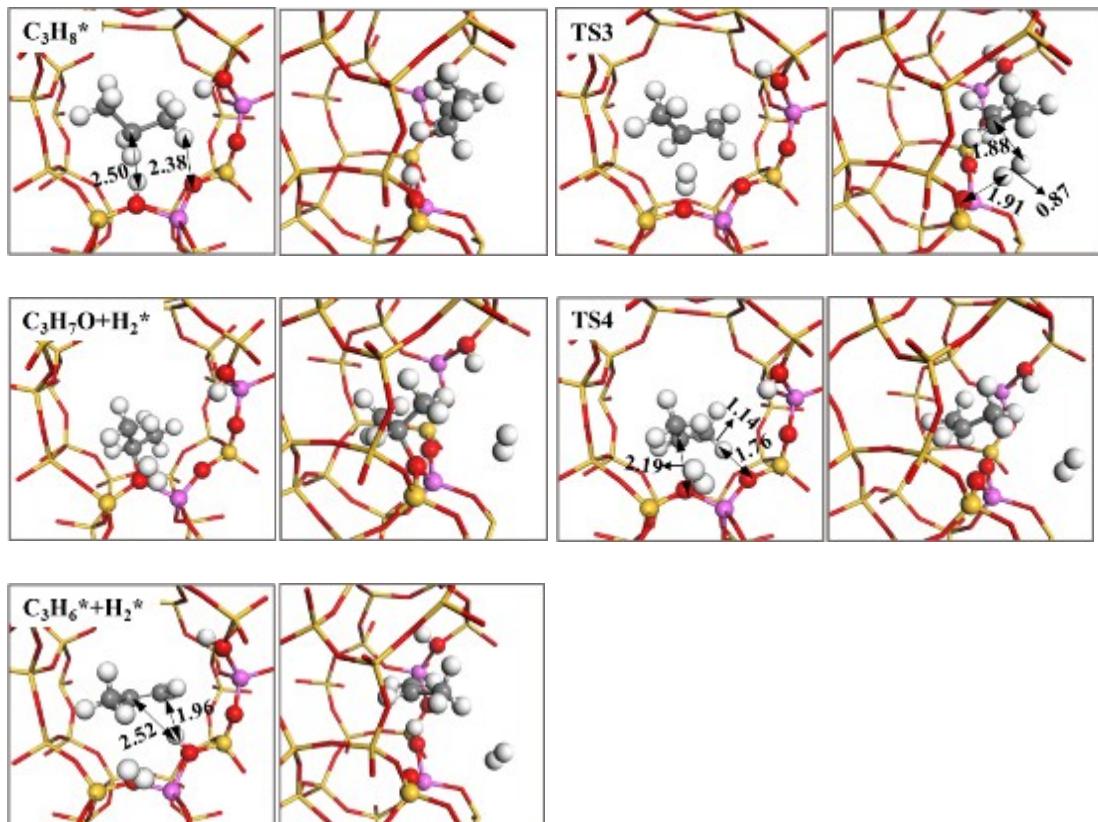
**Figure S6.** Optimized structures of reactant, intermediates and product associated with dehydrogenation of  $\text{C}_6\text{H}_{10}+\text{Ga}(\text{H})$  and  $\text{C}_6\text{H}_8+\text{Ga}(\text{H})$  species in benzene production over P/Ga/ZSM-5 in the presence of  $\text{CO}_2$ . (Yellow: Si, Pink: Al, Brown: Ga, Red: O, Grey: C, White: H, Bright green: H of  $\text{H}_3\text{PO}_4$ , Bright blue: H of ZSM-5, Dark blue: P, Black: C of  $\text{CO}_2$ , Purple: O of  $\text{CO}_2$ ).



**Figure S7.** Optimized structures of reactant, intermediates, transition states, and product associated with propane cracking to methane and ethylene over HZSM-5 (Yellow: Si, Pink: Al, Red: O, White: H, Grey: C).



**Figure S8.** Energy diagrams of propane cracking to methane and ethylene as well as propane dehydrogenation to propene over HZSM-5. (The optimized structures of all states involved in the two conversion pathways are provided in **Figure S6** and **Figure S8**, respectively).



**Figure S9.** Optimized structures of reactant, intermediate, transition states, and product associated with propane dehydrogenation to propene reaction over HZSM-5 (Yellow: Si, Pink: Al, Red: O, White: H, Grey: C).

**Table S1.** TGA results of spent catalysts normalized by propane conversion.

Catalyst	Treatment	Weight loss/%
P/Ga/ZSM-5	C <sub>3</sub> -CO <sub>2</sub>	10.0
	C <sub>3</sub> -Ar	10.3
Ga/ZSM-5	C <sub>3</sub> -CO <sub>2</sub>	41.3
	C <sub>3</sub> -Ar	30.5

Note: The spent catalysts were those underwent 14 hours on stream.

**Table S2.** Structure files in fractional coordinates for all computed structures.

<b>a) structures involved in propane dehydrogenation to propene over P/Ga/ZSM-5 (states shown in Fig. 4)</b>			
<b>P/Ga/ZSM-5 (Brønsted acid site)</b>			
SI2	0.42228	0.05905	0.64956
SI3	0.30639	0.03057	0.79768
SI4	0.28048	0.05785	0.01897
SI5	0.12157	0.06398	0.01352
SI6	0.06697	0.02994	0.80187
SI7	0.18234	0.06125	0.66829
SI8	0.42115	0.82742	0.67445
SI9	0.30364	0.87129	0.81013
SI10	0.26748	0.83066	0.02887
SI11	0.11273	0.82748	0.01753
SI12	0.06541	0.87221	0.80325
SI13	0.18187	0.82753	0.67467
SI14	0.07722	0.94227	0.15369
SI15	0.19466	0.97059	0.29831
SI16	0.21856	0.93985	0.52093
SI17	0.37889	0.93352	0.516
SI18	0.43417	0.96903	0.30559
SI19	0.31953	0.93915	0.16874
SI20	0.08243	0.17333	0.16741
SI21	0.19597	0.13	0.30959
SI22	0.23272	0.17019	0.52592
SI23	0.38738	0.17369	0.51018
SI24	0.43568	0.12715	0.29844
SI25	0.31648	0.17023	0.17337
SI26	0.58017	0.55826	0.34812
SI27	0.69011	0.53408	0.19178

SI28	0.71714	0.55892	0.97472
SI29	0.87558	0.56607	0.98371
SI30	0.93163	0.53077	0.19384
SI31	0.81295	0.55559	0.32272
SI32	0.57867	0.32923	0.3273
SI33	0.69452	0.3765	0.18811
SI34	0.73031	0.32852	0.97256
SI35	0.88471	0.32738	0.9845
SI36	0.93667	0.37254	0.19483
SI37	0.92454	0.44272	0.84963
SI38	0.78018	0.43867	0.4804
SI39	0.62016	0.43288	0.48884
SI40	0.56382	0.4692	0.70006
SI41	0.67698	0.43615	0.83337
SI42	0.91784	0.67565	0.82978
SI43	0.8024	0.63778	0.69164
SI44	0.76499	0.66677	0.4722
SI45	0.61011	0.67246	0.48782
SI46	0.56185	0.62696	0.70064
SI47	0.68123	0.67557	0.82205
SI48	0.57959	0.94211	0.35625
SI49	0.69272	0.96666	0.20581
SI50	0.7218	0.94028	0.98651
SI51	0.88046	0.93592	0.99278
SI52	0.93306	0.96882	0.20195
SI53	0.8168	0.94155	0.34062
SI54	0.57829	0.17384	0.32741
SI55	0.69551	0.12292	0.19436
SI56	0.73445	0.16849	0.97594
SI57	0.88872	0.17317	0.98056
SI58	0.9384	0.12639	0.19192
SI59	0.81956	0.16553	0.32317
SI60	0.92358	0.05469	0.85219
SI61	0.80322	0.02432	0.70696
SI62	0.78292	0.06265	0.4871
SI63	0.62182	0.07094	0.48788
SI64	0.56769	0.03242	0.69846
SI65	0.68022	0.05733	0.84187
SI66	0.92028	0.82795	0.83372
SI67	0.80367	0.86429	0.68761
SI68	0.76783	0.82498	0.47064
SI69	0.61351	0.82619	0.49193
SI70	0.56543	0.87488	0.70146
SI71	0.683	0.83021	0.82847

SI72	0.41921	0.44235	0.64911
SI73	0.30603	0.46948	0.79774
SI74	0.28364	0.44173	0.02119
SI75	0.1255	0.43598	0.01356
SI76	0.07254	0.47146	0.80381
SI77	0.18428	0.44156	0.66384
SI78	0.41975	0.67354	0.67293
SI79	0.30231	0.62806	0.80694
SI80	0.26651	0.67012	0.02543
SI81	0.11187	0.67406	0.01464
SI82	0.06315	0.62946	0.80353
SI83	0.17985	0.66983	0.67228
SI84	0.07596	0.55686	0.14747
SI85	0.19387	0.52862	0.29287
SI86	0.21899	0.5619	0.51297
SI87	0.37903	0.56879	0.51168
SI88	0.43523	0.53187	0.30229
SI89	0.32068	0.56114	0.16616
SI90	0.08291	0.32673	0.16493
SI91	0.19573	0.36938	0.30864
SI92	0.23235	0.33044	0.52625
SI93	0.38692	0.32785	0.51147
SI94	0.43451	0.37437	0.29859
SI95	0.31706	0.32803	0.17347
O96	0.35845	0.06796	0.72328
O97	0.31685	0.05829	0.91049
O98	0.20064	0.0474	0.00569
O99	0.08892	0.06895	0.90323
O100	0.10549	0.06165	0.70622
O101	0.23009	0.04653	0.76407
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O103	0.30558	0.85537	0.92849
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O140	0.64259	0.57107	0.27332
O141	0.67966	0.56712	0.08211
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O145	0.7678	0.54633	0.22314
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O147	0.69239	0.34899	0.07441
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O192	0.81233	0.14506	0.98183
O193	0.91964	0.16832	0.09208
O194	0.89644	0.1562	0.28562
O195	0.76907	0.12732	0.24655
O196	0.6708	0.04524	0.19883
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O200	0.59509	0.13857	0.43392
O201	0.80197	0.86566	0.37869
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O205	0.01767	0.13524	0.21424
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O220	0.9326	0.1281	0.90369
O221	0.92034	0.99745	0.93922
O222	0.89418	0.8663	0.93346
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O224	0.68662	0.00428	0.93329
O225	0.70909	0.87228	0.92401
O226	0.48885	0.04719	0.71596
O227	0.48588	0.86545	0.7217
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O234	0.357	0.67356	0.74952
O235	0.3044	0.64721	0.92411
O236	0.18866	0.64723	0.01812
O237	0.08523	0.67305	0.90037
O238	0.10248	0.65797	0.70577
O239	0.22804	0.64241	0.76191
O240	0.32199	0.54946	0.79239
O241	0.08364	0.55125	0.82208
O242	0.43197	0.37425	0.58472
O243	0.40544	0.50399	0.57289
O244	0.39831	0.63769	0.56899
O245	0.19707	0.36598	0.62209
O246	0.19921	0.49509	0.57582
O247	0.19384	0.6293	0.56929

O248	0.99415	0.45432	0.78857
O249	0.98319	0.63601	0.78585
O250	0.14131	0.56477	0.21816
O251	0.18274	0.55801	0.40468
O252	0.29895	0.56366	0.49837
O253	0.41454	0.5713	0.40354
O254	0.39631	0.56523	0.20837
O255	0.27007	0.54346	0.25779
O256	0.13893	0.32571	0.25246
O257	0.19135	0.35262	0.42691
O258	0.30969	0.3542	0.51605
O259	0.41386	0.3323	0.3978
O260	0.39431	0.34322	0.20351
O261	0.26974	0.35003	0.26743
O262	0.1801	0.44824	0.2895
O263	0.41479	0.45296	0.31354
O264	0.06605	0.62594	0.08434
O265	0.08295	0.49424	0.06976
O266	0.11262	0.36356	0.06594
O267	0.30155	0.63376	0.11987
O268	0.3185	0.50276	0.08166
O269	0.29747	0.36972	0.07364
O270	0.51459	0.54029	0.28205
O271	0.51411	0.36714	0.2789
O272	0.44005	0.75045	0.64764
O273	0.19405	0.74864	0.65071
O274	0.2728	0.7502	0.04117
O275	0.10769	0.75042	0.05634
O276	0.06352	0.24993	0.13681
O277	0.30664	0.2492	0.14849
O278	0.22706	0.25036	0.54276
O279	0.39152	0.25066	0.54943
O280	0.56001	0.25148	0.34977
O281	0.80202	0.24288	0.33804
O282	0.72903	0.24805	0.95751
O283	0.89093	0.25075	0.94385
O284	0.93922	0.75122	0.86374
O285	0.6858	0.75229	0.86184
O286	0.77034	0.74582	0.44386
O287	0.60637	0.74998	0.45065
O288	0.97353	0.27806	0.42596
O289	0.92483	0.18282	0.53597
O290	0.8827	0.30423	0.55715
O291	-0.00055	0.26578	0.60792

GA29	0.93106	0.4247	0.60883
H293	0.94579	0.30406	0.37349
H294	0.83645	0.33458	0.4964
H295	0.88328	0.16567	0.50369
H296	0.03831	0.29043	0.58386
AL29	0.81689	0.32685	0.31879
AL29	0.80153	0.47651	0.70654
P299	0.94115	0.25938	0.52848
<b>TS0</b>			
SI2	0.42292	0.05919	0.64914
SI3	0.30668	0.03046	0.79705
SI4	0.28087	0.05774	0.01863
SI5	0.12191	0.06348	0.0135
SI6	0.06718	0.0294	0.80164
SI7	0.18223	0.06101	0.66762
SI8	0.42124	0.82731	0.67473
SI9	0.30346	0.87122	0.80969
SI10	0.26734	0.83072	0.02868
SI11	0.11269	0.82753	0.01761
SI12	0.06537	0.87161	0.8029
SI13	0.1818	0.82712	0.67441
SI14	0.07718	0.94213	0.15392
SI15	0.19492	0.97062	0.29795
SI16	0.21858	0.93943	0.52091
SI17	0.37908	0.93354	0.51629
SI18	0.43436	0.96896	0.30563
SI19	0.31998	0.9392	0.16819
SI20	0.08298	0.17323	0.16675
SI21	0.19636	0.12996	0.30926
SI22	0.23251	0.1704	0.5258
SI23	0.38704	0.17367	0.51004
SI24	0.43591	0.12739	0.29835
SI25	0.31684	0.17	0.17311
SI26	0.58015	0.55925	0.34658
SI27	0.6888	0.53328	0.1908
SI28	0.71596	0.55849	0.97381
SI29	0.874	0.56536	0.98037
SI30	0.93211	0.53033	0.19081
SI31	0.81286	0.55684	0.32012
SI32	0.58059	0.32948	0.32726
SI33	0.69402	0.376	0.18524
SI34	0.73016	0.32813	0.97119
SI35	0.88451	0.32654	0.98438

SI36	0.93729	0.37193	0.19495
SI37	0.92522	0.44101	0.8469
SI38	0.78166	0.43723	0.47522
SI39	0.62278	0.43506	0.4879
SI40	0.56411	0.46924	0.6985
SI41	0.67784	0.4352	0.83088
SI42	0.91772	0.67566	0.82782
SI43	0.80369	0.63768	0.68774
SI44	0.76468	0.66762	0.46898
SI45	0.61002	0.67285	0.48648
SI46	0.56208	0.62717	0.69993
SI47	0.68206	0.67527	0.82006
SI48	0.57959	0.94249	0.35831
SI49	0.69372	0.96681	0.20932
SI50	0.72177	0.93904	0.98984
SI51	0.88066	0.93571	0.99434
SI52	0.93295	0.96935	0.20351
SI53	0.81805	0.94354	0.34552
SI54	0.57842	0.17419	0.33047
SI55	0.69629	0.12254	0.19785
SI56	0.73445	0.16808	0.97883
SI57	0.88874	0.1726	0.98156
SI58	0.93886	0.12673	0.19265
SI59	0.8204	0.16556	0.32536
SI60	0.92382	0.054	0.85333
SI61	0.80252	0.02427	0.70883
SI62	0.78327	0.06492	0.48917
SI63	0.62232	0.07132	0.48896
SI64	0.5688	0.03195	0.69984
SI65	0.67953	0.05537	0.84695
SI66	0.92033	0.82809	0.83552
SI67	0.80361	0.86535	0.68849
SI68	0.76795	0.82532	0.47235
SI69	0.61365	0.82657	0.49383
SI70	0.56539	0.87422	0.70345
SI71	0.68327	0.83065	0.82975
SI72	0.41894	0.44221	0.64874
SI73	0.30601	0.46936	0.79739
SI74	0.28367	0.44134	0.02117
SI75	0.12567	0.43604	0.01266
SI76	0.07342	0.4719	0.80278
SI77	0.18449	0.44249	0.66181
SI78	0.42022	0.67346	0.67191
SI79	0.30262	0.62757	0.80564

SI80	0.26639	0.67033	0.02413
SI81	0.11194	0.67426	0.01362
SI82	0.06336	0.6298	0.80287
SI83	0.18005	0.66923	0.67073
SI84	0.07594	0.55674	0.14552
SI85	0.19403	0.52821	0.29079
SI86	0.21898	0.56255	0.51064
SI87	0.37915	0.56895	0.51094
SI88	0.43533	0.53149	0.30122
SI89	0.32112	0.56084	0.16431
SI90	0.08345	0.32647	0.16397
SI91	0.19634	0.36913	0.30806
SI92	0.23204	0.33045	0.52585
SI93	0.38662	0.32779	0.51082
SI94	0.43536	0.37391	0.2983
SI95	0.31781	0.32784	0.17367
O96	0.35933	0.06767	0.7234
O97	0.31674	0.05836	0.90983
O98	0.201	0.04677	0.00642
O99	0.08957	0.06802	0.90301
O100	0.10546	0.06124	0.706
O101	0.23048	0.04627	0.7629
O102	0.361	0.82721	0.7557
O103	0.30529	0.85504	0.92799
O104	0.18952	0.85416	0.02318
O105	0.08655	0.83152	0.90344
O106	0.10442	0.83868	0.70802
O107	0.23015	0.85184	0.76545
O108	0.31976	0.94998	0.79024
O109	0.08589	0.95018	0.81332
O110	0.43201	0.12721	0.58341
O111	0.41393	0.99596	0.57389
O112	0.39733	0.86366	0.57217
O113	0.1995	0.1343	0.62206
O114	0.19097	0.00319	0.58347
O115	0.19731	0.86899	0.57306
O116	0.98772	0.03927	0.78215
O117	0.98528	0.86464	0.78623
O118	0.14228	0.93299	0.22488
O119	0.18562	0.94194	0.41032
O120	0.2991	0.9447	0.5141
O121	0.40783	0.92906	0.40361
O122	0.39671	0.93997	0.20719
O123	0.27104	0.95569	0.26221

O124	0.14142	0.17436	0.2504
O125	0.19145	0.14808	0.42677
O126	0.31007	0.14706	0.51327
O127	0.41488	0.17053	0.39646
O128	0.39431	0.15429	0.20173
O129	0.27086	0.14792	0.26831
O130	0.18028	0.05086	0.29198
O131	0.41897	0.04876	0.31895
O132	0.06645	0.87364	0.08963
O133	0.08527	0.00477	0.0772
O134	0.10974	0.13555	0.06689
O135	0.30338	0.86507	0.12428
O136	0.31132	0.99551	0.08175
O137	0.29556	0.12882	0.07354
O138	0.51385	0.95659	0.2907
O139	0.51508	0.13786	0.27592
O140	0.64203	0.57233	0.27094
O141	0.67753	0.56515	0.08044
O142	0.79546	0.55056	0.99455
O143	0.91121	0.56797	0.08768
O144	0.89033	0.56011	0.28488
O145	0.76659	0.54475	0.22236
O146	0.64028	0.33049	0.24636
O147	0.6902	0.35115	0.07002
O148	0.80797	0.35363	0.97637
O149	0.91136	0.32969	0.09828
O150	0.90207	0.34139	0.29481
O151	0.76814	0.3678	0.22891
O152	0.66956	0.45414	0.19244
O153	0.91771	0.4504	0.17873
O154	0.56665	0.62803	0.40867
O155	0.59593	0.49915	0.42523
O156	0.60496	0.36578	0.43017
O157	0.79428	0.62676	0.37436
O158	0.80388	0.49415	0.39691
O159	0.80228	0.36235	0.43753
O160	0.01047	0.54467	0.2148
O161	0.01793	0.36542	0.20644
O162	0.87188	0.42995	0.75299
O163	0.82608	0.44889	0.57931
O164	0.70345	0.443	0.50189
O165	0.58795	0.43191	0.59655
O166	0.59997	0.43721	0.79589
O167	0.72528	0.44808	0.73599

O168	0.86244	0.68212	0.73984
O169	0.80835	0.64883	0.5673
O170	0.68708	0.64616	0.48765
O171	0.57825	0.66679	0.59706
O172	0.6047	0.66059	0.79027
O173	0.73005	0.66446	0.723
O174	0.81513	0.5606	0.71836
O175	0.58225	0.54865	0.68811
O176	0.93128	0.3734	0.91296
O177	0.90474	0.5042	0.91421
O178	0.88724	0.63608	0.92393
O179	0.6932	0.36089	0.87564
O180	0.68904	0.49209	0.91706
O181	0.70377	0.62646	0.91073
O182	0.48453	0.45881	0.71474
O183	0.48281	0.63481	0.72459
O184	0.64256	0.92901	0.2845
O185	0.69245	0.92914	0.10189
O186	0.80159	0.95374	0.99148
O187	0.90548	0.92608	0.10883
O188	0.89442	0.94827	0.30555
O189	0.7692	0.96328	0.25329
O190	0.64324	0.16849	0.25839
O191	0.69903	0.1497	0.08408
O192	0.81232	0.14463	0.9839
O193	0.92004	0.16881	0.0928
O194	0.89686	0.15596	0.2863
O195	0.7696	0.12527	0.25079
O196	0.67095	0.04491	0.19813
O197	0.9207	0.04805	0.17694
O198	0.56755	0.87582	0.42606
O199	0.59277	0.00561	0.43261
O200	0.59297	0.1389	0.43783
O201	0.80318	0.86753	0.3831
O202	0.80789	0.99518	0.43848
O203	0.81949	0.13014	0.4376
O204	0.01167	0.95433	0.22298
O205	0.01824	0.13552	0.21429
O206	0.8567	0.05428	0.78614
O207	0.8067	0.06645	0.6051
O208	0.70308	0.07131	0.47875
O209	0.60009	0.07245	0.60526
O210	0.60411	0.05592	0.80301
O211	0.72841	0.03207	0.75615

O212	0.86045	0.82929	0.75475
O213	0.80884	0.83624	0.57584
O214	0.69127	0.85121	0.48739
O215	0.58843	0.82837	0.609
O216	0.60637	0.85042	0.80241
O217	0.7298	0.8492	0.73352
O218	0.81729	0.94567	0.68731
O219	0.58152	0.95244	0.6792
O220	0.9325	0.12748	0.90477
O221	0.92095	0.99694	0.94071
O222	0.89626	0.86571	0.9369
O223	0.69799	0.13003	0.88656
O224	0.68418	0.00287	0.9395
O225	0.7079	0.87099	0.92777
O226	0.48997	0.04774	0.71463
O227	0.48578	0.86499	0.72331
O228	0.35639	0.42958	0.72355
O229	0.31318	0.43848	0.90861
O230	0.20388	0.4563	0.02059
O231	0.10358	0.43008	0.89634
O232	0.10718	0.44921	0.69778
O233	0.22963	0.45875	0.75979
O234	0.35696	0.67302	0.74742
O235	0.30398	0.64883	0.92198
O236	0.18861	0.6471	0.01676
O237	0.08524	0.67391	0.89929
O238	0.10275	0.65752	0.70483
O239	0.22849	0.64011	0.7589
O240	0.32369	0.54908	0.79453
O241	0.08315	0.55167	0.82304
O242	0.43177	0.37438	0.58393
O243	0.40411	0.50411	0.57344
O244	0.39989	0.63777	0.56737
O245	0.19827	0.36693	0.62185
O246	0.19956	0.49551	0.57299
O247	0.1929	0.62982	0.56652
O248	0.99468	0.45471	0.78909
O249	0.98338	0.6364	0.7847
O250	0.14154	0.56414	0.21563
O251	0.18321	0.5586	0.40202
O252	0.29905	0.56556	0.49708
O253	0.41501	0.57027	0.40309
O254	0.39644	0.56546	0.20776
O255	0.2702	0.54263	0.25523

O256	0.14041	0.32537	0.25
O257	0.19138	0.35227	0.42604
O258	0.30955	0.35418	0.51458
O259	0.41426	0.33218	0.39748
O260	0.39542	0.34243	0.20307
O261	0.27083	0.35047	0.26768
O262	0.18003	0.44791	0.28872
O263	0.41518	0.45254	0.31158
O264	0.06595	0.62596	0.08277
O265	0.08196	0.4942	0.06734
O266	0.11183	0.36364	0.06434
O267	0.30182	0.6333	0.11766
O268	0.31995	0.5025	0.0796
O269	0.29802	0.36955	0.07389
O270	0.51471	0.54007	0.28118
O271	0.51531	0.36731	0.28079
O272	0.44045	0.75046	0.64747
O273	0.19465	0.74821	0.65124
O274	0.27238	0.75027	0.04156
O275	0.10787	0.75038	0.05621
O276	0.06411	0.24976	0.13556
O277	0.30676	0.24905	0.14883
O278	0.22772	0.25045	0.54301
O279	0.39142	0.25068	0.54909
O280	0.56144	0.25226	0.35284
O281	0.80088	0.24269	0.33512
O282	0.72876	0.24754	0.95794
O283	0.89031	0.25006	0.94366
O284	0.93838	0.75082	0.86378
O285	0.68907	0.75199	0.85857
O286	0.76983	0.74674	0.44175
O287	0.60658	0.75068	0.45111
O288	0.95605	0.26438	0.42442
O289	0.92158	0.19147	0.56849
O290	0.87827	0.31296	0.56118
O291	0.99779	0.29061	0.60362
GA29	0.91365	0.40745	0.61939
H293	0.93833	0.29906	0.37355
H294	0.84253	0.32742	0.50476
H295	0.88956	0.16894	0.52295
H296	0.98508	0.36838	0.60565
AL29	0.81546	0.32683	0.31639
AL29	0.80165	0.47689	0.70303
P299	0.94222	0.2648	0.53854

**P/Ga/ZSM-5 ([GaH]<sup>2+</sup> site)**

SI2	0.42306	0.05921	0.64909
SI3	0.30677	0.03046	0.79698
SI4	0.28085	0.05765	0.01859
SI5	0.12192	0.06314	0.01341
SI6	0.06709	0.02913	0.80155
SI7	0.18222	0.06081	0.6675
SI8	0.42132	0.82727	0.6749
SI9	0.30346	0.87122	0.80968
SI10	0.26727	0.83078	0.02869
SI11	0.11267	0.82749	0.01779
SI12	0.06519	0.87117	0.80292
SI13	0.18182	0.8269	0.67448
SI14	0.07709	0.94201	0.15408
SI15	0.19494	0.97053	0.29799
SI16	0.21863	0.93915	0.52095
SI17	0.37914	0.93348	0.5164
SI18	0.43436	0.96892	0.30571
SI19	0.32004	0.9392	0.16816
SI20	0.0832	0.17307	0.16646
SI21	0.19646	0.12986	0.30925
SI22	0.23253	0.17039	0.52584
SI23	0.38707	0.17372	0.51007
SI24	0.4359	0.12732	0.29834
SI25	0.31686	0.16987	0.17309
SI26	0.57902	0.55972	0.34572
SI27	0.68836	0.53334	0.19045
SI28	0.71548	0.5583	0.97422
SI29	0.87343	0.5632	0.97737
SI30	0.93218	0.5292	0.18939
SI31	0.81271	0.55804	0.31752
SI32	0.58066	0.32932	0.32705
SI33	0.69419	0.37577	0.18474
SI34	0.73001	0.32771	0.97142
SI35	0.8844	0.3263	0.98637
SI36	0.93747	0.37074	0.19765
SI37	0.92579	0.43844	0.84454
SI38	0.77946	0.44142	0.47515
SI39	0.62062	0.4358	0.48662
SI40	0.56452	0.46935	0.69832
SI41	0.67957	0.43496	0.8307
SI42	0.91746	0.67483	0.8272
SI43	0.80454	0.63491	0.68733

SI44	0.76471	0.66725	0.46897
SI45	0.60995	0.67293	0.48592
SI46	0.56232	0.62733	0.69959
SI47	0.68268	0.67433	0.81942
SI48	0.57956	0.94254	0.35864
SI49	0.69402	0.96679	0.20998
SI50	0.72172	0.93844	0.99022
SI51	0.88069	0.93549	0.99456
SI52	0.93284	0.96945	0.20414
SI53	0.81821	0.94353	0.34653
SI54	0.57843	0.17403	0.33078
SI55	0.69667	0.1226	0.19842
SI56	0.73453	0.16774	0.97922
SI57	0.88874	0.17244	0.98209
SI58	0.93897	0.12697	0.19341
SI59	0.82075	0.16563	0.3266
SI60	0.92383	0.05394	0.85366
SI61	0.80254	0.02425	0.70917
SI62	0.78333	0.06505	0.48968
SI63	0.6224	0.0713	0.48923
SI64	0.56901	0.03168	0.70008
SI65	0.67952	0.05481	0.84754
SI66	0.92014	0.82752	0.83602
SI67	0.80367	0.8657	0.68875
SI68	0.76792	0.82519	0.47301
SI69	0.61369	0.8266	0.4941
SI70	0.5655	0.87388	0.70394
SI71	0.68353	0.83038	0.82968
SI72	0.41939	0.44223	0.64925
SI73	0.30626	0.46922	0.79734
SI74	0.28378	0.4412	0.02124
SI75	0.12598	0.43612	0.01258
SI76	0.07436	0.47165	0.80258
SI77	0.18496	0.44282	0.66079
SI78	0.42048	0.6734	0.67175
SI79	0.30278	0.62736	0.80531
SI80	0.26623	0.67042	0.02374
SI81	0.11181	0.67424	0.01346
SI82	0.06337	0.62963	0.80276
SI83	0.18015	0.66891	0.67036
SI84	0.07565	0.55657	0.14481
SI85	0.19386	0.52798	0.29004
SI86	0.2192	0.56279	0.50972
SI87	0.37943	0.56889	0.51102

SI88	0.43517	0.53162	0.30053
SI89	0.32095	0.56073	0.16341
SI90	0.08376	0.3262	0.16373
SI91	0.19655	0.36893	0.30789
SI92	0.23225	0.3304	0.52566
SI93	0.38693	0.32793	0.51075
SI94	0.4357	0.3738	0.29788
SI95	0.31798	0.32769	0.17372
O96	0.35954	0.06767	0.72351
O97	0.31669	0.05842	0.90976
O98	0.201	0.04644	0.00637
O99	0.0896	0.06767	0.90292
O100	0.10543	0.061	0.70594
O101	0.23059	0.04629	0.76265
O102	0.361	0.82719	0.75575
O103	0.30519	0.85515	0.92801
O104	0.18945	0.85431	0.02333
O105	0.08659	0.83145	0.90361
O106	0.10443	0.8384	0.70811
O107	0.23015	0.8519	0.76539
O108	0.31982	0.94999	0.79022
O109	0.08541	0.94986	0.81305
O110	0.43209	0.12725	0.58334
O111	0.41396	0.99599	0.57381
O112	0.39753	0.86369	0.57236
O113	0.19919	0.13414	0.62178
O114	0.19093	0.00295	0.58342
O115	0.19725	0.86873	0.57304
O116	0.98764	0.03942	0.78216
O117	0.98516	0.86378	0.78634
O118	0.14221	0.93294	0.22503
O119	0.18575	0.94172	0.4103
O120	0.29913	0.94451	0.51442
O121	0.40774	0.929	0.40364
O122	0.39675	0.93994	0.20721
O123	0.27104	0.95577	0.2621
O124	0.1416	0.17423	0.25016
O125	0.19148	0.14819	0.4267
O126	0.31009	0.14706	0.51359
O127	0.4147	0.1705	0.39635
O128	0.39434	0.15411	0.20157
O129	0.27098	0.14773	0.2684
O130	0.18021	0.05079	0.29222
O131	0.41895	0.04871	0.31902

O132	0.06633	0.87348	0.08987
O133	0.08518	0.00457	0.07722
O134	0.10974	0.1352	0.06672
O135	0.30338	0.86509	0.12428
O136	0.31145	0.9955	0.08168
O137	0.29534	0.12875	0.07358
O138	0.51385	0.95655	0.29087
O139	0.51511	0.1377	0.2761
O140	0.642	0.57161	0.27185
O141	0.67607	0.5648	0.08014
O142	0.79493	0.55067	0.9959
O143	0.91305	0.56329	0.08283
O144	0.8898	0.56163	0.28088
O145	0.76616	0.54626	0.22008
O146	0.64119	0.33041	0.24752
O147	0.68943	0.3504	0.06999
O148	0.80784	0.35328	0.97754
O149	0.9106	0.32892	0.10084
O150	0.90286	0.34012	0.29816
O151	0.76897	0.36726	0.2262
O152	0.67018	0.45393	0.19268
O153	0.91753	0.44913	0.18226
O154	0.56631	0.62861	0.40785
O155	0.59153	0.49906	0.42457
O156	0.60413	0.36575	0.4302
O157	0.79429	0.62739	0.37328
O158	0.80325	0.49439	0.39241
O159	0.79669	0.36414	0.43361
O160	0.0103	0.54418	0.21411
O161	0.01819	0.36453	0.20726
O162	0.87613	0.4235	0.74665
O163	0.82372	0.44837	0.5761
O164	0.70092	0.44636	0.49789
O165	0.58719	0.43185	0.596
O166	0.60204	0.43731	0.79395
O167	0.72938	0.4469	0.73881
O168	0.86222	0.68109	0.73921
O169	0.8081	0.64714	0.56688
O170	0.68692	0.64604	0.48677
O171	0.57822	0.66685	0.59653
O172	0.60505	0.6608	0.78975
O173	0.73054	0.66069	0.72317
O174	0.81809	0.55809	0.71745
O175	0.58232	0.5488	0.68758

O176	0.9317	0.37319	0.91571
O177	0.90027	0.50243	0.90628
O178	0.88742	0.63451	0.92302
O179	0.69304	0.36038	0.87609
O180	0.68906	0.49177	0.91745
O181	0.70326	0.62653	0.91182
O182	0.48498	0.45871	0.71548
O183	0.4831	0.63499	0.7247
O184	0.64261	0.92913	0.28495
O185	0.69299	0.9289	0.1027
O186	0.80156	0.95332	0.99092
O187	0.9051	0.92642	0.10938
O188	0.89456	0.94821	0.30633
O189	0.76939	0.96345	0.25432
O190	0.64345	0.16829	0.25909
O191	0.6992	0.14965	0.08463
O192	0.81242	0.14422	0.98429
O193	0.92001	0.16868	0.09338
O194	0.8974	0.15691	0.28728
O195	0.77009	0.1259	0.25109
O196	0.67149	0.04493	0.19861
O197	0.92053	0.04831	0.17843
O198	0.56753	0.87597	0.42659
O199	0.59263	0.00572	0.43285
O200	0.59286	0.13891	0.43832
O201	0.80323	0.86749	0.38389
O202	0.80824	0.99516	0.4396
O203	0.81967	0.13005	0.43821
O204	0.01161	0.95433	0.22311
O205	0.01844	0.13567	0.21457
O206	0.85672	0.05435	0.78643
O207	0.80635	0.06706	0.60589
O208	0.70313	0.07125	0.47847
O209	0.60066	0.07219	0.60576
O210	0.60415	0.05564	0.80341
O211	0.72851	0.03134	0.75695
O212	0.86005	0.82947	0.75565
O213	0.80881	0.83611	0.57644
O214	0.69129	0.8513	0.48775
O215	0.58847	0.8282	0.60929
O216	0.60643	0.84977	0.80281
O217	0.72965	0.85077	0.73382
O218	0.81796	0.94594	0.68656
O219	0.58167	0.95213	0.67976

O220	0.93256	0.12739	0.90526
O221	0.92099	0.99676	0.94085
O222	0.89672	0.86538	0.93764
O223	0.69806	0.12942	0.88724
O224	0.68389	0.00219	0.94002
O225	0.70756	0.87015	0.92869
O226	0.49017	0.0477	0.71436
O227	0.48584	0.86487	0.72373
O228	0.35692	0.42933	0.72409
O229	0.31251	0.43784	0.90833
O230	0.20407	0.45651	0.02228
O231	0.10549	0.43002	0.89567
O232	0.10782	0.45005	0.69698
O233	0.23013	0.45919	0.7586
O234	0.35705	0.67279	0.74693
O235	0.30371	0.64926	0.92139
O236	0.18848	0.6471	0.0167
O237	0.08526	0.67394	0.89905
O238	0.10295	0.65709	0.70477
O239	0.22874	0.6394	0.75802
O240	0.32421	0.5489	0.79536
O241	0.08273	0.55145	0.82367
O242	0.43196	0.37448	0.58405
O243	0.40409	0.50419	0.5742
O244	0.40053	0.63775	0.56702
O245	0.19844	0.36702	0.62148
O246	0.2001	0.49541	0.57148
O247	0.19274	0.62985	0.56578
O248	0.99606	0.45246	0.78955
O249	0.98354	0.63636	0.78418
O250	0.14127	0.56368	0.21489
O251	0.18358	0.55894	0.401
O252	0.29933	0.56608	0.49685
O253	0.41528	0.56968	0.40316
O254	0.39591	0.5657	0.2077
O255	0.2699	0.54205	0.25382
O256	0.14095	0.32494	0.2494
O257	0.19147	0.35187	0.4258
O258	0.30974	0.35408	0.51424
O259	0.41478	0.33241	0.3975
O260	0.39561	0.34207	0.203
O261	0.27114	0.35044	0.26783
O262	0.17991	0.44765	0.28887
O263	0.41571	0.45249	0.31077

O264	0.06575	0.62601	0.08258
O265	0.08163	0.49427	0.0661
O266	0.11164	0.36379	0.06419
O267	0.30174	0.63325	0.11701
O268	0.32065	0.5025	0.07848
O269	0.2982	0.36946	0.07404
O270	0.51415	0.54151	0.27863
O271	0.51557	0.36693	0.2796
O272	0.44051	0.75047	0.64746
O273	0.19477	0.74798	0.65156
O274	0.27221	0.75034	0.04149
O275	0.10788	0.75033	0.05625
O276	0.06452	0.24955	0.1348
O277	0.30673	0.24892	0.1489
O278	0.22766	0.25042	0.5433
O279	0.39155	0.25075	0.54893
O280	0.56144	0.25215	0.35262
O281	0.80113	0.24287	0.33733
O282	0.72897	0.24712	0.95803
O283	0.89031	0.25	0.94478
O284	0.93752	0.75006	0.86393
O285	0.69076	0.75145	0.85589
O286	0.76993	0.74656	0.44285
O287	0.60668	0.75085	0.45095
O288	0.96137	0.27027	0.44443
O289	0.92059	0.19953	0.58664
O290	0.87006	0.31914	0.55988
O291	0.97929	0.31051	0.6295
GA29	0.92084	0.3973	0.61989
H293	0.9425	0.30027	0.38957
H294	0.82568	0.33818	0.48977
H295	0.8947	0.17297	0.53777
H296	0.96707	0.44836	0.56706
AL29	0.81601	0.32613	0.3132
AL29	0.8054	0.47395	0.69958
P299	0.93505	0.27392	0.55433
<b>C<sub>3</sub>H<sub>8</sub>*</b>			
SI2	0.42591	0.05796	0.64677
SI3	0.30832	0.027	0.79146
SI4	0.28295	0.05549	0.01448
SI5	0.12388	0.06081	0.0131
SI6	0.06951	0.02877	0.80235
SI7	0.18204	0.05606	0.6602

SI8	0.42229	0.82511	0.67527
SI9	0.30631	0.86907	0.81066
SI10	0.26929	0.82986	0.03029
SI11	0.11502	0.82551	0.01777
SI12	0.06647	0.87085	0.80422
SI13	0.18359	0.82709	0.67571
SI14	0.0782	0.94113	0.15175
SI15	0.19796	0.97186	0.29631
SI16	0.21998	0.93625	0.51719
SI17	0.38026	0.93275	0.51679
SI18	0.43554	0.96641	0.30734
SI19	0.32331	0.94081	0.16339
SI20	0.08564	0.17147	0.16784
SI21	0.19984	0.13093	0.31187
SI22	0.2356	0.17148	0.52978
SI23	0.38975	0.17321	0.51035
SI24	0.43831	0.12419	0.30043
SI25	0.32099	0.1655	0.17109
SI26	0.57604	0.5562	0.35433
SI27	0.69294	0.52748	0.20471
SI28	0.71334	0.55948	0.98909
SI29	0.87258	0.56221	0.97895
SI30	0.93214	0.52622	0.19035
SI31	0.81969	0.55255	0.33407
SI32	0.58215	0.32796	0.33362
SI33	0.69737	0.37219	0.18965
SI34	0.73021	0.32506	0.97657
SI35	0.8845	0.32498	0.99403
SI36	0.93837	0.3681	0.20307
SI37	0.92588	0.43656	0.85103
SI38	0.77632	0.43974	0.48426
SI39	0.61788	0.4355	0.4905
SI40	0.5681	0.46921	0.70375
SI41	0.67369	0.44148	0.85389
SI42	0.917	0.67499	0.8311
SI43	0.80642	0.63266	0.69111
SI44	0.76724	0.66697	0.47104
SI45	0.61252	0.67201	0.4875
SI46	0.56466	0.62698	0.70185
SI47	0.68316	0.67031	0.82569
SI48	0.58107	0.94206	0.36147
SI49	0.6983	0.96734	0.21433
SI50	0.72278	0.93378	0.99425
SI51	0.88217	0.93493	0.99738

SI52	0.93395	0.96924	0.20803
SI53	0.82207	0.94359	0.35425
SI54	0.58035	0.17222	0.33646
SI55	0.70007	0.1236	0.20209
SI56	0.7353	0.16782	0.98211
SI57	0.88969	0.17199	0.98593
SI58	0.94081	0.12713	0.1982
SI59	0.82331	0.16623	0.33183
SI60	0.9254	0.05384	0.85715
SI61	0.80319	0.02356	0.71314
SI62	0.78441	0.06476	0.49387
SI63	0.62396	0.06961	0.49286
SI64	0.57123	0.02872	0.70354
SI65	0.67973	0.05072	0.85472
SI66	0.92237	0.82755	0.84056
SI67	0.80411	0.86603	0.69412
SI68	0.77052	0.8237	0.47845
SI69	0.61609	0.82528	0.49657
SI70	0.56657	0.87051	0.70697
SI71	0.68415	0.82771	0.83367
SI72	0.42349	0.44484	0.63871
SI73	0.30502	0.47026	0.7885
SI74	0.28607	0.432	0.00679
SI75	0.12675	0.43176	0.0036
SI76	0.0723	0.46877	0.79506
SI77	0.18276	0.4472	0.64766
SI78	0.4244	0.67063	0.66016
SI79	0.30195	0.62717	0.79529
SI80	0.27096	0.67261	0.01107
SI81	0.11641	0.67165	0.00903
SI82	0.0621	0.62782	0.79907
SI83	0.17863	0.66808	0.66533
SI84	0.07905	0.55207	0.13991
SI85	0.20324	0.52649	0.28356
SI86	0.22335	0.56828	0.50548
SI87	0.38362	0.5697	0.50238
SI88	0.4334	0.52968	0.29026
SI89	0.3267	0.55482	0.13869
SI90	0.08443	0.32573	0.15813
SI91	0.2042	0.36614	0.30217
SI92	0.23509	0.32798	0.52157
SI93	0.38964	0.32722	0.50675
SI94	0.43927	0.3717	0.29345
SI95	0.32499	0.32384	0.16521

O96	0.36129	0.06523	0.71943
O97	0.31263	0.05994	0.902
O98	0.20284	0.0421	0.01301
O99	0.09629	0.06897	0.90008
O100	0.1063	0.05737	0.70313
O101	0.23255	0.03596	0.75048
O102	0.36184	0.82261	0.75604
O103	0.30747	0.852	0.92869
O104	0.19152	0.85324	0.02241
O105	0.08765	0.8303	0.90428
O106	0.10638	0.84006	0.70868
O107	0.2324	0.85369	0.7651
O108	0.32647	0.94731	0.79311
O109	0.08591	0.94942	0.81747
O110	0.4355	0.12683	0.58292
O111	0.41781	0.99565	0.56937
O112	0.39831	0.86374	0.57474
O113	0.19995	0.13039	0.61925
O114	0.18619	0.00094	0.57099
O115	0.19929	0.86653	0.57214
O116	0.98991	0.03996	0.78694
O117	0.98665	0.86219	0.78612
O118	0.14452	0.93783	0.22094
O119	0.19299	0.93342	0.40298
O120	0.30041	0.94573	0.51983
O121	0.40602	0.92529	0.40254
O122	0.3991	0.94047	0.20613
O123	0.27325	0.96375	0.25288
O124	0.14484	0.17344	0.25009
O125	0.19664	0.15702	0.42599
O126	0.31279	0.14697	0.51779
O127	0.41491	0.16927	0.39536
O128	0.39786	0.14749	0.20071
O129	0.27382	0.14444	0.26551
O130	0.18149	0.05147	0.30735
O131	0.42193	0.04607	0.32511
O132	0.0694	0.87013	0.09287
O133	0.08314	0.00143	0.06989
O134	0.11121	0.1318	0.06913
O135	0.30452	0.86579	0.1253
O136	0.31912	0.99314	0.07061
O137	0.29872	0.12571	0.07088
O138	0.51495	0.95317	0.29365
O139	0.5178	0.13514	0.28095

O140	0.64397	0.55872	0.28905
O141	0.68846	0.57235	0.10335
O142	0.79364	0.54576	0.98578
O143	0.90533	0.56273	0.0895
O144	0.8947	0.55643	0.28848
O145	0.76941	0.53096	0.24502
O146	0.64716	0.331	0.26289
O147	0.69111	0.33707	0.08067
O148	0.80773	0.35141	0.98457
O149	0.9092	0.32425	0.10938
O150	0.905	0.34081	0.30644
O151	0.77269	0.36827	0.23039
O152	0.67225	0.45009	0.18275
O153	0.91855	0.44608	0.18209
O154	0.5673	0.62759	0.41159
O155	0.57674	0.49622	0.43766
O156	0.59856	0.36402	0.44023
O157	0.80023	0.62528	0.37938
O158	0.81766	0.49535	0.42199
O159	0.79468	0.36329	0.43903
O160	0.01137	0.54067	0.20396
O161	0.01931	0.36124	0.20793
O162	0.86867	0.42009	0.76313
O163	0.80253	0.43468	0.59828
O164	0.69714	0.45229	0.47436
O165	0.60049	0.43027	0.6081
O166	0.59845	0.43966	0.8069
O167	0.7259	0.46681	0.7719
O168	0.85979	0.68239	0.74606
O169	0.80776	0.65058	0.5726
O170	0.68936	0.64489	0.48477
O171	0.58349	0.66652	0.59982
O172	0.60519	0.66042	0.79431
O173	0.73101	0.64814	0.73304
O174	0.82863	0.55628	0.71056
O175	0.58514	0.54858	0.69098
O176	0.93236	0.37397	0.92739
O177	0.90691	0.50396	0.91042
O178	0.88772	0.63431	0.92737
O179	0.69179	0.36525	0.88896
O180	0.6742	0.49314	0.94903
O181	0.69795	0.62654	0.92508
O182	0.48788	0.45835	0.7087
O183	0.48471	0.63457	0.72225

O184	0.64483	0.93188	0.28835
O185	0.7	0.92605	0.10991
O186	0.80255	0.94817	0.98496
O187	0.90226	0.92811	0.11428
O188	0.89797	0.94724	0.31179
O189	0.77206	0.96441	0.26409
O190	0.64606	0.16582	0.26653
O191	0.70209	0.15626	0.0913
O192	0.81317	0.14409	0.98724
O193	0.92095	0.16746	0.09723
O194	0.9	0.15782	0.2925
O195	0.7732	0.12621	0.25573
O196	0.67727	0.04524	0.19493
O197	0.92215	0.04845	0.18544
O198	0.57066	0.87507	0.42888
O199	0.59138	0.00556	0.43611
O200	0.59417	0.13833	0.44529
O201	0.80742	0.8679	0.39299
O202	0.81364	0.99557	0.44731
O203	0.82092	0.13026	0.44361
O204	0.01297	0.95291	0.22146
O205	0.02055	0.13559	0.21757
O206	0.85917	0.05285	0.7881
O207	0.80358	0.06881	0.61166
O208	0.70444	0.06815	0.47667
O209	0.60549	0.06871	0.61058
O210	0.60498	0.05223	0.8081
O211	0.7305	0.02843	0.76574
O212	0.85964	0.83212	0.76513
O213	0.80909	0.83147	0.5847
O214	0.69376	0.8499	0.49188
O215	0.58987	0.82603	0.61123
O216	0.60658	0.84445	0.80561
O217	0.73005	0.85411	0.7409
O218	0.81871	0.94607	0.68404
O219	0.58325	0.94893	0.68482
O220	0.93342	0.12745	0.90834
O221	0.92163	0.9974	0.94534
O222	0.90427	0.86516	0.94459
O223	0.69701	0.12489	0.89684
O224	0.68273	-0.00319	0.94567
O225	0.70448	0.86461	0.93715
O226	0.49232	0.04592	0.71355
O227	0.48672	0.86181	0.72565

O228	0.35789	0.43986	0.70916
O229	0.30763	0.42583	0.89023
O230	0.20611	0.44448	0.01893
O231	0.10852	0.42871	0.88569
O232	0.10607	0.45021	0.68829
O233	0.23042	0.46524	0.7419
O234	0.35525	0.66224	0.72137
O235	0.30376	0.66748	0.90045
O236	0.19385	0.64608	0.00778
O237	0.08692	0.66986	0.89624
O238	0.10161	0.65527	0.70054
O239	0.22741	0.63208	0.74711
O240	0.32128	0.54869	0.81328
O241	0.07781	0.54865	0.81687
O242	0.43431	0.37436	0.57963
O243	0.41588	0.50422	0.55626
O244	0.41615	0.63728	0.54986
O245	0.19734	0.37234	0.60582
O246	0.19367	0.50109	0.55829
O247	0.19081	0.6352	0.55555
O248	0.9943	0.44545	0.78775
O249	0.98224	0.63747	0.78391
O250	0.1418	0.5535	0.21597
O251	0.20409	0.56772	0.38802
O252	0.30363	0.56944	0.52112
O253	0.40056	0.56943	0.38431
O254	0.40084	0.55674	0.18706
O255	0.27313	0.53918	0.22638
O256	0.14642	0.33195	0.23509
O257	0.19809	0.33586	0.4142
O258	0.31228	0.35294	0.51064
O259	0.4168	0.33081	0.39295
O260	0.40215	0.33927	0.19643
O261	0.27744	0.34861	0.25682
O262	0.1949	0.44688	0.30466
O263	0.41816	0.45003	0.30521
O264	0.07306	0.62344	0.08193
O265	0.08604	0.49263	0.057
O266	0.10411	0.36081	0.05252
O267	0.31287	0.62756	0.08928
O268	0.32451	0.49609	0.05464
O269	0.3066	0.36263	0.0622
O270	0.51283	0.54423	0.28113
O271	0.51963	0.3653	0.27864

O272	0.44158	0.74918	0.64376
O273	0.19529	0.74753	0.65741
O274	0.27431	0.74973	0.04839
O275	0.11166	0.74753	0.0526
O276	0.06794	0.24771	0.13488
O277	0.31389	0.24454	0.14571
O278	0.23204	0.25048	0.55794
O279	0.3953	0.25061	0.54701
O280	0.56264	0.25043	0.35607
O281	0.80282	0.24325	0.34251
O282	0.72969	0.24575	0.9492
O283	0.89141	0.24962	0.94893
O284	0.93827	0.74978	0.86785
O285	0.69579	0.74851	0.85293
O286	0.77247	0.74605	0.44264
O287	0.60915	0.74986	0.45211
O288	0.95	0.26119	0.4627
O289	0.91089	0.18831	0.60175
O290	0.85275	0.30458	0.5734
O291	0.9615	0.30165	0.64907
GA29	0.90171	0.38453	0.63477
H293	0.93846	0.29537	0.4101
H294	0.81511	0.33219	0.49632
H295	0.88532	0.16153	0.55248
H296	0.93868	0.43512	0.56907
H297	0.01034	0.48676	0.55329
H298	0.96341	0.48608	0.44158
H299	0.04025	0.3861	0.4563
H300	0.10978	0.4408	0.45816
H301	0.05948	0.43554	0.34992
H302	0.04912	0.57169	0.37142
H303	0.08336	0.57524	0.49382
H304	-0.00016	0.6003	0.47302
AL30	0.81829	0.32654	0.31876
AL30	0.80099	0.475	0.7156
P307	0.92034	0.26352	0.57122
C308	0.01429	0.4924	0.47167
C309	0.05817	0.43583	0.43194
C310	0.0382	0.5637	0.45077
<b>TS1</b>			
SI2	0.42433	0.05806	0.64757
SI3	0.3061	0.02746	0.79362
SI4	0.28061	0.05857	0.01421

SI5	0.12145	0.0627	0.01448
SI6	0.06802	0.02893	0.80253
SI7	0.1803	0.05721	0.66101
SI8	0.42112	0.8264	0.67353
SI9	0.3054	0.86902	0.8135
SI10	0.26673	0.82919	0.0323
SI11	0.11238	0.82697	0.01807
SI12	0.06608	0.87157	0.80335
SI13	0.18368	0.82801	0.67597
SI14	0.07621	0.94216	0.15374
SI15	0.19548	0.97242	0.29671
SI16	0.2188	0.93863	0.51876
SI17	0.37837	0.93442	0.51713
SI18	0.43143	0.96867	0.30671
SI19	0.3204	0.94324	0.16146
SI20	0.08219	0.17216	0.16841
SI21	0.19521	0.13039	0.31355
SI22	0.23314	0.17214	0.52994
SI23	0.38739	0.17414	0.5118
SI24	0.43485	0.12651	0.30064
SI25	0.31576	0.16749	0.17446
SI26	0.57485	0.5574	0.35276
SI27	0.68679	0.53049	0.19609
SI28	0.71327	0.56257	0.98528
SI29	0.87174	0.56769	0.98037
SI30	0.93235	0.53007	0.18858
SI31	0.81403	0.55322	0.32205
SI32	0.5772	0.32832	0.33088
SI33	0.69338	0.37481	0.18975
SI34	0.72782	0.32468	0.97558
SI35	0.88236	0.32665	0.98696
SI36	0.93522	0.37146	0.1959
SI37	0.92437	0.44245	0.85068
SI38	0.77817	0.43778	0.47505
SI39	0.61839	0.43414	0.48656
SI40	0.57044	0.47062	0.70003
SI41	0.67985	0.43911	0.84595
SI42	0.91774	0.6759	0.82584
SI43	0.80533	0.63435	0.68764
SI44	0.76443	0.66658	0.46864
SI45	0.60964	0.6737	0.48521
SI46	0.56195	0.62818	0.69738
SI47	0.68131	0.6726	0.81981
SI48	0.57767	0.94248	0.36055

SI49	0.69331	0.96625	0.21294
SI50	0.72168	0.93469	0.99272
SI51	0.88121	0.93407	0.99544
SI52	0.93197	0.96887	0.20415
SI53	0.81878	0.9448	0.35209
SI54	0.57747	0.17262	0.33216
SI55	0.69479	0.12133	0.19783
SI56	0.73424	0.16671	0.97923
SI57	0.88914	0.17319	0.98126
SI58	0.93856	0.12562	0.19125
SI59	0.81833	0.16425	0.32409
SI60	0.92362	0.05287	0.85505
SI61	0.80231	0.02329	0.708
SI62	0.78294	0.06677	0.49151
SI63	0.62206	0.07077	0.49068
SI64	0.56942	0.03015	0.7013
SI65	0.67996	0.05082	0.84976
SI66	0.92205	0.82875	0.83528
SI67	0.80294	0.86631	0.68969
SI68	0.76863	0.82337	0.47426
SI69	0.6144	0.82633	0.49409
SI70	0.56602	0.87227	0.70396
SI71	0.68295	0.82965	0.83159
SI72	0.42392	0.4443	0.64595
SI73	0.30454	0.47284	0.79177
SI74	0.2835	0.43465	0.01312
SI75	0.12659	0.43448	0.0137
SI76	0.07644	0.47447	0.80598
SI77	0.18063	0.44771	0.65038
SI78	0.42062	0.67226	0.66379
SI79	0.30142	0.6296	0.80286
SI80	0.26598	0.67228	0.01952
SI81	0.1117	0.67434	0.01124
SI82	0.06326	0.63161	0.80064
SI83	0.17973	0.66999	0.66785
SI84	0.07629	0.5557	0.14372
SI85	0.19752	0.52757	0.28587
SI86	0.21825	0.56565	0.50754
SI87	0.37877	0.56739	0.50894
SI88	0.43053	0.52983	0.29571
SI89	0.32283	0.55401	0.14719
SI90	0.0811	0.32601	0.16115
SI91	0.19661	0.36947	0.30586
SI92	0.23268	0.32953	0.52503

SI93	0.38705	0.32818	0.5109
SI94	0.43432	0.37167	0.2955
SI95	0.31756	0.32604	0.16887
O96	0.3592	0.06329	0.71932
O97	0.30972	0.06466	0.90144
O98	0.20054	0.04499	0.0128
O99	0.09232	0.0687	0.90207
O100	0.1049	0.05976	0.70495
O101	0.23073	0.03473	0.75018
O102	0.36171	0.82541	0.75588
O103	0.30605	0.8468	0.9297
O104	0.18933	0.85341	0.02176
O105	0.08533	0.83112	0.90438
O106	0.10626	0.83911	0.70931
O107	0.23185	0.85451	0.766
O108	0.32425	0.94813	0.80339
O109	0.08687	0.94993	0.81573
O110	0.43247	0.12756	0.5849
O111	0.41855	0.99605	0.56894
O112	0.39635	0.86446	0.57283
O113	0.19942	0.13169	0.62173
O114	0.18273	0.00307	0.57012
O115	0.19839	0.86883	0.57342
O116	0.98828	0.03815	0.78543
O117	0.98628	0.86504	0.78327
O118	0.14203	0.93605	0.22372
O119	0.19425	0.93407	0.40357
O120	0.299	0.94961	0.52564
O121	0.40074	0.92766	0.40128
O122	0.39606	0.94271	0.20466
O123	0.27015	0.96741	0.25
O124	0.14115	0.17381	0.25116
O125	0.19255	0.15673	0.42771
O126	0.31029	0.14804	0.51595
O127	0.41421	0.17085	0.39771
O128	0.39342	0.15302	0.20351
O129	0.26965	0.14198	0.26757
O130	0.17551	0.05123	0.3086
O131	0.41712	0.04836	0.32312
O132	0.06684	0.87275	0.09138
O133	0.08226	0.00407	0.07498
O134	0.10865	0.13445	0.06842
O135	0.30165	0.86786	0.12506
O136	0.31666	0.99501	0.06781

O137	0.29638	0.12818	0.07241
O138	0.5108	0.955	0.29507
O139	0.51423	0.13541	0.27864
O140	0.64056	0.56265	0.28307
O141	0.67613	0.57204	0.09275
O142	0.7934	0.55994	0.0041
O143	0.91413	0.56625	0.08346
O144	0.88986	0.56154	0.2805
O145	0.76465	0.53805	0.229
O146	0.64175	0.33281	0.25958
O147	0.69186	0.33824	0.08158
O148	0.8053	0.35161	0.97808
O149	0.90707	0.32789	0.10219
O150	0.9006	0.34162	0.2968
O151	0.76706	0.37351	0.23733
O152	0.66711	0.4521	0.18007
O153	0.9171	0.45006	0.17911
O154	0.56498	0.62884	0.40922
O155	0.58107	0.49818	0.4362
O156	0.59208	0.36447	0.43777
O157	0.79379	0.62247	0.37709
O158	0.8132	0.48917	0.39787
O159	0.80131	0.3585	0.44187
O160	0.01087	0.54372	0.21342
O161	0.01571	0.36368	0.20616
O162	0.87849	0.42717	0.74957
O163	0.80922	0.44415	0.58308
O164	0.69811	0.44249	0.46554
O165	0.60252	0.43111	0.60482
O166	0.60392	0.44502	0.80279
O167	0.73355	0.45313	0.76074
O168	0.86098	0.68299	0.74016
O169	0.80724	0.64979	0.56809
O170	0.68637	0.64637	0.48641
O171	0.57813	0.66939	0.59602
O172	0.60345	0.66169	0.78874
O173	0.73015	0.65386	0.7268
O174	0.82459	0.5583	0.71283
O175	0.58368	0.55042	0.68302
O176	0.92944	0.377	0.92192
O177	0.89361	0.50489	0.91001
O178	0.88835	0.63755	0.92376
O179	0.68735	0.36277	0.88829
O180	0.68787	0.49226	0.93812

O181	0.69692	0.62691	0.91651
O182	0.49094	0.45632	0.7105
O183	0.48216	0.63418	0.72016
O184	0.63963	0.92913	0.28495
O185	0.69695	0.92662	0.1073
O186	0.80163	0.94824	0.98595
O187	0.90237	0.92485	0.11168
O188	0.89399	0.95038	0.30754
O189	0.76678	0.96409	0.26373
O190	0.64166	0.16691	0.25897
O191	0.69867	0.15074	0.08525
O192	0.81271	0.14561	0.98701
O193	0.92272	0.16859	0.09098
O194	0.89386	0.1528	0.28285
O195	0.76747	0.12201	0.25204
O196	0.66963	0.04357	0.19521
O197	0.92159	0.04701	0.17304
O198	0.56699	0.8764	0.42991
O199	0.59091	0.00623	0.43344
O200	0.59318	0.13893	0.44404
O201	0.80675	0.86851	0.39099
O202	0.81106	0.99688	0.44502
O203	0.81677	0.1321	0.43786
O204	0.01063	0.95293	0.22305
O205	0.01753	0.1349	0.21702
O206	0.85738	0.05057	0.78614
O207	0.80482	0.07075	0.60868
O208	0.70262	0.06909	0.47918
O209	0.60115	0.07127	0.60757
O210	0.60466	0.05278	0.80521
O211	0.7291	0.02709	0.75943
O212	0.85974	0.83316	0.75922
O213	0.80605	0.82989	0.58157
O214	0.69204	0.85061	0.48578
O215	0.59087	0.8267	0.61016
O216	0.60572	0.84809	0.80388
O217	0.72964	0.85558	0.7395
O218	0.81753	0.94618	0.67621
O219	0.58163	0.95066	0.67985
O220	0.93102	0.1277	0.90251
O221	0.92025	0.99741	0.94467
O222	0.90236	0.86495	0.93982
O223	0.69942	0.12515	0.88914
O224	0.68324	0.99815	0.94235

O225	0.70378	0.86559	0.93542
O226	0.49059	0.0469	0.71504
O227	0.48623	0.86292	0.72192
O228	0.36081	0.43873	0.72152
O229	0.29932	0.43008	0.89465
O230	0.20481	0.44993	0.03515
O231	0.11335	0.43319	0.89433
O232	0.10599	0.44933	0.69908
O233	0.23269	0.47077	0.73608
O234	0.35497	0.66847	0.73398
O235	0.30186	0.66529	0.91146
O236	0.18862	0.64756	0.01042
O237	0.08335	0.67599	0.89777
O238	0.1022	0.6598	0.70235
O239	0.22751	0.63563	0.75254
O240	0.32242	0.55102	0.81468
O241	0.08669	0.5545	0.82153
O242	0.43213	0.37458	0.58401
O243	0.41421	0.50515	0.56636
O244	0.40431	0.63783	0.55639
O245	0.1953	0.37207	0.61201
O246	0.183	0.49946	0.55642
O247	0.19093	0.63374	0.56035
O248	0.99724	0.45857	0.80489
O249	0.9831	0.63585	0.78234
O250	0.14172	0.5615	0.2142
O251	0.19814	0.56878	0.39044
O252	0.29847	0.5597	0.52213
O253	0.39956	0.56799	0.39239
O254	0.39662	0.56028	0.19558
O255	0.27047	0.53216	0.23422
O256	0.13976	0.32956	0.24408
O257	0.19498	0.34122	0.41918
O258	0.30987	0.3547	0.5152
O259	0.41381	0.33196	0.39695
O260	0.39478	0.33854	0.20144
O261	0.26969	0.35668	0.25649
O262	0.17902	0.44919	0.3058
O263	0.4141	0.45021	0.30676
O264	0.06712	0.62483	0.08072
O265	0.082	0.49314	0.06541
O266	0.10526	0.36169	0.05793
O267	0.30349	0.62653	0.10162
O268	0.32559	0.49659	0.06072

O269	0.30327	0.363	0.06276
O270	0.50999	0.54264	0.28408
O271	0.51398	0.36435	0.27582
O272	0.43973	0.74999	0.643
O273	0.1972	0.74895	0.65485
O274	0.27039	0.74955	0.05623
O275	0.10775	0.74974	0.05656
O276	0.06324	0.24852	0.13684
O277	0.30333	0.2467	0.15408
O278	0.22948	0.25131	0.55674
O279	0.39212	0.25128	0.5501
O280	0.5594	0.25049	0.35308
O281	0.79735	0.24156	0.32591
O282	0.72709	0.24513	0.95101
O283	0.8909	0.25087	0.94361
O284	0.93981	0.75101	0.85987
O285	0.69275	0.75027	0.8507
O286	0.77045	0.74553	0.43836
O287	0.60678	0.75126	0.4485
O288	0.93835	0.24884	0.413
O289	0.94495	0.19022	0.57627
O290	0.88781	0.30677	0.56777
O291	0.01237	0.29689	0.55301
GA29	0.93659	0.37055	0.65972
H293	0.93053	0.28866	0.36494
H294	0.83075	0.33645	0.49522
H295	0.90851	0.16165	0.55158
H296	0.9705	0.32783	0.74289
H297	0.99995	0.36166	0.55371
H298	0.92708	0.42052	0.48886
H299	0.02991	0.37485	0.40778
H300	0.08042	0.42683	0.48452
H301	0.02471	0.46377	0.39704
H302	0.96762	0.53476	0.50674
H303	0.02539	0.51222	0.60121
H304	0.9382	0.51209	0.62642
AL30	0.81439	0.32533	0.3154
AL30	0.80649	0.47419	0.70374
P307	0.94665	0.26187	0.52646
C308	0.97427	0.42798	0.5296
C309	0.03096	0.42196	0.45011
C310	0.97618	0.50038	0.57

### C<sub>3</sub>H<sub>7</sub>Ga(H)

SI2	0.42318	0.05962	0.64936
SI3	0.30634	0.03023	0.79652
SI4	0.28054	0.0577	0.01844
SI5	0.12139	0.06338	0.01481
SI6	0.06722	0.02898	0.80252
SI7	0.18131	0.06113	0.66667
SI8	0.42081	0.82732	0.67535
SI9	0.30346	0.87099	0.81087
SI10	0.26678	0.8307	0.0298
SI11	0.11237	0.82768	0.01844
SI12	0.06548	0.87127	0.8035
SI13	0.18202	0.82735	0.67502
SI14	0.07649	0.94211	0.15473
SI15	0.19443	0.97099	0.29802
SI16	0.21835	0.93993	0.52111
SI17	0.37873	0.93418	0.5173
SI18	0.43332	0.96841	0.30604
SI19	0.31965	0.93978	0.16743
SI20	0.08225	0.1734	0.16742
SI21	0.19561	0.12994	0.30993
SI22	0.23194	0.17117	0.52646
SI23	0.3866	0.17417	0.51031
SI24	0.43512	0.12665	0.29877
SI25	0.31627	0.16935	0.17378
SI26	0.57764	0.55894	0.34859
SI27	0.68888	0.53332	0.19302
SI28	0.71296	0.56056	0.97927
SI29	0.87145	0.56556	0.98234
SI30	0.9315	0.53058	0.19264
SI31	0.81274	0.55672	0.32037
SI32	0.57712	0.32872	0.32692
SI33	0.69491	0.37553	0.18899
SI34	0.73026	0.32705	0.97348
SI35	0.88507	0.32736	0.98351
SI36	0.93711	0.37179	0.19619
SI37	0.9247	0.44271	0.84743
SI38	0.77773	0.4401	0.4755
SI39	0.61695	0.43385	0.48564
SI40	0.5659	0.46974	0.70004
SI41	0.6786	0.43728	0.83831
SI42	0.91783	0.67516	0.8292
SI43	0.80444	0.63702	0.6901
SI44	0.7639	0.66703	0.47129
SI45	0.60928	0.67311	0.48667

SI46	0.56119	0.62774	0.69962
SI47	0.68106	0.67524	0.82067
SI48	0.57783	0.94267	0.36075
SI49	0.69388	0.96715	0.21339
SI50	0.72106	0.93794	0.99375
SI51	0.88022	0.93506	0.99602
SI52	0.93223	0.96905	0.20518
SI53	0.81855	0.94347	0.35042
SI54	0.57741	0.17315	0.33088
SI55	0.69519	0.12251	0.19745
SI56	0.73447	0.16787	0.97884
SI57	0.88892	0.17292	0.98254
SI58	0.93841	0.12634	0.19364
SI59	0.81901	0.16442	0.32596
SI60	0.92349	0.05337	0.85502
SI61	0.80162	0.02314	0.71088
SI62	0.7811	0.0635	0.49189
SI63	0.62075	0.07089	0.49013
SI64	0.56907	0.03173	0.70125
SI65	0.67906	0.05309	0.85113
SI66	0.92073	0.82779	0.83744
SI67	0.80319	0.86538	0.69068
SI68	0.76745	0.82427	0.47477
SI69	0.61339	0.82659	0.49519
SI70	0.5651	0.87402	0.70454
SI71	0.68233	0.83095	0.83244
SI72	0.41999	0.44268	0.6486
SI73	0.30602	0.46947	0.79708
SI74	0.28299	0.44026	0.0204
SI75	0.12584	0.43657	0.01455
SI76	0.07533	0.47527	0.80667
SI77	0.18335	0.44367	0.66107
SI78	0.4199	0.67339	0.67001
SI79	0.30168	0.62771	0.80408
SI80	0.26549	0.67083	0.02273
SI81	0.11131	0.67514	0.01372
SI82	0.06404	0.63155	0.80365
SI83	0.17928	0.6697	0.66933
SI84	0.07509	0.55722	0.14526
SI85	0.19374	0.52823	0.28881
SI86	0.21797	0.5633	0.50997
SI87	0.37895	0.56889	0.51051
SI88	0.43452	0.5319	0.29872
SI89	0.32098	0.5595	0.16073

SI90	0.08302	0.32654	0.1641
SI91	0.19518	0.36951	0.3081
SI92	0.23161	0.33114	0.52591
SI93	0.38636	0.32868	0.50968
SI94	0.43424	0.37362	0.29516
SI95	0.31579	0.32728	0.173
O96	0.35945	0.06732	0.72352
O97	0.31499	0.05947	0.90876
O98	0.2005	0.0465	0.00938
O99	0.09013	0.06762	0.90363
O100	0.10488	0.06135	0.70662
O101	0.23035	0.04519	0.76057
O102	0.36086	0.82682	0.75684
O103	0.30505	0.85447	0.92908
O104	0.18912	0.85452	0.02372
O105	0.0866	0.83128	0.90411
O106	0.10456	0.83841	0.70858
O107	0.23011	0.85212	0.76631
O108	0.32003	0.9498	0.79193
O109	0.08624	0.94984	0.81364
O110	0.43157	0.12799	0.58413
O111	0.41472	0.99649	0.57368
O112	0.39646	0.86436	0.57356
O113	0.19844	0.13485	0.62226
O114	0.189	0.00413	0.58104
O115	0.19742	0.86969	0.57407
O116	0.98762	0.03858	0.78427
O117	0.98538	0.86439	0.78705
O118	0.14181	0.93304	0.22525
O119	0.18667	0.94068	0.40966
O120	0.29887	0.94659	0.51667
O121	0.40643	0.92879	0.4041
O122	0.39614	0.93953	0.20723
O123	0.27055	0.95848	0.26036
O124	0.14124	0.17458	0.25023
O125	0.19112	0.14943	0.42698
O126	0.30951	0.14787	0.51444
O127	0.41422	0.17002	0.3967
O128	0.39392	0.15444	0.2023
O129	0.27041	0.14619	0.26859
O130	0.17805	0.05097	0.29466
O131	0.41759	0.04816	0.31896
O132	0.06586	0.87395	0.08976
O133	0.08415	0.00514	0.07862

O134	0.10849	0.13566	0.06729
O135	0.30244	0.86538	0.12538
O136	0.31232	0.99515	0.07936
O137	0.29566	0.12851	0.07369
O138	0.51271	0.95547	0.29133
O139	0.51454	0.13563	0.27702
O140	0.64317	0.56748	0.27911
O141	0.675	0.56934	0.08621
O142	0.79266	0.55479	0.99953
O143	0.91053	0.56656	0.08842
O144	0.89037	0.562	0.28613
O145	0.7669	0.5462	0.22176
O146	0.64104	0.33269	0.25402
O147	0.69297	0.34479	0.07704
O148	0.80804	0.35311	0.97584
O149	0.91126	0.33139	0.09786
O150	0.90319	0.33784	0.29498
O151	0.76835	0.36904	0.23615
O152	0.67135	0.45385	0.18719
O153	0.91681	0.45038	0.18503
O154	0.56599	0.62908	0.40789
O155	0.5852	0.49871	0.42987
O156	0.59243	0.3647	0.43355
O157	0.79332	0.62523	0.3776
O158	0.80424	0.49117	0.39131
O159	0.80461	0.36239	0.44166
O160	0.01004	0.54525	0.21539
O161	0.01784	0.36601	0.20619
O162	0.87797	0.43093	0.74733
O163	0.81353	0.45199	0.57931
O164	0.69761	0.43879	0.47773
O165	0.59276	0.43164	0.60046
O166	0.6016	0.43966	0.79848
O167	0.73015	0.45128	0.74994
O168	0.86276	0.68308	0.74121
O169	0.80778	0.64946	0.56962
O170	0.68611	0.64586	0.48976
O171	0.57632	0.66727	0.59637
O172	0.60372	0.66231	0.78892
O173	0.73039	0.66292	0.72583
O174	0.8184	0.56083	0.72112
O175	0.58201	0.54947	0.68795
O176	0.93191	0.37407	0.91191
O177	0.8976	0.50217	0.91694

O178	0.88736	0.63557	0.92528
O179	0.69037	0.36208	0.88289
O180	0.68583	0.49225	0.9283
O181	0.69956	0.62671	0.91291
O182	0.48615	0.45797	0.71387
O183	0.48182	0.63482	0.72454
O184	0.6419	0.93069	0.28866
O185	0.69499	0.92762	0.10748
O186	0.801	0.95228	0.99009
O187	0.90321	0.92584	0.11152
O188	0.89431	0.94893	0.30813
O189	0.76849	0.96492	0.26055
O190	0.64216	0.16796	0.25861
O191	0.69876	0.15073	0.08445
O192	0.81249	0.14502	0.98507
O193	0.91985	0.16899	0.0942
O194	0.89537	0.15401	0.28758
O195	0.76835	0.12535	0.25083
O196	0.67064	0.04471	0.19706
O197	0.92099	0.04766	0.177
O198	0.56666	0.87589	0.42842
O199	0.5878	0.00617	0.43553
O200	0.59289	0.13925	0.43915
O201	0.80423	0.8673	0.38755
O202	0.80988	0.99445	0.44472
O203	0.81611	0.12924	0.43867
O204	0.01091	0.95353	0.22391
O205	0.01761	0.13607	0.21615
O206	0.85687	0.05309	0.78659
O207	0.80145	0.06784	0.6089
O208	0.70126	0.06749	0.47565
O209	0.60141	0.07274	0.60763
O210	0.60408	0.05421	0.8054
O211	0.72862	0.02725	0.76275
O212	0.86004	0.83048	0.75818
O213	0.80706	0.83314	0.57979
O214	0.69098	0.85139	0.48823
O215	0.58872	0.82797	0.61066
O216	0.60557	0.85059	0.80404
O217	0.7296	0.85187	0.73815
O218	0.81776	0.94558	0.68363
O219	0.58095	0.95224	0.67946
O220	0.93215	0.12719	0.90569
O221	0.92035	0.99679	0.94312

O222	0.89797	0.86518	0.9398
O223	0.69824	0.12817	0.88798
O224	0.68233	0.00217	0.94595
O225	0.70489	0.87004	0.93271
O226	0.49035	0.04866	0.71479
O227	0.48544	0.86479	0.72387
O228	0.35748	0.43065	0.72389
O229	0.31053	0.4359	0.90691
O230	0.2037	0.45791	0.02423
O231	0.10579	0.43114	0.89745
O232	0.10658	0.4498	0.70078
O233	0.23017	0.46042	0.75656
O234	0.35547	0.67208	0.74317
O235	0.30249	0.65252	0.91884
O236	0.18778	0.64743	0.0159
O237	0.0849	0.67699	0.89928
O238	0.10192	0.65965	0.70443
O239	0.22766	0.63835	0.75591
O240	0.32359	0.54916	0.79886
O241	0.08864	0.55471	0.825
O242	0.4316	0.37499	0.58291
O243	0.40511	0.50479	0.57364
O244	0.40136	0.63817	0.56429
O245	0.19665	0.36791	0.62099
O246	0.1958	0.49632	0.57082
O247	0.19067	0.63071	0.56427
O248	0.99568	0.46344	0.79825
O249	0.98376	0.63544	0.78715
O250	0.14097	0.56473	0.21477
O251	0.1849	0.55984	0.39956
O252	0.29841	0.56544	0.50172
O253	0.41233	0.56919	0.40094
O254	0.39571	0.5658	0.20535
O255	0.26968	0.54036	0.25073
O256	0.13943	0.3251	0.25087
O257	0.19083	0.35253	0.42609
O258	0.30909	0.35492	0.5147
O259	0.41362	0.33326	0.39606
O260	0.39329	0.34215	0.2012
O261	0.26953	0.35106	0.26716
O262	0.178	0.44815	0.28906
O263	0.4158	0.4526	0.308
O264	0.06516	0.626	0.08142
O265	0.08075	0.49401	0.06819

O266	0.11212	0.36368	0.06487
O267	0.30125	0.63159	0.11371
O268	0.322	0.50062	0.07673
O269	0.29561	0.36798	0.07256
O270	0.51359	0.54284	0.2784
O271	0.51343	0.36474	0.27317
O272	0.43989	0.75067	0.64693
O273	0.19544	0.74856	0.65134
O274	0.27151	0.75034	0.04418
O275	0.10763	0.75079	0.05834
O276	0.06336	0.24989	0.13585
O277	0.30489	0.24827	0.1502
O278	0.22713	0.25125	0.54429
O279	0.39114	0.25149	0.54776
O280	0.5592	0.25103	0.35049
O281	0.80096	0.24188	0.33853
O282	0.72906	0.24684	0.95466
O283	0.89166	0.25034	0.9446
O284	0.93884	0.75044	0.86493
O285	0.68893	0.75207	0.85855
O286	0.76863	0.74606	0.44205
O287	0.60648	0.75101	0.4515
O288	0.95838	0.25429	0.42072
O289	0.90313	0.1901	0.56251
O290	0.89719	0.31954	0.55906
O291	1.00538	0.25494	0.59507
GA29	0.94199	0.40115	0.63343
H293	0.93998	0.28916	0.37148
H294	0.83791	0.34339	0.49309
H295	0.87022	0.16942	0.51522
H296	0.98539	0.35084	0.7023
H297	1.00579	0.29127	0.6475
H298	0.92465	0.464	0.47338
H299	1.01004	0.37684	0.43377
H300	0.06973	0.41732	0.51071
H301	0.04135	0.4567	0.39985
H302	0.00087	0.56259	0.4846
H303	0.03337	0.53323	0.59947
H304	0.94844	0.55929	0.59168
AL30	0.81709	0.32536	0.31765
AL30	0.80522	0.47642	0.7026
P307	0.93912	0.25656	0.53317
C308	0.96929	0.46159	0.52112
C309	0.02535	0.42583	0.46406

C310	0.98864	0.53289	0.55183
<b>TS2</b>			
SI2	0.42407	0.05806	0.64834
SI3	0.30564	0.0283	0.7945
SI4	0.28034	0.05982	0.01515
SI5	0.12093	0.06383	0.01482
SI6	0.06751	0.02898	0.80269
SI7	0.17993	0.05768	0.66113
SI8	0.42055	0.82694	0.67347
SI9	0.30439	0.8699	0.81341
SI10	0.26637	0.82934	0.03207
SI11	0.11193	0.8273	0.01855
SI12	0.06502	0.87128	0.80389
SI13	0.18274	0.82854	0.67661
SI14	0.07594	0.94288	0.15383
SI15	0.19523	0.97241	0.29702
SI16	0.21832	0.93865	0.51903
SI17	0.37816	0.9344	0.51699
SI18	0.43136	0.96926	0.30617
SI19	0.32006	0.94355	0.16143
SI20	0.0815	0.17278	0.1688
SI21	0.1952	0.13053	0.31338
SI22	0.23253	0.17264	0.52991
SI23	0.38699	0.17435	0.51277
SI24	0.43512	0.12746	0.3013
SI25	0.316	0.16848	0.17541
SI26	0.57694	0.55851	0.34936
SI27	0.68717	0.53104	0.19313
SI28	0.71387	0.56047	0.97972
SI29	0.87204	0.56528	0.98019
SI30	0.93222	0.53061	0.19009
SI31	0.81282	0.55561	0.31971
SI32	0.57864	0.32846	0.32964
SI33	0.69375	0.37429	0.1885
SI34	0.72998	0.32566	0.97353
SI35	0.8846	0.3264	0.98438
SI36	0.93677	0.37204	0.19646
SI37	0.92439	0.44124	0.84721
SI38	0.78067	0.43859	0.47584
SI39	0.61991	0.43534	0.48805
SI40	0.56722	0.47016	0.70142
SI41	0.67976	0.43611	0.83818
SI42	0.91824	0.67462	0.82528

SI43	0.80399	0.63522	0.68756
SI44	0.76352	0.66674	0.46899
SI45	0.60888	0.67323	0.48499
SI46	0.56121	0.628	0.69847
SI47	0.68086	0.67409	0.81943
SI48	0.5765	0.94258	0.36234
SI49	0.69344	0.96675	0.21594
SI50	0.72044	0.93525	0.99594
SI51	0.88016	0.9332	0.99648
SI52	0.93152	0.96899	0.20542
SI53	0.81902	0.94431	0.35388
SI54	0.57782	0.17318	0.33475
SI55	0.69526	0.12187	0.20022
SI56	0.73404	0.16681	0.98127
SI57	0.88842	0.17222	0.985
SI58	0.93788	0.12585	0.19535
SI59	0.81875	0.1639	0.32775
SI60	0.92326	0.05293	0.85674
SI61	0.80146	0.02336	0.71221
SI62	0.78119	0.0648	0.49381
SI63	0.6209	0.07003	0.49223
SI64	0.56949	0.03007	0.70312
SI65	0.6789	0.05112	0.85403
SI66	0.92099	0.82749	0.83746
SI67	0.80226	0.86639	0.69293
SI68	0.76746	0.82402	0.47668
SI69	0.61323	0.82632	0.49547
SI70	0.56505	0.87235	0.70523
SI71	0.68163	0.83012	0.83415
SI72	0.42209	0.4442	0.64729
SI73	0.30459	0.47255	0.79395
SI74	0.283	0.43628	0.01572
SI75	0.12549	0.43481	0.01398
SI76	0.0754	0.47539	0.80614
SI77	0.18116	0.44788	0.65448
SI78	0.41995	0.67297	0.66667
SI79	0.30203	0.62952	0.80531
SI80	0.26536	0.67191	0.02267
SI81	0.11113	0.67488	0.01183
SI82	0.06428	0.63192	0.8011
SI83	0.18095	0.67035	0.66932
SI84	0.07573	0.55627	0.14398
SI85	0.19582	0.52822	0.28736
SI86	0.21835	0.56575	0.50794

SI87	0.3794	0.56805	0.50918
SI88	0.43257	0.53029	0.29717
SI89	0.32206	0.55533	0.15281
SI90	0.08187	0.32653	0.16361
SI91	0.19604	0.37	0.30818
SI92	0.23249	0.33054	0.52718
SI93	0.38701	0.32829	0.51196
SI94	0.4346	0.37224	0.29722
SI95	0.31698	0.32712	0.17205
O96	0.35921	0.06366	0.7205
O97	0.30915	0.06569	0.90218
O98	0.20021	0.04699	0.01471
O99	0.09272	0.06855	0.90187
O100	0.10446	0.05935	0.70487
O101	0.23045	0.03566	0.75052
O102	0.36023	0.82664	0.75422
O103	0.30539	0.8464	0.92905
O104	0.18895	0.85356	0.02231
O105	0.08515	0.83108	0.90476
O106	0.10511	0.83886	0.70963
O107	0.23059	0.8562	0.76628
O108	0.32357	0.94897	0.80498
O109	0.08543	0.94972	0.81571
O110	0.43206	0.1275	0.5855
O111	0.4178	0.99588	0.57014
O112	0.39695	0.86416	0.57142
O113	0.19868	0.13219	0.62163
O114	0.18309	0.00352	0.57033
O115	0.19716	0.86909	0.57374
O116	0.9878	0.0389	0.78667
O117	0.9851	0.86391	0.78528
O118	0.14169	0.93629	0.22384
O119	0.19356	0.9342	0.40394
O120	0.29866	0.94869	0.52562
O121	0.40064	0.92872	0.40111
O122	0.39581	0.94329	0.20432
O123	0.26996	0.96677	0.25068
O124	0.14127	0.17349	0.25019
O125	0.19232	0.15705	0.42741
O126	0.30982	0.14852	0.51662
O127	0.41401	0.17113	0.39877
O128	0.39377	0.15439	0.20439
O129	0.2698	0.1422	0.26792
O130	0.17575	0.05132	0.30861

O131	0.41776	0.04907	0.32236
O132	0.0664	0.87362	0.0911
O133	0.08208	0.00509	0.07571
O134	0.10675	0.1358	0.06745
O135	0.30176	0.86825	0.1242
O136	0.31585	0.99583	0.06849
O137	0.29719	0.12933	0.07298
O138	0.51065	0.95473	0.29442
O139	0.51455	0.13693	0.27992
O140	0.64142	0.56679	0.27761
O141	0.6747	0.5671	0.08592
O142	0.79338	0.5593	0.00275
O143	0.91368	0.56546	0.08397
O144	0.88942	0.56288	0.28135
O145	0.76516	0.5412	0.22431
O146	0.64081	0.33021	0.25323
O147	0.69221	0.34349	0.07661
O148	0.80756	0.35221	0.97678
O149	0.91136	0.33111	0.09827
O150	0.90203	0.33964	0.29518
O151	0.76729	0.37015	0.23588
O152	0.66793	0.45201	0.18701
O153	0.91694	0.45064	0.18316
O154	0.56508	0.62939	0.40655
O155	0.58727	0.49978	0.43244
O156	0.59803	0.36618	0.43361
O157	0.79244	0.6247	0.37494
O158	0.80889	0.4916	0.39556
O159	0.80312	0.36054	0.44037
O160	0.01061	0.54511	0.21465
O161	0.01742	0.36614	0.20795
O162	0.87748	0.42878	0.74688
O163	0.81966	0.44587	0.58047
O164	0.70091	0.44313	0.48422
O165	0.59491	0.43171	0.60247
O166	0.60238	0.44112	0.80114
O167	0.72941	0.44835	0.74632
O168	0.86192	0.68157	0.73876
O169	0.80703	0.64781	0.56722
O170	0.68568	0.64592	0.48713
O171	0.57653	0.66698	0.59494
O172	0.60312	0.66365	0.78764
O173	0.72966	0.65876	0.72484
O174	0.81888	0.55867	0.71634

O175	0.58304	0.54988	0.6886
O176	0.93118	0.37289	0.91199
O177	0.89282	0.50025	0.91361
O178	0.88937	0.63405	0.92132
O179	0.69056	0.3608	0.88238
O180	0.69163	0.49084	0.92721
O181	0.69725	0.62559	0.91271
O182	0.48763	0.45762	0.7149
O183	0.4816	0.6343	0.72187
O184	0.63993	0.93053	0.28909
O185	0.69663	0.92637	0.11089
O186	0.80054	0.94753	0.98756
O187	0.90173	0.92532	0.11277
O188	0.89412	0.94937	0.30896
O189	0.76712	0.96466	0.26597
O190	0.64252	0.16707	0.26258
O191	0.69865	0.15144	0.08775
O192	0.81208	0.14401	0.98757
O193	0.91914	0.16958	0.09689
O194	0.89509	0.1523	0.29005
O195	0.76839	0.12305	0.25362
O196	0.6703	0.04413	0.19747
O197	0.92033	0.04741	0.17616
O198	0.56584	0.87592	0.43051
O199	0.58715	0.00605	0.43687
O200	0.59258	0.13871	0.44278
O201	0.80589	0.86816	0.39252
O202	0.81175	0.99612	0.44733
O203	0.81511	0.13134	0.44185
O204	0.01035	0.95354	0.22319
O205	0.01721	0.13501	0.21773
O206	0.857	0.05319	0.78759
O207	0.80012	0.06917	0.61147
O208	0.70121	0.06623	0.47634
O209	0.60237	0.07116	0.61005
O210	0.60399	0.05222	0.80783
O211	0.72893	0.02586	0.76589
O212	0.8586	0.83148	0.7614
O213	0.80486	0.83129	0.58382
O214	0.69079	0.85109	0.48764
O215	0.58936	0.82655	0.61134
O216	0.60443	0.84753	0.80503
O217	0.72879	0.85572	0.74234
O218	0.8182	0.94617	0.68229

O219	0.58164	0.95058	0.68145
O220	0.93201	0.12609	0.90932
O221	0.91918	0.99555	0.94357
O222	0.90095	0.86342	0.94215
O223	0.69759	0.12618	0.89158
O224	0.68207	0.9998	0.94839
O225	0.70107	0.86699	0.93768
O226	0.49062	0.04703	0.71526
O227	0.48515	0.86387	0.72289
O228	0.35787	0.43673	0.72036
O229	0.30321	0.43174	0.89873
O230	0.20382	0.45235	0.03059
O231	0.10881	0.43216	0.89556
O232	0.10558	0.45048	0.69962
O233	0.23081	0.46987	0.74423
O234	0.3553	0.67078	0.73902
O235	0.30233	0.66187	0.91606
O236	0.18793	0.64786	0.01238
O237	0.08385	0.67708	0.8977
O238	0.1033	0.65932	0.70246
O239	0.22818	0.63648	0.75513
O240	0.32409	0.55096	0.81143
O241	0.08765	0.55501	0.82396
O242	0.43224	0.37498	0.58471
O243	0.41273	0.50546	0.56846
O244	0.40194	0.63829	0.56023
O245	0.1967	0.37227	0.61655
O246	0.18626	0.49984	0.5614
O247	0.19362	0.63432	0.56212
O248	0.99576	0.46235	0.80127
O249	0.98427	0.63621	0.78133
O250	0.14187	0.5627	0.21301
O251	0.19259	0.56781	0.39321
O252	0.29893	0.55988	0.51311
O253	0.40568	0.56974	0.39524
O254	0.39651	0.5613	0.19909
O255	0.27048	0.53418	0.24139
O256	0.14065	0.32793	0.24655
O257	0.19356	0.34483	0.42301
O258	0.30989	0.35483	0.51583
O259	0.41402	0.332	0.39811
O260	0.39454	0.34014	0.20277
O261	0.26997	0.35663	0.2616
O262	0.17735	0.44937	0.30239

O263	0.41502	0.45097	0.3096
O264	0.06606	0.62497	0.07994
O265	0.08094	0.49303	0.06689
O266	0.10726	0.36189	0.06068
O267	0.30188	0.62778	0.10775
O268	0.32384	0.49789	0.06646
O269	0.30077	0.36467	0.06704
O270	0.51212	0.54111	0.28187
O271	0.51426	0.36446	0.27772
O272	0.43976	0.75037	0.64462
O273	0.19742	0.74954	0.65665
O274	0.26989	0.74978	0.05619
O275	0.10675	0.75019	0.05764
O276	0.06223	0.24942	0.13909
O277	0.30332	0.24777	0.15595
O278	0.22894	0.25187	0.55619
O279	0.39208	0.25143	0.55143
O280	0.56068	0.25123	0.35636
O281	0.79942	0.24142	0.33328
O282	0.72869	0.24552	0.95452
O283	0.89085	0.24938	0.94575
O284	0.93869	0.74966	0.86186
O285	0.69183	0.75089	0.85528
O286	0.76925	0.74604	0.44187
O287	0.60621	0.75113	0.45025
O288	0.95212	0.25271	0.42435
O289	0.9082	0.19179	0.57426
O290	0.89091	0.31933	0.56022
O291	0.00527	0.27086	0.59794
GA29	0.9257	0.40389	0.61882
H293	0.93889	0.28992	0.37685
H294	0.83631	0.33905	0.49256
H295	0.87516	0.17169	0.52787
H296	0.97934	0.35566	0.70857
H297	0.9922	0.32149	0.66912
H298	0.92784	0.46667	0.46253
H299	0.01546	0.37996	0.43299
H300	0.07006	0.42046	0.51763
H301	0.047	0.46089	0.40463
H302	0.9982	0.56647	0.49096
H303	0.02838	0.5334	0.60516
H304	0.943	0.55722	0.59386
AL30	0.81627	0.32484	0.31553
AL30	0.80465	0.47448	0.7027

P307	0.94189	0.25926	0.53999
C308	0.96936	0.46326	0.51642
C309	0.02845	0.42881	0.46587
C310	0.9852	0.53374	0.55459
<b>C<sub>3</sub>H<sub>7</sub>Ga+H<sub>2</sub>*</b>			
SI2	0.42441	0.05737	0.64869
SI3	0.30479	0.02743	0.79368
SI4	0.28105	0.06061	0.0147
SI5	0.12148	0.06376	0.01526
SI6	0.06804	0.02969	0.80278
SI7	0.17939	0.05649	0.65862
SI8	0.42044	0.82656	0.67342
SI9	0.30365	0.86919	0.81355
SI10	0.26591	0.82917	0.03262
SI11	0.11151	0.8273	0.01844
SI12	0.06418	0.87151	0.80364
SI13	0.18195	0.82836	0.67637
SI14	0.07577	0.94311	0.15362
SI15	0.19597	0.97298	0.29657
SI16	0.21862	0.93771	0.51841
SI17	0.37818	0.93441	0.51724
SI18	0.43118	0.96944	0.30651
SI19	0.3207	0.94481	0.15929
SI20	0.08151	0.17252	0.16957
SI21	0.19621	0.13044	0.31356
SI22	0.23357	0.17277	0.53029
SI23	0.38803	0.17432	0.51429
SI24	0.43624	0.12783	0.30244
SI25	0.31718	0.1682	0.17565
SI26	0.57478	0.56062	0.34443
SI27	0.68668	0.53147	0.18879
SI28	0.714	0.55778	0.97475
SI29	0.87228	0.56157	0.9726
SI30	0.93191	0.52946	0.18605
SI31	0.81274	0.56007	0.31227
SI32	0.58043	0.32923	0.32848
SI33	0.69379	0.37314	0.18267
SI34	0.72775	0.32442	0.97157
SI35	0.88196	0.32623	0.98614
SI36	0.93596	0.37109	0.19948
SI37	0.92356	0.43712	0.8384
SI38	0.77667	0.44503	0.46705
SI39	0.61761	0.43977	0.48344

SI40	0.56786	0.47075	0.69937
SI41	0.68039	0.43375	0.83374
SI42	0.91703	0.67434	0.8235
SI43	0.80382	0.63486	0.68508
SI44	0.76399	0.66731	0.46706
SI45	0.60945	0.67381	0.48188
SI46	0.56208	0.62821	0.69649
SI47	0.68151	0.67362	0.81631
SI48	0.57694	0.94322	0.36348
SI49	0.69465	0.96686	0.21824
SI50	0.72075	0.93342	0.99728
SI51	0.88054	0.93278	0.99807
SI52	0.9311	0.97009	0.20811
SI53	0.81988	0.94486	0.35791
SI54	0.57886	0.17395	0.33811
SI55	0.69718	0.12249	0.20439
SI56	0.73335	0.16588	0.98468
SI57	0.88707	0.17174	0.98977
SI58	0.9377	0.12729	0.20035
SI59	0.81981	0.16554	0.33311
SI60	0.92361	0.05365	0.86
SI61	0.80194	0.02407	0.71514
SI62	0.7822	0.06603	0.49694
SI63	0.62159	0.07073	0.49426
SI64	0.56947	0.0287	0.70464
SI65	0.6784	0.04988	0.85621
SI66	0.92083	0.82708	0.8402
SI67	0.80171	0.86729	0.69676
SI68	0.76791	0.82479	0.48044
SI69	0.61381	0.82696	0.49736
SI70	0.56503	0.87097	0.70717
SI71	0.68142	0.82914	0.83652
SI72	0.42246	0.44574	0.64643
SI73	0.30353	0.47367	0.79386
SI74	0.28243	0.43382	0.01328
SI75	0.12469	0.43331	0.01135
SI76	0.07471	0.47181	0.80191
SI77	0.18201	0.44898	0.65004
SI78	0.42058	0.67208	0.66451
SI79	0.30175	0.63006	0.80577
SI80	0.26502	0.67301	0.02088
SI81	0.11068	0.67431	0.00977
SI82	0.06229	0.62987	0.79924
SI83	0.18048	0.66964	0.66922

SI84	0.07577	0.55519	0.14177
SI85	0.19621	0.52765	0.28668
SI86	0.21909	0.56683	0.5059
SI87	0.37986	0.56814	0.50663
SI88	0.43136	0.53067	0.29343
SI89	0.32082	0.55381	0.14771
SI90	0.08079	0.32671	0.16315
SI91	0.19677	0.36999	0.30767
SI92	0.23369	0.32977	0.52568
SI93	0.38842	0.32837	0.51228
SI94	0.43644	0.37214	0.29706
SI95	0.31805	0.32695	0.17216
O96	0.35919	0.06197	0.72022
O97	0.30626	0.06677	0.89991
O98	0.20091	0.04787	0.01998
O99	0.09629	0.0686	0.90068
O100	0.10412	0.05894	0.70336
O101	0.23031	0.03345	0.74679
O102	0.35939	0.8266	0.75299
O103	0.30452	0.84402	0.92845
O104	0.18854	0.85355	0.0227
O105	0.08476	0.83181	0.90471
O106	0.10437	0.83936	0.70924
O107	0.22993	0.85641	0.76565
O108	0.32286	0.94841	0.80809
O109	0.08401	0.95007	0.81536
O110	0.43279	0.1275	0.58755
O111	0.41852	0.99614	0.5687
O112	0.39816	0.86426	0.57103
O113	0.19829	0.13112	0.61963
O114	0.1815	0.0025	0.56739
O115	0.19668	0.86824	0.57286
O116	0.98837	0.04162	0.78953
O117	0.9843	0.86314	0.78551
O118	0.14141	0.93772	0.22414
O119	0.1969	0.93269	0.40194
O120	0.29875	0.94839	0.52958
O121	0.39863	0.92908	0.40042
O122	0.39606	0.94412	0.20389
O123	0.26976	0.96961	0.24653
O124	0.14233	0.17283	0.24932
O125	0.19422	0.15923	0.42641
O126	0.31082	0.14846	0.51832
O127	0.41475	0.17104	0.4002

O128	0.39496	0.15495	0.20554
O129	0.27062	0.14002	0.26652
O130	0.17594	0.05136	0.31328
O131	0.41866	0.04941	0.32268
O132	0.06643	0.8731	0.09251
O133	0.08187	0.0043	0.07353
O134	0.10503	0.13536	0.06749
O135	0.30186	0.86942	0.12299
O136	0.31811	0.99637	0.06519
O137	0.29984	0.12994	0.0718
O138	0.51043	0.95423	0.29655
O139	0.51576	0.13787	0.28223
O140	0.63993	0.56572	0.27342
O141	0.67385	0.5656	0.08014
O142	0.79376	0.55503	0.997
O143	0.9152	0.55764	0.07502
O144	0.88872	0.56781	0.2716
O145	0.76414	0.54641	0.21794
O146	0.6429	0.33004	0.25255
O147	0.68543	0.34402	0.07019
O148	0.80477	0.35159	0.98167
O149	0.91188	0.3329	0.09805
O150	0.9009	0.33746	0.29731
O151	0.76938	0.36501	0.22087
O152	0.67077	0.45169	0.18598
O153	0.9156	0.44979	0.1908
O154	0.56574	0.63223	0.40071
O155	0.57986	0.5017	0.42858
O156	0.59979	0.36886	0.43076
O157	0.79328	0.6283	0.37042
O158	0.80886	0.49491	0.38569
O159	0.79256	0.36602	0.43049
O160	0.01016	0.54384	0.21105
O161	0.01668	0.36507	0.21105
O162	0.87796	0.42602	0.73568
O163	0.81583	0.45222	0.57141
O164	0.69735	0.45528	0.47616
O165	0.59423	0.43391	0.59839
O166	0.603	0.43851	0.79676
O167	0.7303	0.44736	0.7427
O168	0.86077	0.68222	0.73694
O169	0.80747	0.64589	0.56431
O170	0.6861	0.64601	0.48348
O171	0.57659	0.66531	0.59119

O172	0.60347	0.66568	0.78458
O173	0.72922	0.65907	0.7202
O174	0.81882	0.55865	0.71616
O175	0.5853	0.55035	0.69032
O176	0.92581	0.37109	0.90822
O177	0.89376	0.49983	0.89948
O178	0.88862	0.63259	0.91887
O179	0.69202	0.35798	0.87577
O180	0.69114	0.48775	0.92404
O181	0.69813	0.62266	0.90666
O182	0.48809	0.46001	0.71339
O183	0.48244	0.63387	0.71982
O184	0.63986	0.93062	0.28935
O185	0.69867	0.92652	0.11323
O186	0.8008	0.9453	0.98553
O187	0.90028	0.92726	0.11533
O188	0.89489	0.94948	0.31224
O189	0.76774	0.96441	0.27
O190	0.64446	0.16671	0.26818
O191	0.69867	0.15298	0.09232
O192	0.8112	0.14219	0.99111
O193	0.91773	0.17028	0.1017
O194	0.89694	0.15592	0.29588
O195	0.77076	0.12457	0.25642
O196	0.67271	0.0446	0.20004
O197	0.91907	0.04894	0.18242
O198	0.56655	0.87739	0.43357
O199	0.58851	0.00762	0.43582
O200	0.59245	0.13983	0.44688
O201	0.80721	0.86887	0.39724
O202	0.81244	0.99687	0.45103
O203	0.81666	0.13181	0.4456
O204	0.01019	0.95455	0.22273
O205	0.01749	0.13526	0.22021
O206	0.85751	0.05413	0.79041
O207	0.80155	0.07028	0.61474
O208	0.70209	0.06767	0.47981
O209	0.60247	0.06981	0.61183
O210	0.60368	0.05107	0.80943
O211	0.72918	0.0267	0.76784
O212	0.857	0.83245	0.7671
O213	0.80462	0.83135	0.58825
O214	0.69127	0.85214	0.49055
O215	0.58947	0.82538	0.61306

O216	0.60402	0.84581	0.80723
O217	0.72796	0.85763	0.74575
O218	0.81854	0.94687	0.68497
O219	0.58185	0.94919	0.68351
O220	0.93186	0.12607	0.91488
O221	0.91962	0.99501	0.94479
O222	0.90353	0.86272	0.94633
O223	0.69602	0.12433	0.89691
O224	0.68161	-0.00298	0.94857
O225	0.70016	0.86435	0.94179
O226	0.49052	0.04554	0.71623
O227	0.485	0.86274	0.7242
O228	0.35848	0.44084	0.72014
O229	0.29969	0.42889	0.89511
O230	0.20321	0.44763	0.0321
O231	0.1105	0.43112	0.89212
O232	0.10665	0.45063	0.69511
O233	0.2313	0.47294	0.73917
O234	0.35555	0.66767	0.73578
O235	0.30226	0.66706	0.91355
O236	0.18787	0.64834	0.00869
O237	0.08216	0.67448	0.89632
O238	0.10307	0.65675	0.70187
O239	0.22808	0.63619	0.75479
O240	0.32183	0.55138	0.81996
O241	0.08159	0.55189	0.82197
O242	0.4318	0.375	0.5875
O243	0.41376	0.50508	0.56416
O244	0.40419	0.6381	0.55692
O245	0.19851	0.37328	0.61351
O246	0.18598	0.50021	0.5559
O247	0.19362	0.63469	0.56131
O248	0.99673	0.45129	0.793
O249	0.98276	0.63664	0.77746
O250	0.14103	0.56022	0.2127
O251	0.19574	0.57046	0.38998
O252	0.2995	0.56073	0.51506
O253	0.40316	0.5697	0.39118
O254	0.39494	0.55965	0.19454
O255	0.26952	0.53157	0.23589
O256	0.14155	0.33005	0.24273
O257	0.19453	0.34092	0.4207
O258	0.31096	0.35397	0.5127
O259	0.41751	0.33286	0.39961

O260	0.39548	0.3389	0.20433
O261	0.27058	0.35838	0.25967
O262	0.17819	0.44947	0.30883
O263	0.41673	0.45091	0.3077
O264	0.06683	0.6248	0.08001
O265	0.0814	0.49312	0.06273
O266	0.10265	0.36141	0.05796
O267	0.30125	0.62663	0.10345
O268	0.32274	0.49705	0.06041
O269	0.30352	0.3634	0.06562
O270	0.51002	0.54535	0.27597
O271	0.5159	0.36442	0.27553
O272	0.43925	0.74996	0.64436
O273	0.19598	0.74914	0.65775
O274	0.26885	0.74991	0.05971
O275	0.10597	0.74974	0.05505
O276	0.06213	0.24913	0.14056
O277	0.30331	0.24754	0.15843
O278	0.22994	0.25171	0.55893
O279	0.39326	0.25156	0.55208
O280	0.56241	0.25241	0.35798
O281	0.79881	0.2426	0.33999
O282	0.72815	0.24406	0.95488
O283	0.88791	0.24866	0.95004
O284	0.93769	0.74881	0.86246
O285	0.69352	0.74977	0.8547
O286	0.76959	0.74718	0.44459
O287	0.60731	0.75232	0.45021
O288	0.95387	0.2627	0.44556
O289	0.9204	0.20628	0.60406
O290	0.86716	0.32222	0.55774
O291	-0.0203	0.3193	0.61918
GA29	0.92177	0.40511	0.60485
H293	0.93821	0.29338	0.38979
H294	0.82118	0.34099	0.48771
H295	0.89509	0.17498	0.56164
H296	0.99735	0.2389	0.82525
H297	1.01087	0.25906	0.78227
H298	0.92562	0.47313	0.45222
H299	0.01512	0.38931	0.41981
H300	0.0659	0.42466	0.51452
H301	0.04808	0.47126	0.40452
H302	-0.00428	0.57187	0.4931
H303	0.0207	0.53516	0.60763

H304	0.936	0.55967	0.5894
AL30	0.81391	0.32527	0.31239
AL30	0.80439	0.47482	0.6967
P307	0.93183	0.27739	0.55588
C308	0.96572	0.46817	0.50812
C309	0.02684	0.43608	0.45968
C310	0.97985	0.53726	0.55297

### C<sub>3</sub>H<sub>7</sub>Ga

SI2	0.42376	0.05896	0.64862
SI3	0.30642	0.02938	0.79536
SI4	0.28056	0.0585	0.01693
SI5	0.12122	0.06309	0.01434
SI6	0.06703	0.02908	0.80206
SI7	0.18078	0.05917	0.66408
SI8	0.42076	0.82726	0.67504
SI9	0.304	0.87051	0.81201
SI10	0.26654	0.83035	0.03104
SI11	0.11218	0.82738	0.01812
SI12	0.06501	0.87103	0.80308
SI13	0.18241	0.82715	0.67607
SI14	0.07618	0.94201	0.154
SI15	0.19453	0.97108	0.29771
SI16	0.21803	0.9385	0.52016
SI17	0.37831	0.93423	0.51705
SI18	0.43287	0.96884	0.30649
SI19	0.3199	0.9414	0.16534
SI20	0.08238	0.17291	0.1678
SI21	0.19574	0.12978	0.3112
SI22	0.23273	0.17152	0.52768
SI23	0.38727	0.17427	0.51125
SI24	0.43578	0.1271	0.30005
SI25	0.31657	0.16852	0.17458
SI26	0.57682	0.55924	0.34664
SI27	0.68833	0.53177	0.19098
SI28	0.71461	0.55886	0.97704
SI29	0.87296	0.56211	0.97587
SI30	0.93243	0.52946	0.18911
SI31	0.81318	0.5587	0.31602
SI32	0.57988	0.32888	0.32804
SI33	0.69466	0.37383	0.18428
SI34	0.72891	0.32531	0.97183
SI35	0.88343	0.32631	0.98589
SI36	0.93692	0.37073	0.1991

SI37	0.92459	0.43792	0.84088
SI38	0.77698	0.44263	0.47083
SI39	0.6174	0.43699	0.48583
SI40	0.56594	0.46978	0.70012
SI41	0.67943	0.43548	0.83521
SI42	0.91723	0.67441	0.8262
SI43	0.80466	0.63455	0.68662
SI44	0.76425	0.66728	0.46864
SI45	0.60965	0.67311	0.48485
SI46	0.56185	0.62773	0.6988
SI47	0.68233	0.67348	0.81844
SI48	0.57784	0.94273	0.36155
SI49	0.69453	0.96704	0.21492
SI50	0.72076	0.93533	0.99465
SI51	0.88032	0.93402	0.99638
SI52	0.93184	0.96959	0.20625
SI53	0.81931	0.9443	0.3531
SI54	0.57847	0.17344	0.33361
SI55	0.69685	0.12258	0.20035
SI56	0.73433	0.16651	0.98064
SI57	0.88839	0.17201	0.98521
SI58	0.93831	0.12707	0.19668
SI59	0.81998	0.16541	0.32962
SI60	0.92339	0.05347	0.85637
SI61	0.80196	0.0237	0.71184
SI62	0.78228	0.0653	0.49324
SI63	0.62172	0.07056	0.49151
SI64	0.5695	0.03045	0.70202
SI65	0.67895	0.05116	0.85242
SI66	0.92067	0.82721	0.83828
SI67	0.80287	0.86665	0.69263
SI68	0.76762	0.82474	0.47675
SI69	0.61345	0.82652	0.49549
SI70	0.56526	0.87274	0.7052
SI71	0.68235	0.82996	0.83307
SI72	0.42073	0.44334	0.64797
SI73	0.30636	0.47045	0.79691
SI74	0.28326	0.43813	0.01856
SI75	0.12567	0.43538	0.01293
SI76	0.0744	0.47177	0.80335
SI77	0.18462	0.44554	0.65826
SI78	0.42064	0.67332	0.66813
SI79	0.30266	0.62796	0.80456
SI80	0.26538	0.67138	0.022

SI81	0.11115	0.67436	0.01149
SI82	0.06278	0.62969	0.80146
SI83	0.18028	0.66865	0.6698
SI84	0.07567	0.55646	0.14351
SI85	0.19446	0.52787	0.28772
SI86	0.21899	0.56461	0.50792
SI87	0.38017	0.56899	0.50893
SI88	0.43436	0.53142	0.29649
SI89	0.32103	0.55776	0.1572
SI90	0.08286	0.32615	0.16441
SI91	0.19575	0.3693	0.30873
SI92	0.23289	0.33082	0.52649
SI93	0.38751	0.32846	0.51012
SI94	0.43593	0.37297	0.29579
SI95	0.31687	0.32693	0.17397
O96	0.3596	0.06609	0.72206
O97	0.31294	0.06196	0.90594
O98	0.20047	0.04655	0.01079
O99	0.09109	0.06773	0.90253
O100	0.1047	0.0607	0.70563
O101	0.23053	0.04066	0.75608
O102	0.36073	0.82628	0.75642
O103	0.30517	0.85181	0.92951
O104	0.18892	0.85428	0.02345
O105	0.08613	0.83149	0.90401
O106	0.1048	0.83825	0.70877
O107	0.2304	0.85373	0.7664
O108	0.32224	0.9493	0.79653
O109	0.08506	0.94974	0.81323
O110	0.43234	0.12782	0.58454
O111	0.41561	0.99651	0.57156
O112	0.39645	0.86454	0.57341
O113	0.19892	0.13312	0.62146
O114	0.18588	0.00292	0.57664
O115	0.19769	0.86831	0.57394
O116	0.98739	0.03935	0.78499
O117	0.98504	0.86311	0.78592
O118	0.14177	0.93408	0.22418
O119	0.18887	0.93681	0.4072
O120	0.29849	0.94724	0.51991
O121	0.40412	0.92844	0.4028
O122	0.39612	0.94161	0.20628
O123	0.27035	0.96181	0.25687
O124	0.14188	0.174	0.24977

O125	0.19193	0.15241	0.42702
O126	0.31019	0.148	0.51535
O127	0.41435	0.17085	0.39733
O128	0.39429	0.15367	0.203
O129	0.2706	0.14361	0.26826
O130	0.17671	0.05075	0.30098
O131	0.4185	0.04868	0.32141
O132	0.06591	0.87308	0.09064
O133	0.08345	0.00429	0.07635
O134	0.10785	0.13502	0.06741
O135	0.30218	0.86656	0.12541
O136	0.31368	0.9953	0.07496
O137	0.2963	0.12882	0.07326
O138	0.51225	0.95531	0.29306
O139	0.51515	0.13713	0.2788
O140	0.64267	0.56591	0.27719
O141	0.67537	0.56694	0.08313
O142	0.79438	0.55278	0.99772
O143	0.91446	0.56004	0.07979
O144	0.88984	0.56522	0.27772
O145	0.76612	0.5454	0.21972
O146	0.64287	0.33105	0.25311
O147	0.68799	0.34385	0.07211
O148	0.80633	0.352	0.97934
O149	0.91136	0.3316	0.09918
O150	0.90229	0.33795	0.298
O151	0.76994	0.3666	0.22412
O152	0.67114	0.45227	0.18603
O153	0.91703	0.44951	0.18914
O154	0.56631	0.62987	0.40512
O155	0.58183	0.49946	0.42925
O156	0.59865	0.36658	0.43222
O157	0.7934	0.62734	0.37276
O158	0.80707	0.49409	0.38993
O159	0.7945	0.36445	0.43261
O160	0.01066	0.54457	0.21386
O161	0.01774	0.36472	0.20861
O162	0.87726	0.42499	0.7404
O163	0.8169	0.44982	0.57457
O164	0.69754	0.45059	0.48225
O165	0.59194	0.43193	0.59983
O166	0.602	0.43902	0.79785
O167	0.72968	0.44909	0.74454
O168	0.86134	0.6818	0.73917

O169	0.8081	0.64732	0.56621
O170	0.68652	0.64599	0.48682
O171	0.57718	0.66632	0.59482
O172	0.60442	0.66229	0.78822
O173	0.72996	0.65796	0.72261
O174	0.82038	0.55813	0.7158
O175	0.58257	0.54937	0.68846
O176	0.92896	0.37215	0.91123
O177	0.89692	0.5009	0.90337
O178	0.88821	0.63334	0.92188
O179	0.69173	0.3601	0.8783
O180	0.68883	0.49053	0.92448
O181	0.70099	0.62549	0.9115
O182	0.48628	0.45834	0.71479
O183	0.48251	0.63522	0.72355
O184	0.64149	0.93066	0.28869
O185	0.69637	0.92701	0.10944
O186	0.80076	0.94874	0.98746
O187	0.90208	0.92684	0.11264
O188	0.89485	0.9488	0.30963
O189	0.76868	0.96459	0.26344
O190	0.64345	0.1674	0.26205
O191	0.69933	0.15151	0.08745
O192	0.81226	0.1432	0.98679
O193	0.91911	0.16929	0.09703
O194	0.89684	0.15593	0.29133
O195	0.77013	0.1252	0.2533
O196	0.67207	0.04474	0.1981
O197	0.92023	0.04845	0.18018
O198	0.56657	0.87599	0.42935
O199	0.5888	0.00609	0.43617
O200	0.59291	0.13892	0.44171
O201	0.80534	0.86826	0.39126
O202	0.81129	0.99586	0.44664
O203	0.81731	0.13078	0.44168
O204	0.0107	0.95382	0.22312
O205	0.0179	0.13586	0.21736
O206	0.85679	0.05403	0.78795
O207	0.80219	0.06928	0.61083
O208	0.70216	0.06768	0.47713
O209	0.60229	0.07156	0.60902
O210	0.60398	0.05279	0.80663
O211	0.72887	0.02649	0.76371
O212	0.85867	0.83118	0.76146

O213	0.80607	0.83254	0.58296
O214	0.69096	0.85161	0.48885
O215	0.58874	0.82688	0.61097
O216	0.60513	0.84785	0.80458
O217	0.72908	0.85571	0.74082
O218	0.81912	0.94645	0.68327
O219	0.58178	0.95092	0.68082
O220	0.93249	0.12654	0.90911
O221	0.91974	0.99595	0.94297
O222	0.9006	0.86396	0.94236
O223	0.69771	0.12586	0.89117
O224	0.68191	-0.00091	0.94581
O225	0.70264	0.86659	0.93658
O226	0.49063	0.04729	0.71446
O227	0.48541	0.86445	0.72392
O228	0.3575	0.43262	0.72214
O229	0.30891	0.43288	0.9041
O230	0.20385	0.45505	0.02453
O231	0.10632	0.42995	0.89553
O232	0.10802	0.45022	0.69783
O233	0.23102	0.46529	0.753
O234	0.35568	0.6709	0.74005
O235	0.30303	0.65718	0.9171
O236	0.18792	0.64739	0.01237
O237	0.08369	0.67473	0.89753
O238	0.10298	0.65656	0.70359
O239	0.22858	0.63581	0.75525
O240	0.32559	0.54957	0.80634
O241	0.08239	0.5517	0.824
O242	0.43227	0.37512	0.58357
O243	0.40761	0.5052	0.57172
O244	0.40331	0.63838	0.56171
O245	0.19959	0.36964	0.62079
O246	0.19491	0.49723	0.56611
O247	0.19226	0.63201	0.56298
O248	0.99622	0.45262	0.79005
O249	0.98307	0.63623	0.78143
O250	0.14169	0.56344	0.21276
O251	0.18741	0.5631	0.39641
O252	0.29959	0.56526	0.50296
O253	0.4117	0.56911	0.39816
O254	0.39557	0.56422	0.2023
O255	0.27013	0.5373	0.24701
O256	0.14046	0.32547	0.24951

O257	0.19169	0.34988	0.42595
O258	0.31024	0.35449	0.51302
O259	0.4155	0.33291	0.39694
O260	0.39463	0.34098	0.20239
O261	0.27029	0.35261	0.26669
O262	0.1776	0.44818	0.29379
O263	0.41701	0.45193	0.30723
O264	0.06573	0.62558	0.08072
O265	0.08118	0.49373	0.06558
O266	0.11026	0.36312	0.06398
O267	0.30086	0.62991	0.11099
O268	0.32247	0.49959	0.07207
O269	0.29772	0.36663	0.07206
O270	0.51316	0.54372	0.2756
O271	0.51548	0.36466	0.27546
O272	0.44007	0.7508	0.64591
O273	0.19593	0.74798	0.65552
O274	0.27058	0.75022	0.04923
O275	0.10736	0.75004	0.05583
O276	0.0636	0.24939	0.13641
O277	0.30486	0.24775	0.1536
O278	0.22839	0.25129	0.54891
O279	0.39214	0.25149	0.54919
O280	0.56149	0.25164	0.35437
O281	0.79975	0.24255	0.33806
O282	0.72872	0.2451	0.95344
O283	0.88988	0.24935	0.94712
O284	0.9377	0.74933	0.86366
O285	0.69252	0.75063	0.8534
O286	0.76933	0.74673	0.44292
O287	0.60676	0.75119	0.45082
O288	0.95436	0.26306	0.44708
O289	0.91869	0.20214	0.60073
O290	0.86708	0.32004	0.56102
O291	-0.02133	0.31428	0.62515
GA29	0.92269	0.40185	0.61087
H293	0.93869	0.29426	0.39188
H294	0.82296	0.33906	0.49023
H295	0.89341	0.17261	0.55536
H296	0.92804	0.46699	0.45583
H297	0.01696	0.3805	0.42822
H298	0.06846	0.41897	0.51898
H299	0.04944	0.46191	0.40603
H300	-0.00031	0.5651	0.49037

H301	0.02605	0.5305	0.60568
H302	0.94152	0.55636	0.58981
AL30	0.8153	0.32551	0.3133
AL30	0.80468	0.47428	0.69878
P305	0.93137	0.27462	0.55793
C306	0.96823	0.46245	0.51175
C307	0.02882	0.42857	0.46426
C308	0.9842	0.53226	0.55268
<b>TS3</b>			
SI2	0.42379	0.05806	0.64801
SI3	0.30573	0.02821	0.79432
SI4	0.28016	0.05896	0.01516
SI5	0.12091	0.06337	0.01449
SI6	0.06707	0.02933	0.80286
SI7	0.1798	0.0573	0.66189
SI8	0.42038	0.82677	0.67399
SI9	0.30421	0.8697	0.81298
SI10	0.26633	0.82942	0.03194
SI11	0.11182	0.82689	0.01808
SI12	0.06486	0.87175	0.80384
SI13	0.18222	0.82796	0.67651
SI14	0.07586	0.9425	0.15349
SI15	0.19505	0.97231	0.29727
SI16	0.21796	0.93798	0.51919
SI17	0.37788	0.93408	0.51698
SI18	0.43179	0.96863	0.30654
SI19	0.32002	0.94288	0.16247
SI20	0.08163	0.17249	0.16863
SI21	0.1953	0.13086	0.31316
SI22	0.23274	0.17203	0.52979
SI23	0.38709	0.17388	0.51164
SI24	0.4353	0.1267	0.30055
SI25	0.31618	0.16813	0.17458
SI26	0.57729	0.55791	0.34946
SI27	0.68973	0.5311	0.19467
SI28	0.71532	0.55897	0.97904
SI29	0.87427	0.56616	0.9827
SI30	0.93103	0.53133	0.19162
SI31	0.81397	0.55401	0.32594
SI32	0.57837	0.32839	0.32975
SI33	0.69337	0.37477	0.18716
SI34	0.7289	0.32596	0.97286
SI35	0.88323	0.32581	0.98761

SI36	0.93507	0.37315	0.19527
SI37	0.92373	0.44109	0.85361
SI38	0.77788	0.43807	0.48243
SI39	0.61721	0.43434	0.48972
SI40	0.56391	0.46911	0.70321
SI41	0.67452	0.43764	0.84063
SI42	0.91658	0.67569	0.82744
SI43	0.80349	0.63629	0.68902
SI44	0.76448	0.6668	0.47015
SI45	0.60977	0.67229	0.48707
SI46	0.56133	0.62704	0.70101
SI47	0.68131	0.6736	0.82071
SI48	0.57721	0.94239	0.36232
SI49	0.69418	0.9674	0.21558
SI50	0.72039	0.93564	0.99541
SI51	0.87994	0.93386	0.99703
SI52	0.93141	0.96882	0.20626
SI53	0.81912	0.94438	0.35413
SI54	0.57786	0.17291	0.33393
SI55	0.69625	0.12307	0.19991
SI56	0.73353	0.1674	0.98042
SI57	0.88793	0.17215	0.98491
SI58	0.93781	0.12585	0.19586
SI59	0.81979	0.16556	0.32887
SI60	0.92299	0.053	0.85691
SI61	0.80122	0.02347	0.71168
SI62	0.78199	0.06574	0.49342
SI63	0.62132	0.07009	0.49219
SI64	0.56917	0.03021	0.70271
SI65	0.67853	0.05143	0.85319
SI66	0.92085	0.82813	0.83801
SI67	0.80201	0.86613	0.69292
SI68	0.76754	0.82393	0.47692
SI69	0.61327	0.82578	0.4959
SI70	0.56482	0.8725	0.70542
SI71	0.68142	0.82975	0.83441
SI72	0.41996	0.44388	0.64564
SI73	0.30346	0.47196	0.79306
SI74	0.2823	0.43624	0.01426
SI75	0.12415	0.43414	0.01102
SI76	0.07138	0.47106	0.80185
SI77	0.181	0.447	0.65453
SI78	0.42013	0.67281	0.66702
SI79	0.30159	0.62897	0.80459

SI80	0.26555	0.67159	0.02213
SI81	0.11109	0.67375	0.01124
SI82	0.06148	0.6293	0.80086
SI83	0.17927	0.66922	0.67034
SI84	0.07555	0.55524	0.14341
SI85	0.19591	0.52744	0.28789
SI86	0.21827	0.56565	0.50799
SI87	0.37951	0.56844	0.50792
SI88	0.43296	0.5308	0.29635
SI89	0.32165	0.55537	0.15267
SI90	0.08087	0.32633	0.16263
SI91	0.19602	0.3687	0.30803
SI92	0.23277	0.32962	0.52682
SI93	0.38707	0.32779	0.51074
SI94	0.43485	0.37266	0.29671
SI95	0.3172	0.32683	0.17107
O96	0.35893	0.06413	0.72023
O97	0.31001	0.0645	0.90274
O98	0.20007	0.04592	0.01278
O99	0.09185	0.06907	0.9021
O100	0.10422	0.05973	0.70518
O101	0.23022	0.03619	0.75182
O102	0.36027	0.82591	0.75517
O103	0.30516	0.84783	0.9293
O104	0.18878	0.8532	0.0227
O105	0.08538	0.83112	0.90415
O106	0.10473	0.8397	0.7091
O107	0.23048	0.85507	0.76609
O108	0.32333	0.94867	0.80236
O109	0.08529	0.95017	0.81622
O110	0.43217	0.12719	0.58452
O111	0.41711	0.99572	0.57025
O112	0.39622	0.86406	0.57231
O113	0.19878	0.13146	0.6212
O114	0.18285	0.00221	0.5724
O115	0.1976	0.86787	0.57328
O116	0.98737	0.03907	0.78631
O117	0.98494	0.86454	0.78569
O118	0.14171	0.93647	0.22349
O119	0.19216	0.93451	0.4045
O120	0.29829	0.94837	0.52407
O121	0.40124	0.92801	0.40154
O122	0.39592	0.94263	0.20487
O123	0.27007	0.96567	0.2522

O124	0.14105	0.17386	0.25065
O125	0.19218	0.15695	0.42744
O126	0.30993	0.14794	0.51586
O127	0.41392	0.17074	0.39757
O128	0.39377	0.15295	0.20335
O129	0.26979	0.1435	0.26791
O130	0.1764	0.05152	0.30788
O131	0.41798	0.04843	0.32261
O132	0.06643	0.87294	0.0913
O133	0.08197	0.00445	0.07488
O134	0.10785	0.1352	0.06811
O135	0.30163	0.86767	0.12479
O136	0.31537	0.99537	0.06985
O137	0.29613	0.12867	0.07297
O138	0.51113	0.95451	0.29472
O139	0.51468	0.13634	0.27915
O140	0.64249	0.56569	0.27867
O141	0.68197	0.57029	0.08887
O142	0.79562	0.54858	0.99009
O143	0.90654	0.57268	0.09375
O144	0.89161	0.55752	0.29049
O145	0.76736	0.53834	0.22984
O146	0.64107	0.33169	0.25452
O147	0.69044	0.34268	0.07601
O148	0.80646	0.35196	0.97859
O149	0.90749	0.32781	0.10329
O150	0.9006	0.34611	0.29801
O151	0.76705	0.37084	0.23414
O152	0.66856	0.45284	0.18321
O153	0.91723	0.45158	0.17468
O154	0.5662	0.62824	0.40858
O155	0.5851	0.49801	0.43134
O156	0.59648	0.36476	0.43527
O157	0.79427	0.625	0.37628
O158	0.80801	0.49238	0.40535
O159	0.80063	0.36131	0.44311
O160	0.01002	0.5447	0.2134
O161	0.01574	0.36521	0.20684
O162	0.86663	0.43041	0.76853
O163	0.81476	0.44544	0.58889
O164	0.69806	0.443	0.48763
O165	0.59056	0.43087	0.60335
O166	0.59684	0.43831	0.80363
O167	0.72139	0.45621	0.74792

O168	0.86021	0.68365	0.74129
O169	0.80805	0.64841	0.56854
O170	0.68675	0.64546	0.488
O171	0.57809	0.66573	0.59756
O172	0.60335	0.6613	0.79136
O173	0.72865	0.66014	0.72381
O174	0.81871	0.56013	0.71914
O175	0.58147	0.54851	0.69124
O176	0.93167	0.3739	0.92149
O177	0.91193	0.50549	0.9246
O178	0.8871	0.63641	0.92451
O179	0.69074	0.36235	0.88148
O180	0.683	0.49152	0.93195
O181	0.70158	0.6253	0.91277
O182	0.48393	0.45852	0.71571
O183	0.48169	0.63499	0.72354
O184	0.64064	0.93123	0.28878
O185	0.69645	0.92709	0.11035
O186	0.80043	0.94856	0.98758
O187	0.90137	0.9256	0.11329
O188	0.89454	0.94861	0.30998
O189	0.76802	0.96474	0.26509
O190	0.64273	0.16743	0.26218
O191	0.69845	0.15252	0.08725
O192	0.81149	0.14427	0.98676
O193	0.91886	0.16853	0.09652
O194	0.89617	0.15357	0.29072
O195	0.76938	0.12603	0.25268
O196	0.67198	0.04505	0.19759
O197	0.91975	0.04734	0.17844
O198	0.56655	0.87525	0.42953
O199	0.58802	0.00561	0.43729
O200	0.59262	0.13841	0.44196
O201	0.80536	0.86828	0.39249
O202	0.8116	0.9963	0.4473
O203	0.81575	0.13152	0.44111
O204	0.01037	0.95333	0.22293
O205	0.0174	0.13448	0.21697
O206	0.85672	0.05259	0.78783
O207	0.80182	0.06961	0.61119
O208	0.70172	0.06693	0.47774
O209	0.60199	0.07139	0.60976
O210	0.60352	0.05245	0.80745
O211	0.72845	0.02687	0.76445

O212	0.85865	0.83206	0.7617
O213	0.80536	0.83125	0.58373
O214	0.69081	0.85056	0.48858
O215	0.58878	0.82667	0.61145
O216	0.60435	0.8478	0.80517
O217	0.72863	0.85422	0.74197
O218	0.81703	0.94607	0.68211
O219	0.58135	0.95069	0.68129
O220	0.93148	0.12648	0.90843
O221	0.9194	0.99612	0.94445
O222	0.90066	0.86418	0.94246
O223	0.69702	0.12633	0.89128
O224	0.68179	-0.00028	0.94703
O225	0.70164	0.86718	0.9372
O226	0.49026	0.04701	0.71497
O227	0.48491	0.86392	0.72322
O228	0.3545	0.43601	0.71617
O229	0.30454	0.43138	0.89804
O230	0.20274	0.45152	0.02534
O231	0.10572	0.43023	0.89328
O232	0.10458	0.44928	0.6957
O233	0.22859	0.46908	0.7467
O234	0.35459	0.67026	0.73777
O235	0.30268	0.66055	0.91584
O236	0.18813	0.64746	0.01201
O237	0.08333	0.67336	0.89745
O238	0.10173	0.65658	0.70297
O239	0.22726	0.63616	0.75591
O240	0.32347	0.55033	0.80931
O241	0.08057	0.55105	0.82115
O242	0.4317	0.37445	0.58425
O243	0.41148	0.50456	0.56563
O244	0.40338	0.63774	0.56037
O245	0.1975	0.37171	0.61622
O246	0.18755	0.49889	0.56128
O247	0.19212	0.63334	0.56297
O248	0.99307	0.45159	0.79168
O249	0.98164	0.63636	0.78187
O250	0.14144	0.56058	0.2132
O251	0.19159	0.56725	0.39361
O252	0.29887	0.56181	0.51203
O253	0.4056	0.5707	0.39385
O254	0.39647	0.56055	0.1977
O255	0.2705	0.53447	0.24208

O256	0.13907	0.32857	0.24668
O257	0.19314	0.34293	0.42275
O258	0.30985	0.35411	0.51376
O259	0.41429	0.33185	0.39711
O260	0.39444	0.34121	0.20207
O261	0.26952	0.35418	0.26132
O262	0.17885	0.44843	0.30407
O263	0.4158	0.45144	0.31013
O264	0.0664	0.62462	0.08105
O265	0.08069	0.49276	0.06513
O266	0.10656	0.36173	0.06015
O267	0.30178	0.62812	0.10832
O268	0.32188	0.49834	0.06579
O269	0.29996	0.36513	0.06713
O270	0.51237	0.54263	0.28074
O271	0.51441	0.36467	0.27696
O272	0.43959	0.75027	0.64475
O273	0.19506	0.74854	0.6574
O274	0.27023	0.74967	0.05432
O275	0.10643	0.74945	0.05543
O276	0.06221	0.24899	0.13823
O277	0.30494	0.24744	0.15344
O278	0.2292	0.25117	0.5569
O279	0.3921	0.25097	0.55015
O280	0.56025	0.25095	0.35465
O281	0.80172	0.24343	0.33471
O282	0.72775	0.24591	0.95227
O283	0.89023	0.24944	0.94641
O284	0.93881	0.75046	0.86301
O285	0.69064	0.75058	0.85695
O286	0.7696	0.74598	0.44208
O287	0.60629	0.7502	0.45217
O288	0.95679	0.25926	0.41408
O289	0.94459	0.1982	0.57717
O290	0.88577	0.31218	0.55397
O291	1.01124	0.30483	0.57406
GA29	0.92072	0.41045	0.61965
H293	0.93778	0.2949	0.3671
H294	0.83478	0.33601	0.49355
H295	0.9074	0.17142	0.55059
H296	0.94321	0.45055	0.43409
H297	0.03528	0.37806	0.39192
H298	0.02813	0.35583	0.52099
H299	0.09125	0.42316	0.47948

H300	0.01362	0.5587	0.45181
H301	0.04448	0.5275	0.5676
H302	0.95755	0.54752	0.55257
AL30	0.81495	0.32751	0.31763
AL30	0.80041	0.47603	0.71146
P305	0.94945	0.27053	0.52926
C306	0.99031	0.45703	0.47519
C307	0.04032	0.40914	0.45919
C308	1.00185	0.52586	0.51626

### C<sub>3</sub>H<sub>6</sub>\*

SI2	0.42338	0.0582	0.64809
SI3	0.30567	0.02839	0.79436
SI4	0.27966	0.05822	0.01543
SI5	0.1206	0.06285	0.01452
SI6	0.06671	0.02947	0.80323
SI7	0.17962	0.05756	0.66254
SI8	0.42017	0.82683	0.67446
SI9	0.30418	0.86999	0.81294
SI10	0.26633	0.82949	0.03179
SI11	0.11182	0.82645	0.01851
SI12	0.06484	0.87206	0.80456
SI13	0.18202	0.82824	0.67663
SI14	0.07568	0.94218	0.15354
SI15	0.19486	0.97257	0.29734
SI16	0.21761	0.93841	0.51918
SI17	0.37754	0.934	0.51709
SI18	0.43176	0.96821	0.3066
SI19	0.31973	0.94234	0.16312
SI20	0.08157	0.17257	0.1685
SI21	0.19497	0.13143	0.3132
SI22	0.23255	0.17191	0.52989
SI23	0.38691	0.17381	0.51125
SI24	0.43487	0.12631	0.30008
SI25	0.31579	0.16822	0.17405
SI26	0.57888	0.55712	0.35048
SI27	0.69106	0.53118	0.19547
SI28	0.71704	0.55916	0.97862
SI29	0.87571	0.56709	0.98654
SI30	0.93023	0.531	0.19485
SI31	0.81421	0.55232	0.32988
SI32	0.57857	0.32861	0.33064
SI33	0.69478	0.37479	0.18988
SI34	0.72976	0.32668	0.97384

SI35	0.88397	0.32625	0.98982
SI36	0.93533	0.3726	0.19672
SI37	0.92466	0.44299	0.86115
SI38	0.78056	0.4365	0.48882
SI39	0.61944	0.43284	0.49174
SI40	0.56368	0.46876	0.70373
SI41	0.67544	0.43829	0.84016
SI42	0.91678	0.67613	0.83015
SI43	0.80311	0.63683	0.69125
SI44	0.76454	0.6665	0.4721
SI45	0.6098	0.6717	0.48884
SI46	0.56112	0.62683	0.7024
SI47	0.68112	0.6739	0.82258
SI48	0.57691	0.94193	0.3621
SI49	0.69352	0.96733	0.2146
SI50	0.72004	0.9368	0.99493
SI51	0.87936	0.93467	0.99674
SI52	0.93142	0.96833	0.20595
SI53	0.8183	0.94333	0.35213
SI54	0.57713	0.17309	0.33284
SI55	0.69502	0.1231	0.1982
SI56	0.7333	0.16809	0.97936
SI57	0.8879	0.17266	0.98409
SI58	0.93784	0.12547	0.19503
SI59	0.81908	0.16488	0.32671
SI60	0.92243	0.05318	0.85593
SI61	0.80056	0.02278	0.71095
SI62	0.78052	0.06387	0.4924
SI63	0.62019	0.07007	0.49121
SI64	0.56881	0.03067	0.70214
SI65	0.67826	0.05215	0.85242
SI66	0.92055	0.82852	0.83739
SI67	0.80205	0.86513	0.69136
SI68	0.76709	0.82325	0.47539
SI69	0.61299	0.82523	0.49572
SI70	0.56464	0.87306	0.70493
SI71	0.68133	0.83	0.83388
SI72	0.42014	0.44344	0.64613
SI73	0.3032	0.4712	0.79232
SI74	0.28324	0.43693	0.01465
SI75	0.12531	0.4344	0.01156
SI76	0.0718	0.47176	0.80314
SI77	0.17997	0.44659	0.65459
SI78	0.42008	0.67295	0.66772

SI79	0.30101	0.62871	0.80361
SI80	0.26613	0.67116	0.02215
SI81	0.11161	0.67323	0.01173
SI82	0.0617	0.6299	0.80095
SI83	0.17873	0.6697	0.66978
SI84	0.07533	0.55484	0.1441
SI85	0.19631	0.52742	0.28789
SI86	0.21844	0.56566	0.50873
SI87	0.37967	0.56828	0.50914
SI88	0.43323	0.53034	0.2979
SI89	0.32271	0.55586	0.15316
SI90	0.08138	0.32627	0.16109
SI91	0.19643	0.36826	0.30676
SI92	0.23248	0.32963	0.52606
SI93	0.38685	0.32775	0.51088
SI94	0.43471	0.37263	0.29712
SI95	0.31795	0.32665	0.1702
O96	0.35857	0.06489	0.72037
O97	0.31018	0.06381	0.90338
O98	0.19963	0.04485	0.01178
O99	0.09103	0.06955	0.90248
O100	0.104	0.06009	0.70568
O101	0.23	0.03682	0.75256
O102	0.3604	0.82577	0.75623
O103	0.30509	0.84961	0.9298
O104	0.1887	0.85299	0.02292
O105	0.0852	0.83116	0.90468
O106	0.10462	0.84014	0.70963
O107	0.2305	0.8549	0.76629
O108	0.3233	0.94885	0.80034
O109	0.0855	0.95049	0.81697
O110	0.43194	0.12713	0.58411
O111	0.41648	0.9957	0.57071
O112	0.39531	0.8641	0.57305
O113	0.19825	0.13189	0.62164
O114	0.18298	0.00278	0.57282
O115	0.19731	0.86851	0.57367
O116	0.98707	0.03898	0.78595
O117	0.98489	0.86546	0.78652
O118	0.1417	0.93686	0.22323
O119	0.19107	0.93522	0.40484
O120	0.29795	0.94863	0.52268
O121	0.40168	0.9277	0.40202
O122	0.39567	0.94208	0.20523

O123	0.27004	0.96532	0.25315
O124	0.14022	0.17445	0.2518
O125	0.19137	0.15679	0.42803
O126	0.3096	0.148	0.51564
O127	0.41359	0.17044	0.39714
O128	0.39315	0.15215	0.2029
O129	0.26931	0.14536	0.2684
O130	0.17676	0.052	0.30699
O131	0.41793	0.04803	0.32263
O132	0.06643	0.87241	0.09197
O133	0.08134	0.00398	0.0745
O134	0.10857	0.13452	0.06913
O135	0.30121	0.86715	0.12561
O136	0.31491	0.99488	0.07059
O137	0.29479	0.12799	0.07356
O138	0.51104	0.95403	0.29402
O139	0.51411	0.13633	0.278
O140	0.64244	0.56678	0.27692
O141	0.68492	0.57001	0.0893
O142	0.79735	0.54719	0.98662
O143	0.90322	0.57426	0.10032
O144	0.89208	0.55581	0.29556
O145	0.76824	0.5378	0.23263
O146	0.64114	0.33187	0.25522
O147	0.69328	0.34238	0.07893
O148	0.80739	0.35218	0.97809
O149	0.9054	0.32661	0.10693
O150	0.90313	0.34385	0.30057
O151	0.76773	0.37062	0.23957
O152	0.66991	0.4528	0.18467
O153	0.91663	0.45104	0.17714
O154	0.56664	0.62687	0.41078
O155	0.59074	0.49717	0.43098
O156	0.59718	0.36379	0.43669
O157	0.79455	0.62337	0.37995
O158	0.80681	0.49031	0.4079
O159	0.80376	0.35972	0.44717
O160	0.00948	0.54473	0.21309
O161	0.01613	0.36525	0.20368
O162	0.86531	0.4335	0.78209
O163	0.8192	0.44462	0.59264
O164	0.70039	0.43795	0.49505
O165	0.5894	0.43048	0.60352
O166	0.59753	0.43844	0.8036

O167	0.72253	0.45567	0.74743
O168	0.85966	0.68366	0.74529
O169	0.80822	0.6506	0.57113
O170	0.68682	0.64516	0.49026
O171	0.57807	0.66619	0.59948
O172	0.60335	0.65974	0.79362
O173	0.72836	0.66182	0.72531
O174	0.81753	0.56058	0.72005
O175	0.58041	0.54825	0.69072
O176	0.93412	0.37539	0.92862
O177	0.91852	0.50768	0.93375
O178	0.88868	0.63758	0.9288
O179	0.69065	0.36347	0.88402
O180	0.68291	0.49301	0.93068
O181	0.70329	0.6266	0.91475
O182	0.4837	0.45757	0.71721
O183	0.4815	0.63549	0.72505
O184	0.64073	0.93134	0.28913
O185	0.6948	0.92725	0.10919
O186	0.8	0.95073	0.98987
O187	0.90202	0.92531	0.11236
O188	0.89402	0.94802	0.30927
O189	0.76785	0.96475	0.2627
O190	0.64198	0.16764	0.26092
O191	0.69753	0.15215	0.08551
O192	0.8113	0.14525	0.98667
O193	0.91904	0.16775	0.09553
O194	0.89576	0.15331	0.28983
O195	0.7684	0.12642	0.25082
O196	0.67116	0.04503	0.19715
O197	0.91979	0.04694	0.17862
O198	0.5664	0.8746	0.42884
O199	0.58689	0.00524	0.43734
O200	0.59173	0.13832	0.44075
O201	0.80414	0.8672	0.38954
O202	0.81003	0.99472	0.44603
O203	0.81574	0.12939	0.43918
O204	0.01032	0.953	0.22334
O205	0.01723	0.1346	0.21678
O206	0.85631	0.05206	0.78649
O207	0.80037	0.06831	0.60972
O208	0.70063	0.06697	0.47539
O209	0.60149	0.07187	0.60897
O210	0.60323	0.05313	0.80671

O211	0.7279	0.02672	0.76386
O212	0.8595	0.83137	0.7589
O213	0.80574	0.83148	0.58135
O214	0.69049	0.85005	0.48814
O215	0.58853	0.82698	0.61126
O216	0.60453	0.8493	0.80478
O217	0.72888	0.85185	0.74033
O218	0.81607	0.94536	0.6819
O219	0.58096	0.95124	0.68021
O220	0.93057	0.12703	0.90641
O221	0.91901	0.9969	0.94437
O222	0.89832	0.8652	0.94046
O223	0.69737	0.12713	0.88947
O224	0.68135	0.00095	0.94687
O225	0.70288	0.86866	0.93507
O226	0.48989	0.04728	0.71493
O227	0.48476	0.86433	0.72299
O228	0.3542	0.435	0.71561
O229	0.30528	0.43204	0.89838
O230	0.20377	0.45238	0.02643
O231	0.10752	0.43124	0.89359
O232	0.10356	0.44865	0.69624
O233	0.2281	0.46636	0.74716
O234	0.35411	0.67053	0.73766
O235	0.30253	0.65888	0.91565
O236	0.18866	0.64691	0.01393
O237	0.08465	0.6735	0.89754
O238	0.10115	0.65755	0.70251
O239	0.22655	0.63682	0.75577
O240	0.32251	0.54994	0.8059
O241	0.08157	0.55174	0.82035
O242	0.43187	0.37426	0.58388
O243	0.412	0.50445	0.56659
O244	0.40377	0.63763	0.56111
O245	0.19491	0.37127	0.61394
O246	0.18752	0.49935	0.56295
O247	0.19198	0.63365	0.56264
O248	0.99346	0.4521	0.79584
O249	0.98173	0.63689	0.78389
O250	0.14102	0.56044	0.21443
O251	0.19246	0.56661	0.39409
O252	0.29904	0.56161	0.51413
O253	0.40527	0.57038	0.39485
O254	0.39746	0.5606	0.1989

O255	0.27074	0.53536	0.24158
O256	0.1392	0.3283	0.24581
O257	0.19341	0.34179	0.42134
O258	0.30952	0.35413	0.51518
O259	0.41331	0.33144	0.3969
O260	0.39511	0.34087	0.20185
O261	0.26995	0.35293	0.26071
O262	0.18059	0.44806	0.303
O263	0.41474	0.45114	0.31078
O264	0.06655	0.62395	0.08071
O265	0.08118	0.49204	0.06645
O266	0.10828	0.3613	0.05902
O267	0.30344	0.62877	0.10852
O268	0.32314	0.49882	0.06619
O269	0.30082	0.3656	0.06685
O270	0.51298	0.54057	0.28441
O271	0.51447	0.36543	0.27894
O272	0.43946	0.75042	0.6451
O273	0.1948	0.74897	0.65658
O274	0.27089	0.74962	0.05226
O275	0.10685	0.74902	0.05587
O276	0.06249	0.24886	0.13682
O277	0.30578	0.24738	0.15082
O278	0.22796	0.25115	0.55685
O279	0.39159	0.25082	0.55002
O280	0.55967	0.25102	0.35389
O281	0.80285	0.24277	0.33747
O282	0.72758	0.24664	0.9523
O283	0.89137	0.25016	0.94699
O284	0.93917	0.75132	0.86415
O285	0.68838	0.7511	0.85916
O286	0.76892	0.74531	0.44097
O287	0.60586	0.74947	0.45289
O288	0.97126	0.26071	0.41004
O289	0.92914	0.17355	0.53641
O290	0.88868	0.29602	0.54911
O291	0.00712	0.26209	0.59065
GA29	0.93833	0.4027	0.62412
H293	0.94549	0.29441	0.36611
H294	0.83486	0.33239	0.49492
H295	0.88659	0.15707	0.506
H296	0.95571	0.46168	0.39378
H297	0.03705	0.37082	0.40059
H298	0.0496	0.26682	0.55574

H299	0.0904	0.42059	0.48651
H300	0.01265	0.57457	0.43648
H301	0.05214	0.53446	0.5404
H302	0.96346	0.54574	0.53654
AL30	0.81712	0.32702	0.32067
AL30	0.80294	0.47537	0.71419
P305	0.94504	0.24957	0.5189
C306	1.00082	0.46777	0.43915
C307	0.0446	0.41695	0.44291
C308	0.00811	0.53364	0.4915

**b) structures involved in propene aromatization to benzene over P/Ga/ZSM-5 (states shown in Fig. 5)**

**2C<sub>3</sub>H<sub>6</sub>\***

SI2	0.42397	0.05648	0.64701
SI3	0.30551	0.02673	0.7935
SI4	0.27945	0.05782	0.01356
SI5	0.12057	0.06201	0.01433
SI6	0.06723	0.02811	0.80358
SI7	0.17929	0.05546	0.66025
SI8	0.42041	0.82601	0.67365
SI9	0.30416	0.86835	0.81336
SI10	0.26575	0.82813	0.03264
SI11	0.11131	0.82516	0.01938
SI12	0.06491	0.87095	0.80553
SI13	0.18173	0.82759	0.67577
SI14	0.07527	0.94178	0.15312
SI15	0.19532	0.97256	0.29595
SI16	0.21755	0.93722	0.51779
SI17	0.37717	0.93289	0.51673
SI18	0.43076	0.96737	0.30695
SI19	0.32011	0.94299	0.16011
SI20	0.08146	0.17166	0.16879
SI21	0.19468	0.13084	0.31412
SI22	0.23254	0.17137	0.53098
SI23	0.38696	0.1731	0.51196
SI24	0.43415	0.12506	0.30099
SI25	0.31541	0.1667	0.17393
SI26	0.57778	0.55544	0.35105
SI27	0.68904	0.53037	0.19449
SI28	0.71649	0.55825	0.97745
SI29	0.87471	0.56592	0.98525
SI30	0.92791	0.5268	0.19124
SI31	0.81307	0.54973	0.33024

SI32	0.57768	0.32783	0.33049
SI33	0.69396	0.37426	0.19033
SI34	0.72957	0.3257	0.97399
SI35	0.88349	0.32441	0.98933
SI36	0.93371	0.37002	0.1943
SI37	0.92538	0.44172	0.86282
SI38	0.78041	0.43449	0.49184
SI39	0.61957	0.43066	0.49234
SI40	0.56304	0.46824	0.70312
SI41	0.67462	0.4375	0.84015
SI42	0.91616	0.67503	0.83001
SI43	0.80351	0.63484	0.69066
SI44	0.76613	0.665	0.47056
SI45	0.61107	0.67038	0.48792
SI46	0.56241	0.62606	0.70187
SI47	0.68173	0.67284	0.82172
SI48	0.57678	0.94127	0.36216
SI49	0.69353	0.96661	0.21445
SI50	0.72	0.93544	0.99456
SI51	0.87946	0.93353	0.99675
SI52	0.93106	0.96822	0.20613
SI53	0.81845	0.94268	0.35296
SI54	0.57639	0.17221	0.33235
SI55	0.69459	0.12254	0.19755
SI56	0.73311	0.16733	0.9787
SI57	0.88782	0.17165	0.98216
SI58	0.93747	0.12541	0.19386
SI59	0.81854	0.16496	0.32569
SI60	0.92261	0.05175	0.85517
SI61	0.80075	0.02204	0.70957
SI62	0.78086	0.06387	0.4918
SI63	0.62058	0.06978	0.4906
SI64	0.56952	0.02936	0.70119
SI65	0.6786	0.05095	0.85194
SI66	0.92064	0.8277	0.83788
SI67	0.80208	0.8648	0.69115
SI68	0.7682	0.82175	0.47552
SI69	0.61379	0.82385	0.49473
SI70	0.56522	0.87186	0.70359
SI71	0.6814	0.82927	0.83314
SI72	0.41982	0.4443	0.64495
SI73	0.30152	0.47216	0.79131
SI74	0.28388	0.43397	0.01179
SI75	0.12617	0.4324	0.00963

SI76	0.07263	0.47033	0.80235
SI77	0.17917	0.44713	0.6509
SI78	0.42088	0.67175	0.66603
SI79	0.30028	0.62902	0.80314
SI80	0.26586	0.67129	0.02139
SI81	0.11123	0.67181	0.01394
SI82	0.06128	0.62862	0.80223
SI83	0.17751	0.66906	0.66879
SI84	0.07447	0.5519	0.14315
SI85	0.19707	0.52609	0.28709
SI86	0.21786	0.56603	0.50802
SI87	0.37843	0.5681	0.50881
SI88	0.43001	0.52843	0.29845
SI89	0.32314	0.55344	0.14751
SI90	0.08052	0.32577	0.15976
SI91	0.19679	0.36724	0.30661
SI92	0.2324	0.32825	0.52563
SI93	0.38697	0.32675	0.51217
SI94	0.434	0.37142	0.29845
SI95	0.31855	0.32517	0.16897
O96	0.35921	0.06189	0.71949
O97	0.30794	0.06514	0.90051
O98	0.1995	0.04332	0.01281
O99	0.09191	0.06937	0.90171
O100	0.10408	0.05771	0.70493
O101	0.23053	0.0332	0.74825
O102	0.36086	0.82532	0.75574
O103	0.30403	0.84496	0.92897
O104	0.18819	0.8519	0.02366
O105	0.08493	0.82943	0.90529
O106	0.10466	0.83966	0.71012
O107	0.23097	0.85453	0.76418
O108	0.32333	0.94753	0.80562
O109	0.08586	0.94926	0.81944
O110	0.43199	0.12586	0.58398
O111	0.41749	0.99444	0.56857
O112	0.39541	0.86288	0.57202
O113	0.19753	0.1304	0.62126
O114	0.18136	0.00191	0.5686
O115	0.19603	0.8676	0.57212
O116	0.98762	0.03736	0.78609
O117	0.98502	0.86451	0.78681
O118	0.14141	0.93724	0.22269
O119	0.19418	0.93306	0.40196

O120	0.29775	0.94794	0.52616
O121	0.39901	0.92614	0.4006
O122	0.39562	0.94277	0.20395
O123	0.26966	0.96778	0.2481
O124	0.13971	0.17358	0.25271
O125	0.1917	0.1575	0.42838
O126	0.30958	0.14749	0.51703
O127	0.41288	0.16998	0.39737
O128	0.39258	0.15005	0.20316
O129	0.26877	0.14373	0.26799
O130	0.17615	0.05141	0.31024
O131	0.41714	0.04702	0.32521
O132	0.06616	0.8716	0.09256
O133	0.08048	0.00313	0.07311
O134	0.10874	0.13346	0.06968
O135	0.3014	0.86752	0.1242
O136	0.3166	0.99436	0.06584
O137	0.29445	0.12713	0.07289
O138	0.51007	0.95298	0.29584
O139	0.51341	0.13457	0.27865
O140	0.6387	0.56646	0.27301
O141	0.68527	0.56951	0.08847
O142	0.79667	0.54454	0.98323
O143	0.90045	0.57293	0.10008
O144	0.89055	0.54853	0.29404
O145	0.76549	0.53642	0.23462
O146	0.63998	0.33114	0.25468
O147	0.69435	0.34044	0.08029
O148	0.80724	0.35113	0.97697
O149	0.90378	0.32178	0.10701
O150	0.90222	0.34345	0.29974
O151	0.76622	0.3715	0.24256
O152	0.66811	0.45192	0.18259
O153	0.91382	0.44745	0.16919
O154	0.5663	0.62483	0.41275
O155	0.59407	0.49533	0.42934
O156	0.5969	0.36185	0.43709
O157	0.79759	0.62251	0.37863
O158	0.80331	0.4898	0.41098
O159	0.80506	0.3586	0.44858
O160	0.00747	0.53903	0.20841
O161	0.01464	0.36395	0.20185
O162	0.86591	0.43184	0.78417
O163	0.82023	0.44271	0.59455

O164	0.70037	0.4333	0.50071
O165	0.58699	0.42955	0.60246
O166	0.59706	0.43672	0.80195
O167	0.72305	0.4545	0.74885
O168	0.85951	0.68255	0.74439
O169	0.80843	0.64827	0.57051
O170	0.68806	0.6438	0.48586
O171	0.5812	0.66556	0.59981
O172	0.60366	0.65895	0.79412
O173	0.72841	0.6591	0.72434
O174	0.81866	0.55889	0.72028
O175	0.58149	0.54738	0.69056
O176	0.93444	0.37475	0.93195
O177	0.91941	0.50752	0.93334
O178	0.88718	0.63688	0.92852
O179	0.68958	0.36313	0.88573
O180	0.68029	0.49318	0.9297
O181	0.70382	0.62646	0.91489
O182	0.48285	0.45885	0.71696
O183	0.4826	0.63459	0.72288
O184	0.63992	0.93085	0.28789
O185	0.69549	0.92638	0.10921
O186	0.80002	0.94871	0.98829
O187	0.90142	0.9252	0.11128
O188	0.89402	0.94783	0.30963
O189	0.7674	0.96363	0.26406
O190	0.64106	0.16667	0.26003
O191	0.6973	0.15181	0.08499
O192	0.81115	0.14447	0.98601
O193	0.91974	0.16675	0.09309
O194	0.89512	0.15488	0.2873
O195	0.76783	0.126	0.25052
O196	0.6714	0.04428	0.19612
O197	0.9189	0.04684	0.17924
O198	0.56715	0.87372	0.42875
O199	0.5875	0.00474	0.43686
O200	0.59156	0.13802	0.44058
O201	0.80551	0.86645	0.3908
O202	0.81006	0.99425	0.44656
O203	0.81683	0.12875	0.43783
O204	0.01005	0.95303	0.22304
O205	0.01684	0.13386	0.21651
O206	0.85692	0.05032	0.78508
O207	0.8003	0.06857	0.6093

O208	0.70101	0.06746	0.47416
O209	0.60222	0.07106	0.60851
O210	0.6036	0.05166	0.80607
O211	0.72841	0.02574	0.76349
O212	0.85914	0.83186	0.76031
O213	0.80593	0.82945	0.58232
O214	0.69141	0.84828	0.48711
O215	0.5894	0.82551	0.61037
O216	0.60442	0.84781	0.80391
O217	0.72879	0.85289	0.7404
O218	0.81605	0.94487	0.67869
O219	0.58197	0.94999	0.67888
O220	0.93035	0.12592	0.90452
O221	0.9188	0.99589	0.94411
O222	0.89953	0.86384	0.94192
O223	0.69722	0.12604	0.88912
O224	0.68165	-0.00022	0.94644
O225	0.70181	0.86725	0.93546
O226	0.49054	0.04572	0.71372
O227	0.48522	0.86363	0.7211
O228	0.35331	0.43859	0.7134
O229	0.30188	0.42876	0.8939
O230	0.20461	0.44815	0.02889
O231	0.1109	0.42998	0.89082
O232	0.10311	0.4481	0.69418
O233	0.22752	0.46942	0.74199
O234	0.35484	0.66759	0.73552
O235	0.30003	0.66423	0.91206
O236	0.18855	0.64593	0.01599
O237	0.08418	0.67125	0.89979
O238	0.10048	0.65761	0.70442
O239	0.22665	0.63557	0.75231
O240	0.32043	0.55013	0.81381
O241	0.08152	0.55038	0.8198
O242	0.43101	0.37385	0.58567
O243	0.41309	0.50389	0.56249
O244	0.40565	0.63715	0.55843
O245	0.19494	0.37167	0.61157
O246	0.18506	0.49893	0.55764
O247	0.1885	0.6332	0.5609
O248	0.99454	0.44942	0.7981
O249	0.98128	0.63534	0.78532
O250	0.13828	0.55635	0.21734
O251	0.19767	0.56847	0.39084

O252	0.29812	0.56246	0.52307
O253	0.39839	0.56967	0.3919
O254	0.39711	0.55727	0.19632
O255	0.26912	0.53312	0.23306
O256	0.13843	0.33021	0.24403
O257	0.19422	0.33723	0.41939
O258	0.30948	0.35262	0.51474
O259	0.41404	0.3299	0.39851
O260	0.39537	0.33859	0.20314
O261	0.26946	0.3528	0.25715
O262	0.18291	0.44737	0.31005
O263	0.41148	0.44928	0.31231
O264	0.06653	0.62265	0.08369
O265	0.08257	0.49134	0.06228
O266	0.10625	0.35981	0.05629
O267	0.30595	0.62669	0.10227
O268	0.32444	0.49666	0.06008
O269	0.30408	0.36326	0.06392
O270	0.50999	0.53829	0.29002
O271	0.51393	0.36619	0.28018
O272	0.43951	0.74952	0.64475
O273	0.1941	0.74828	0.65544
O274	0.26985	0.74872	0.05746
O275	0.10621	0.74785	0.05719
O276	0.06268	0.24793	0.13708
O277	0.30562	0.24589	0.15105
O278	0.22779	0.25032	0.56011
O279	0.39202	0.2499	0.55171
O280	0.55814	0.25014	0.35211
O281	0.80119	0.24256	0.33717
O282	0.72725	0.2458	0.95102
O283	0.89099	0.24898	0.94391
O284	0.93876	0.75025	0.86344
O285	0.68994	0.7503	0.85638
O286	0.77105	0.74398	0.44043
O287	0.60658	0.74812	0.45157
O288	0.97169	0.25994	0.40665
O289	0.93204	0.17173	0.53226
O290	0.89107	0.29434	0.54864
O291	0.0089	0.26196	0.58737
GA29	0.94004	0.39973	0.62576
H293	0.9457	0.29429	0.36428
H294	0.83665	0.33135	0.49537
H295	0.89005	0.15486	0.50071

H296	0.95467	0.46873	0.39952
H297	0.0361	0.37757	0.39275
H298	0.05244	0.24942	0.56048
H299	0.08827	0.41997	0.48791
H300	0.00902	0.5779	0.46523
H301	0.04878	0.52964	0.56052
H302	0.96003	0.54006	0.55755
H303	0.99374	0.77608	0.41535
H304	0.11401	0.7423	0.4549
H305	0.92458	0.68205	0.35765
H306	0.00087	0.63459	0.32269
H307	0.11085	0.7697	0.32958
H308	0.11192	0.68184	0.35674
AL30	0.81636	0.32681	0.32143
AL31	0.80375	0.47363	0.71589
P311	0.94699	0.24821	0.51601
C312	-0.00095	0.471	0.44712
C313	0.04293	0.42018	0.44288
C314	0.0051	0.53218	0.51125
C315	0.01757	0.73081	0.38516
C316	0.97897	0.68021	0.35407
C317	0.09226	0.73076	0.38125

### C<sub>6</sub>H<sub>13</sub>

SI2	0.42615	0.0561	0.64477
SI3	0.30656	0.02563	0.78931
SI4	0.28176	0.05862	0.01051
SI5	0.12226	0.06192	0.0123
SI6	0.06996	0.0268	0.80023
SI7	0.18053	0.05406	0.65466
SI8	0.42163	0.82538	0.6715
SI9	0.30555	0.86766	0.81107
SI10	0.26729	0.82812	0.03043
SI11	0.11292	0.82496	0.0155
SI12	0.0665	0.86954	0.80091
SI13	0.18397	0.82669	0.67303
SI14	0.07672	0.94103	0.1503
SI15	0.19661	0.97177	0.293
SI16	0.21953	0.93611	0.51458
SI17	0.3787	0.93289	0.51505
SI18	0.43162	0.96774	0.30504
SI19	0.32155	0.94402	0.15648
SI20	0.08303	0.17159	0.16603
SI21	0.19685	0.12873	0.3101

SI22	0.23453	0.17063	0.52682
SI23	0.38881	0.17268	0.51001
SI24	0.43647	0.12545	0.29902
SI25	0.31766	0.16579	0.17164
SI26	0.5788	0.55564	0.34423
SI27	0.6905	0.52964	0.18726
SI28	0.7197	0.55681	0.97188
SI29	0.87861	0.56274	0.97623
SI30	0.93061	0.52644	0.18592
SI31	0.81291	0.55034	0.32119
SI32	0.58029	0.32724	0.32526
SI33	0.6956	0.37332	0.18184
SI34	0.73296	0.32546	0.96848
SI35	0.88753	0.32405	0.9863
SI36	0.93618	0.36901	0.19424
SI37	0.92525	0.43852	0.85028
SI38	0.77908	0.43431	0.48251
SI39	0.61864	0.43196	0.48672
SI40	0.5656	0.46642	0.70085
SI41	0.67919	0.43731	0.8332
SI42	0.91742	0.67517	0.82204
SI43	0.80635	0.63326	0.68356
SI44	0.7664	0.66418	0.46431
SI45	0.61162	0.66961	0.48296
SI46	0.56474	0.62464	0.69865
SI47	0.68551	0.67137	0.81534
SI48	0.57824	0.94106	0.35951
SI49	0.69562	0.96569	0.2118
SI50	0.72188	0.93312	0.99189
SI51	0.88164	0.93349	0.99458
SI52	0.93234	0.96837	0.20532
SI53	0.82025	0.94253	0.35247
SI54	0.57904	0.17134	0.33069
SI55	0.69805	0.12168	0.1958
SI56	0.73575	0.16718	0.9772
SI57	0.89045	0.17083	0.97978
SI58	0.93968	0.12603	0.19348
SI59	0.82052	0.16618	0.32351
SI60	0.92461	0.0513	0.85228
SI61	0.80227	0.02215	0.70614
SI62	0.78288	0.06495	0.48899
SI63	0.62265	0.06936	0.48856
SI64	0.57163	0.02835	0.69978
SI65	0.68059	0.04993	0.85078

SI66	0.9223	0.82791	0.8358
SI67	0.80271	0.8655	0.68959
SI68	0.76957	0.82116	0.47521
SI69	0.61499	0.82344	0.49296
SI70	0.56628	0.87054	0.70245
SI71	0.68284	0.828	0.83055
SI72	0.42358	0.44437	0.64285
SI73	0.30465	0.472	0.79171
SI74	0.28565	0.4314	0.00754
SI75	0.12623	0.43216	0.00619
SI76	0.07036	0.46881	0.79556
SI77	0.18392	0.44562	0.65188
SI78	0.42439	0.67055	0.6629
SI79	0.30383	0.62875	0.80346
SI80	0.26857	0.67217	0.01707
SI81	0.11359	0.67139	0.00868
SI82	0.06221	0.62826	0.79651
SI83	0.18274	0.66808	0.66909
SI84	0.07777	0.55293	0.14434
SI85	0.19998	0.52606	0.28755
SI86	0.22693	0.564	0.50907
SI87	0.38667	0.56683	0.50505
SI88	0.43308	0.52832	0.29149
SI89	0.32372	0.55206	0.1427
SI90	0.08208	0.32607	0.15977
SI91	0.19796	0.36782	0.30704
SI92	0.23418	0.32748	0.5248
SI93	0.38866	0.32661	0.51057
SI94	0.43655	0.37056	0.29532
SI95	0.31878	0.32452	0.16983
O96	0.3611	0.06086	0.71685
O97	0.30674	0.06486	0.89563
O98	0.20161	0.04549	0.01563
O99	0.09621	0.06743	0.89796
O100	0.1058	0.05732	0.70141
O101	0.23225	0.03062	0.74136
O102	0.36152	0.82409	0.75276
O103	0.3057	0.844	0.92656
O104	0.18972	0.85176	0.01997
O105	0.08623	0.82884	0.90153
O106	0.10638	0.8375	0.70615
O107	0.23206	0.85446	0.76226
O108	0.32512	0.94672	0.80365
O109	0.08795	0.94775	0.81403

O110	0.43395	0.12576	0.58246
O111	0.41992	0.99418	0.56596
O112	0.3971	0.86269	0.5699
O113	0.19893	0.12886	0.61588
O114	0.18106	0.00024	0.56326
O115	0.19829	0.86639	0.56922
O116	0.99027	0.03674	0.7847
O117	0.98662	0.86307	0.78178
O118	0.14254	0.93581	0.22052
O119	0.19827	0.93088	0.39796
O120	0.29937	0.94826	0.5267
O121	0.39911	0.92656	0.39828
O122	0.39663	0.94328	0.2018
O123	0.27031	0.96986	0.24267
O124	0.14369	0.17199	0.24595
O125	0.1952	0.15778	0.42286
O126	0.31166	0.14633	0.51449
O127	0.41533	0.17011	0.39569
O128	0.39518	0.15156	0.20153
O129	0.27114	0.13745	0.2625
O130	0.17553	0.04985	0.31034
O131	0.41838	0.04748	0.32261
O132	0.06756	0.87103	0.08893
O133	0.08256	0.00249	0.07046
O134	0.10666	0.13377	0.06432
O135	0.30242	0.86843	0.12142
O136	0.31937	0.9948	0.06129
O137	0.29991	0.12818	0.06738
O138	0.51082	0.95267	0.29476
O139	0.51582	0.13399	0.27689
O140	0.64192	0.56472	0.26941
O141	0.68612	0.56916	0.08143
O142	0.80002	0.54337	0.97936
O143	0.9061	0.57036	0.09065
O144	0.89151	0.54982	0.28712
O145	0.76782	0.53712	0.22339
O146	0.64259	0.33083	0.24935
O147	0.69241	0.34134	0.0703
O148	0.81077	0.34955	0.97981
O149	0.91158	0.32179	0.1022
O150	0.90174	0.34333	0.29741
O151	0.76921	0.36894	0.22856
O152	0.66993	0.45126	0.17636
O153	0.91784	0.44683	0.16721

O154	0.56788	0.62584	0.40443
O155	0.5887	0.49557	0.42475
O156	0.59758	0.36249	0.4315
O157	0.79711	0.62355	0.36956
O158	0.80288	0.49147	0.402
O159	0.80182	0.36057	0.44059
O160	0.00968	0.541	0.20838
O161	0.01725	0.36399	0.20587
O162	0.862	0.42875	0.78101
O163	0.81855	0.44791	0.58358
O164	0.69863	0.4392	0.49177
O165	0.58692	0.42918	0.5977
O166	0.60085	0.43407	0.79808
O167	0.72403	0.45963	0.74069
O168	0.86111	0.68368	0.73583
O169	0.8105	0.64537	0.56235
O170	0.68876	0.64317	0.4814
O171	0.58136	0.66259	0.59432
O172	0.60723	0.65871	0.78856
O173	0.73105	0.65676	0.71689
O174	0.8257	0.55847	0.71409
O175	0.58312	0.54591	0.68955
O176	0.93694	0.37221	0.92174
O177	0.92285	0.50465	0.92269
O178	0.89073	0.6338	0.91881
O179	0.69832	0.36277	0.8751
O180	0.68395	0.49111	0.92559
O181	0.70807	0.62469	0.90779
O182	0.48545	0.45678	0.71785
O183	0.48544	0.63477	0.72298
O184	0.64051	0.93067	0.28361
O185	0.69896	0.92464	0.10728
O186	0.80196	0.9456	0.98248
O187	0.90176	0.9266	0.11141
O188	0.89575	0.94643	0.30841
O189	0.76867	0.96231	0.26384
O190	0.64419	0.16425	0.25986
O191	0.70052	0.15319	0.08437
O192	0.81386	0.14386	0.98403
O193	0.92345	0.16485	0.08968
O194	0.89754	0.15792	0.28509
O195	0.77131	0.12423	0.24869
O196	0.67479	0.0434	0.19102
O197	0.92054	0.04737	0.1817

O198	0.56902	0.87362	0.42652
O199	0.58992	0.00446	0.43385
O200	0.59283	0.13765	0.4398
O201	0.8075	0.86667	0.3923
O202	0.81267	0.99524	0.44459
O203	0.81871	0.12989	0.43569
O204	0.01139	0.95228	0.21989
O205	0.01909	0.13432	0.21651
O206	0.8596	0.0489	0.78118
O207	0.8015	0.06956	0.60697
O208	0.70297	0.0675	0.47124
O209	0.60469	0.06924	0.60665
O210	0.60569	0.05114	0.80447
O211	0.73063	0.02572	0.76198
O212	0.85915	0.83429	0.76175
O213	0.80691	0.8273	0.58275
O214	0.69278	0.84761	0.48655
O215	0.58988	0.82473	0.60826
O216	0.60534	0.84496	0.80214
O217	0.72919	0.85531	0.73879
O218	0.81682	0.94516	0.67278
O219	0.58364	0.94871	0.67919
O220	0.93249	0.12636	0.89926
O221	0.92007	0.99697	0.94309
O222	0.9052	0.86432	0.94122
O223	0.69917	0.12455	0.8897
O224	0.68353	0.99742	0.9437
O225	0.70233	0.86453	0.93453
O226	0.49266	0.04519	0.71159
O227	0.48616	0.86293	0.71991
O228	0.35515	0.444	0.7076
O229	0.3082	0.42521	0.89113
O230	0.20581	0.44546	0.01696
O231	0.10535	0.4301	0.88904
O232	0.10669	0.44865	0.69025
O233	0.22946	0.46792	0.7462
O234	0.35675	0.66317	0.72848
O235	0.30627	0.66771	0.90972
O236	0.19135	0.64699	0.00524
O237	0.08313	0.66934	0.89637
O238	0.10487	0.65577	0.70069
O239	0.22899	0.63595	0.75677
O240	0.32098	0.54971	0.82027
O241	0.07734	0.54908	0.81378

O242	0.43164	0.37242	0.58701
O243	0.42242	0.5027	0.55739
O244	0.41371	0.63623	0.55383
O245	0.19889	0.36964	0.61443
O246	0.19449	0.49638	0.55795
O247	0.19824	0.6313	0.56304
O248	0.99359	0.44493	0.78208
O249	0.98332	0.63892	0.7723
O250	0.13954	0.55862	0.22274
O251	0.20619	0.56734	0.39197
O252	0.30681	0.56044	0.52355
O253	0.40337	0.56889	0.38713
O254	0.39749	0.55692	0.19133
O255	0.26995	0.53077	0.22805
O256	0.14132	0.33027	0.24192
O257	0.19454	0.33864	0.42012
O258	0.31105	0.35218	0.51105
O259	0.41745	0.3315	0.39797
O260	0.3959	0.33668	0.20265
O261	0.27109	0.35462	0.25817
O262	0.18236	0.44793	0.31027
O263	0.41565	0.44909	0.30609
O264	0.0713	0.62283	0.08254
O265	0.08728	0.4919	0.0649
O266	0.106	0.36027	0.05509
O267	0.30573	0.62525	0.09802
O268	0.32467	0.49503	0.05598
O269	0.30398	0.36166	0.06392
O270	0.51243	0.54053	0.27832
O271	0.51581	0.3636	0.27359
O272	0.44075	0.74894	0.64284
O273	0.19757	0.7474	0.65391
O274	0.27157	0.74884	0.05711
O275	0.10834	0.74734	0.05215
O276	0.06448	0.24826	0.13616
O277	0.30416	0.24519	0.15466
O278	0.23045	0.24926	0.55739
O279	0.39322	0.24956	0.54924
O280	0.56155	0.24953	0.3485
O281	0.80055	0.24299	0.33169
O282	0.73103	0.24522	0.94678
O283	0.89508	0.24811	0.94104
O284	0.93862	0.74985	0.85989
O285	0.6945	0.74891	0.84946

O286	0.7724	0.74373	0.43815
O287	0.60769	0.7479	0.44928
O288	0.96168	0.27069	0.43535
O289	0.92522	0.17733	0.55373
O290	0.86582	0.28975	0.56251
O291	0.98618	0.27609	0.61956
GA29	0.01749	0.26256	0.76008
H293	0.93775	0.29882	0.38266
H294	0.83895	0.31982	0.51156
H295	0.88754	0.15852	0.51439
H296	0.97079	0.59174	0.58398
H297	0.08098	0.53762	0.55739
H298	0.0839	0.62009	0.50737
H299	0.07592	0.55065	0.42574
H300	0.97695	0.62833	0.36442
H301	0.98602	0.6827	0.47034
H302	0.90745	0.64389	0.44444
H303	0.92218	0.42127	0.45278
H304	0.03778	0.43202	0.37211
H305	0.8925	0.52421	0.51147
H306	0.95369	0.43047	0.56841
H307	0.03276	0.36627	0.46071
H308	0.07446	0.44155	0.49226
AL30	0.81468	0.32816	0.31917
AL31	0.80616	0.47294	0.70634
P311	0.93381	0.2557	0.54237
C312	0.98631	0.57703	0.5058
C313	0.06122	0.57043	0.49895
C314	0.96151	0.63729	0.44191
C315	0.96479	0.4471	0.48938
C316	0.94615	0.51693	0.49844
C317	0.03168	0.42102	0.45198

### **C<sub>6</sub>H<sub>12</sub>+Ga(H)**

SI2	0.42612	0.055	0.6446
SI3	0.30634	0.02498	0.78902
SI4	0.28162	0.05909	0.00972
SI5	0.1223	0.06172	0.01204
SI6	0.07035	0.02579	0.79994
SI7	0.18077	0.05261	0.65307
SI8	0.42197	0.8248	0.67079
SI9	0.30566	0.86768	0.81077
SI10	0.26793	0.82781	0.02988
SI11	0.11361	0.82465	0.01601

SI12	0.06652	0.86832	0.80186
SI13	0.18413	0.8269	0.67313
SI14	0.07714	0.94094	0.15017
SI15	0.19756	0.97128	0.2923
SI16	0.22013	0.93504	0.51329
SI17	0.37948	0.93164	0.51413
SI18	0.43173	0.968	0.30403
SI19	0.32215	0.94467	0.15438
SI20	0.08269	0.17071	0.16594
SI21	0.19696	0.12815	0.3105
SI22	0.23427	0.17022	0.52745
SI23	0.38853	0.1721	0.51095
SI24	0.4361	0.12582	0.29971
SI25	0.31762	0.16572	0.17136
SI26	0.57838	0.5544	0.34838
SI27	0.68635	0.52845	0.18939
SI28	0.71491	0.55758	0.97599
SI29	0.87337	0.56315	0.97804
SI30	0.93114	0.52682	0.18607
SI31	0.81068	0.55018	0.31894
SI32	0.58115	0.32675	0.32838
SI33	0.69399	0.37259	0.18389
SI34	0.7314	0.32359	0.97041
SI35	0.88545	0.3228	0.98342
SI36	0.93655	0.3689	0.19266
SI37	0.92702	0.43813	0.84782
SI38	0.78017	0.43125	0.47776
SI39	0.62176	0.43141	0.49117
SI40	0.56496	0.46662	0.70162
SI41	0.67898	0.43427	0.83539
SI42	0.91826	0.67287	0.82267
SI43	0.80535	0.63333	0.68248
SI44	0.76342	0.66429	0.46332
SI45	0.60874	0.66976	0.48337
SI46	0.56314	0.62448	0.69877
SI47	0.68355	0.67159	0.81697
SI48	0.57735	0.94036	0.35951
SI49	0.69434	0.96451	0.21248
SI50	0.72161	0.93276	0.99269
SI51	0.88135	0.93175	0.99362
SI52	0.93283	0.96691	0.20297
SI53	0.82001	0.94242	0.35071
SI54	0.57882	0.17132	0.33239
SI55	0.69608	0.11983	0.1966

SI56	0.73506	0.16488	0.97861
SI57	0.88936	0.16935	0.98067
SI58	0.93942	0.12416	0.19195
SI59	0.81936	0.16357	0.32184
SI60	0.92484	0.05021	0.85202
SI61	0.80251	0.02105	0.70594
SI62	0.78221	0.06398	0.48859
SI63	0.62219	0.06812	0.48875
SI64	0.57151	0.02759	0.69984
SI65	0.68074	0.04895	0.85055
SI66	0.92175	0.82615	0.8342
SI67	0.80264	0.86433	0.68798
SI68	0.76783	0.82096	0.47293
SI69	0.61315	0.82308	0.4924
SI70	0.56608	0.86999	0.70247
SI71	0.68285	0.82798	0.83069
SI72	0.42298	0.44358	0.64555
SI73	0.30377	0.47223	0.79294
SI74	0.28664	0.43223	0.01121
SI75	0.12834	0.4324	0.01087
SI76	0.07698	0.47214	0.80156
SI77	0.18316	0.44563	0.65146
SI78	0.4232	0.67007	0.66441
SI79	0.30342	0.62891	0.80566
SI80	0.26946	0.67197	0.02044
SI81	0.1148	0.67185	0.01192
SI82	0.06543	0.62972	0.80009
SI83	0.18325	0.66878	0.67038
SI84	0.07775	0.55299	0.14598
SI85	0.2005	0.52599	0.28832
SI86	0.22582	0.56354	0.50976
SI87	0.38546	0.56576	0.50742
SI88	0.4325	0.52611	0.29487
SI89	0.32516	0.55228	0.14504
SI90	0.08276	0.32532	0.16071
SI91	0.1987	0.36759	0.30788
SI92	0.23391	0.32698	0.52624
SI93	0.38835	0.3257	0.5136
SI94	0.43629	0.36933	0.29884
SI95	0.31998	0.32412	0.17103
O96	0.36123	0.05989	0.71676
O97	0.30498	0.06573	0.89412
O98	0.2017	0.04559	0.01791
O99	0.09779	0.06626	0.89705

O100	0.10618	0.054	0.69988
O101	0.23267	0.02779	0.7389
O102	0.36089	0.82451	0.75019
O103	0.30617	0.84183	0.92525
O104	0.19043	0.85164	0.01896
O105	0.08623	0.82721	0.90227
O106	0.10654	0.83671	0.70687
O107	0.23202	0.85599	0.76176
O108	0.32604	0.94661	0.80677
O109	0.08722	0.94649	0.81576
O110	0.43403	0.12451	0.582
O111	0.42024	0.99292	0.56601
O112	0.39937	0.86124	0.56752
O113	0.19931	0.12768	0.61605
O114	0.18216	0.00008	0.55984
O115	0.19747	0.86605	0.56862
O116	0.9907	0.03616	0.78507
O117	0.98665	0.8613	0.7823
O118	0.14307	0.93581	0.22003
O119	0.20027	0.92916	0.39615
O120	0.3001	0.94572	0.52707
O121	0.39951	0.92643	0.39707
O122	0.39706	0.94411	0.20037
O123	0.27079	0.97044	0.24038
O124	0.14327	0.17039	0.24591
O125	0.1955	0.15792	0.42278
O126	0.31153	0.1458	0.51483
O127	0.41498	0.17037	0.39645
O128	0.39508	0.15165	0.20193
O129	0.27096	0.13726	0.26185
O130	0.17645	0.04905	0.31205
O131	0.41878	0.04765	0.32299
O132	0.06812	0.87114	0.08845
O133	0.08237	0.00256	0.07065
O134	0.10587	0.13353	0.06363
O135	0.30344	0.86898	0.11957
O136	0.3202	0.99525	0.05904
O137	0.30063	0.1284	0.06666
O138	0.51092	0.95277	0.29298
O139	0.51545	0.13512	0.27775
O140	0.64019	0.56555	0.27215
O141	0.6773	0.56635	0.08287
O142	0.7947	0.55023	0.99392
O143	0.91058	0.56764	0.08549

O144	0.88777	0.55282	0.28118
O145	0.76419	0.53588	0.22266
O146	0.64177	0.32796	0.24928
O147	0.69198	0.34159	0.07195
O148	0.80887	0.34992	0.9761
O149	0.91141	0.32417	0.09805
O150	0.90152	0.34137	0.29424
O151	0.76781	0.36976	0.2302
O152	0.66591	0.44981	0.18134
O153	0.91816	0.44709	0.16953
O154	0.56469	0.62462	0.40684
O155	0.59499	0.49609	0.42948
O156	0.60383	0.3627	0.4323
O157	0.79291	0.62177	0.36991
O158	0.80098	0.49007	0.40043
O159	0.80109	0.35723	0.43783
O160	0.00966	0.54174	0.21045
O161	0.01731	0.36319	0.2052
O162	0.87592	0.42733	0.75187
O163	0.82505	0.44009	0.5817
O164	0.70232	0.43822	0.50618
O165	0.58689	0.42795	0.59977
O166	0.60163	0.43506	0.79822
O167	0.72801	0.45023	0.74367
O168	0.86343	0.67951	0.73367
O169	0.80691	0.64622	0.56219
O170	0.68588	0.64347	0.4821
O171	0.57888	0.66301	0.59488
O172	0.60571	0.65953	0.78764
O173	0.73117	0.6557	0.72123
O174	0.82192	0.55666	0.7088
O175	0.58333	0.54588	0.68924
O176	0.93264	0.37029	0.91377
O177	0.90253	0.49996	0.9154
O178	0.88763	0.63237	0.91778
O179	0.6941	0.3594	0.8778
O180	0.68692	0.48983	0.92417
O181	0.70232	0.62443	0.91073
O182	0.4854	0.45637	0.71991
O183	0.48388	0.63262	0.72367
O184	0.64046	0.92855	0.28547
O185	0.6976	0.92389	0.10757
O186	0.80165	0.94522	0.98462
O187	0.90291	0.9238	0.10982

O188	0.89524	0.9463	0.30595
O189	0.76803	0.96216	0.26258
O190	0.64358	0.16428	0.26057
O191	0.69854	0.15014	0.08446
O192	0.8129	0.14145	0.98655
O193	0.92243	0.16585	0.09093
O194	0.89586	0.15214	0.28466
O195	0.76958	0.12119	0.24861
O196	0.67163	0.0419	0.19327
O197	0.92176	0.04548	0.17543
O198	0.56668	0.87337	0.42713
O199	0.58855	0.00383	0.43387
O200	0.59295	0.13688	0.44073
O201	0.80633	0.86671	0.39092
O202	0.81333	0.99541	0.44265
O203	0.81569	0.13071	0.43625
O204	0.01171	0.9512	0.22002
O205	0.01848	0.13362	0.21621
O206	0.8599	0.04803	0.78039
O207	0.8006	0.0682	0.60652
O208	0.70232	0.06505	0.47063
O209	0.60477	0.06849	0.60694
O210	0.60581	0.05007	0.80445
O211	0.73092	0.02425	0.7623
O212	0.85973	0.83159	0.7576
O213	0.80491	0.82651	0.58068
O214	0.69091	0.84701	0.48415
O215	0.58959	0.82388	0.60842
O216	0.60542	0.84473	0.8021
O217	0.72953	0.85424	0.73881
O218	0.81708	0.94399	0.67239
O219	0.58355	0.948	0.67864
O220	0.93158	0.12408	0.90238
O221	0.92007	0.99439	0.94108
O222	0.9025	0.86219	0.93897
O223	0.69915	0.12385	0.88882
O224	0.68343	0.9971	0.94433
O225	0.70244	0.86433	0.93457
O226	0.49262	0.04442	0.71117
O227	0.4861	0.86232	0.72058
O228	0.35535	0.44243	0.71153
O229	0.30523	0.42631	0.89333
O230	0.20731	0.44635	0.02838
O231	0.11253	0.43149	0.89209

O232	0.10675	0.44976	0.69326
O233	0.22967	0.46928	0.74426
O234	0.35608	0.66437	0.73119
O235	0.30648	0.66676	0.91268
O236	0.19227	0.64634	0.01033
O237	0.0854	0.67233	0.89891
O238	0.10511	0.65861	0.70254
O239	0.22861	0.63662	0.75937
O240	0.32139	0.54985	0.82028
O241	0.08686	0.55211	0.81908
O242	0.4318	0.3719	0.58928
O243	0.42203	0.50238	0.56084
O244	0.41139	0.63576	0.55566
O245	0.19859	0.36975	0.61499
O246	0.19234	0.49601	0.55685
O247	0.19918	0.63104	0.56537
O248	0.99826	0.45521	0.7985
O249	0.98533	0.63527	0.78025
O250	0.14038	0.55822	0.22253
O251	0.20619	0.56785	0.39231
O252	0.30578	0.55789	0.52468
O253	0.40345	0.56757	0.38989
O254	0.399	0.55633	0.19423
O255	0.27091	0.53073	0.22949
O256	0.14164	0.33004	0.24331
O257	0.19544	0.33829	0.42069
O258	0.31109	0.35176	0.51376
O259	0.41757	0.33015	0.40118
O260	0.39731	0.3345	0.20543
O261	0.27181	0.35431	0.25862
O262	0.18337	0.44775	0.31087
O263	0.41303	0.44731	0.30825
O264	0.07127	0.62259	0.08321
O265	0.08616	0.49132	0.06682
O266	0.10686	0.36001	0.05655
O267	0.30779	0.62592	0.1014
O268	0.32698	0.49593	0.0572
O269	0.30714	0.36233	0.06541
O270	0.51258	0.53464	0.28466
O271	0.51633	0.36475	0.28059
O272	0.44155	0.74798	0.64441
O273	0.19933	0.74781	0.6547
O274	0.27225	0.74893	0.05912
O275	0.1098	0.74765	0.05593

O276	0.06467	0.24774	0.13748
O277	0.30436	0.24518	0.15435
O278	0.23088	0.24877	0.55825
O279	0.3934	0.24863	0.55204
O280	0.56196	0.24952	0.35339
O281	0.79958	0.24079	0.32575
O282	0.73008	0.24348	0.9507
O283	0.89088	0.24654	0.94165
O284	0.93794	0.74804	0.85919
O285	0.69391	0.74877	0.85064
O286	0.76994	0.74344	0.43543
O287	0.60472	0.74763	0.44836
O288	0.95052	0.2518	0.4225
O289	0.90563	0.18724	0.56834
O290	0.88639	0.31476	0.55943
O291	1.0017	0.26813	0.6006
GA29	0.91718	0.4038	0.61493
H293	0.93823	0.29025	0.37692
H294	0.84746	0.32397	0.50801
H295	0.87352	0.16842	0.51897
H296	0.97352	0.59802	0.5942
H297	0.08148	0.5441	0.55725
H298	0.08292	0.62711	0.50918
H299	0.07093	0.55886	0.42671
H300	0.97297	0.63601	0.37229
H301	0.98497	0.69045	0.47669
H302	0.90614	0.65184	0.4566
H303	0.91932	0.43047	0.43257
H304	0.04087	0.42881	0.36572
H305	0.89063	0.53345	0.49633
H306	0.99081	0.39018	0.64117
H307	0.02663	0.37444	0.46761
H308	0.0685	0.45148	0.48746
AL30	0.81506	0.32549	0.31496
AL31	0.80502	0.4728	0.70398
P311	0.94273	0.25383	0.53925
C312	0.98459	0.58479	0.51547
C313	0.05934	0.57777	0.50181
C314	0.96011	0.64428	0.45113
C315	0.9613	0.46048	0.46186
C316	0.94422	0.52354	0.49205
C317	0.02803	0.42779	0.44567

**C<sub>6</sub>H<sub>11</sub>Ga+H<sub>2</sub>\***

SI2	0.42597	0.05411	0.6439
SI3	0.3058	0.02418	0.78719
SI4	0.28261	0.05819	0.00926
SI5	0.12285	0.06053	0.01053
SI6	0.0708	0.02542	0.79806
SI7	0.18033	0.05109	0.65029
SI8	0.42242	0.82396	0.67143
SI9	0.30474	0.86648	0.80903
SI10	0.26759	0.82651	0.02859
SI11	0.113	0.82375	0.01614
SI12	0.0658	0.8675	0.80107
SI13	0.18299	0.82394	0.67325
SI14	0.07683	0.94035	0.14944
SI15	0.19775	0.96938	0.29327
SI16	0.21991	0.93135	0.51333
SI17	0.37949	0.93039	0.51366
SI18	0.43176	0.96643	0.30349
SI19	0.32208	0.94277	0.15391
SI20	0.08216	0.16881	0.16457
SI21	0.19853	0.12615	0.30827
SI22	0.23635	0.16915	0.52447
SI23	0.39068	0.17128	0.51003
SI24	0.43789	0.12407	0.29907
SI25	0.31967	0.16388	0.16989
SI26	0.57416	0.55687	0.34511
SI27	0.68817	0.5289	0.19161
SI28	0.71287	0.55531	0.97845
SI29	0.87204	0.55911	0.97099
SI30	0.93223	0.5255	0.18276
SI31	0.8147	0.55655	0.31455
SI32	0.57968	0.32643	0.32597
SI33	0.69546	0.37122	0.18254
SI34	0.72895	0.32174	0.9712
SI35	0.88337	0.32262	0.98168
SI36	0.93715	0.36679	0.19403
SI37	0.92362	0.43492	0.83613
SI38	0.7734	0.44106	0.46538
SI39	0.61474	0.43549	0.48078
SI40	0.5693	0.46803	0.69827
SI41	0.67764	0.43372	0.84038
SI42	0.91619	0.672	0.82213
SI43	0.80346	0.63426	0.68341
SI44	0.76322	0.66683	0.46265
SI45	0.60898	0.67114	0.4802

SI46	0.56407	0.62531	0.69687
SI47	0.68189	0.67053	0.81903
SI48	0.57782	0.94068	0.35991
SI49	0.69547	0.96449	0.21475
SI50	0.72217	0.93174	0.99392
SI51	0.88164	0.9306	0.99473
SI52	0.93197	0.96786	0.20421
SI53	0.821	0.94321	0.35409
SI54	0.58005	0.17067	0.33403
SI55	0.69856	0.11974	0.20107
SI56	0.73459	0.16354	0.98083
SI57	0.88831	0.16872	0.98374
SI58	0.93782	0.12514	0.19587
SI59	0.82053	0.16358	0.33008
SI60	0.92596	0.04988	0.85598
SI61	0.80307	0.02111	0.71115
SI62	0.78372	0.0641	0.49359
SI63	0.62298	0.06822	0.49069
SI64	0.57086	0.02565	0.70112
SI65	0.67931	0.04803	0.85284
SI66	0.9216	0.82456	0.83676
SI67	0.80214	0.86382	0.69211
SI68	0.76749	0.8229	0.47591
SI69	0.61357	0.82448	0.49476
SI70	0.56624	0.86826	0.70534
SI71	0.68267	0.82602	0.83447
SI72	0.42483	0.44367	0.63933
SI73	0.30867	0.46866	0.79361
SI74	0.28649	0.42982	0.00773
SI75	0.12745	0.4298	0.00684
SI76	0.0729	0.46695	0.79732
SI77	0.18753	0.44271	0.65643
SI78	0.42389	0.66892	0.66218
SI79	0.30402	0.62576	0.80245
SI80	0.26749	0.67028	0.01575
SI81	0.11264	0.67057	0.00838
SI82	0.0612	0.62554	0.79898
SI83	0.18122	0.66515	0.67074
SI84	0.07879	0.55127	0.14364
SI85	0.19849	0.52336	0.28913
SI86	0.22528	0.56299	0.51039
SI87	0.38552	0.56771	0.50245
SI88	0.4327	0.52846	0.28853
SI89	0.32132	0.55096	0.14529

SI90	0.08391	0.32336	0.16179
SI91	0.19836	0.36511	0.3087
SI92	0.23704	0.32579	0.52673
SI93	0.39129	0.32536	0.50837
SI94	0.43727	0.36992	0.29228
SI95	0.31843	0.32278	0.1701
O96	0.36082	0.05939	0.71549
O97	0.30485	0.06371	0.89316
O98	0.2025	0.04685	0.02002
O99	0.10062	0.06482	0.89451
O100	0.10562	0.05395	0.69711
O101	0.23205	0.0287	0.73763
O102	0.36022	0.82338	0.74889
O103	0.3055	0.84202	0.92414
O104	0.18995	0.85042	0.01984
O105	0.08608	0.82782	0.90234
O106	0.10543	0.83497	0.7064
O107	0.23098	0.85369	0.76124
O108	0.32468	0.94548	0.80289
O109	0.08654	0.94587	0.81206
O110	0.43553	0.12412	0.58274
O111	0.41902	0.99315	0.56367
O112	0.40138	0.86093	0.56782
O113	0.19882	0.12535	0.60934
O114	0.18151	-0.0039	0.56035
O115	0.1974	0.86202	0.56802
O116	0.99107	0.03763	0.78637
O117	0.98581	0.86015	0.7834
O118	0.14217	0.93621	0.2206
O119	0.20033	0.92585	0.39594
O120	0.29981	0.94257	0.52758
O121	0.3989	0.9251	0.39633
O122	0.39707	0.94255	0.19982
O123	0.27053	0.96788	0.24007
O124	0.14384	0.16633	0.24264
O125	0.19869	0.15985	0.4182
O126	0.31365	0.14461	0.51447
O127	0.41677	0.16876	0.39554
O128	0.39716	0.15067	0.20139
O129	0.27212	0.13328	0.25773
O130	0.17832	0.04721	0.31669
O131	0.41915	0.04621	0.32179
O132	0.06785	0.8695	0.09029
O133	0.08341	0.00012	0.06699

O134	0.10316	0.13174	0.06128
O135	0.30367	0.86704	0.11856
O136	0.31999	0.9938	0.05904
O137	0.30414	0.12768	0.06381
O138	0.51104	0.95139	0.29341
O139	0.5176	0.13265	0.2793
O140	0.64169	0.56033	0.27897
O141	0.67683	0.56765	0.0861
O142	0.79349	0.54713	0.99141
O143	0.91334	0.55784	0.07504
O144	0.89058	0.56146	0.27236
O145	0.7658	0.54203	0.2211
O146	0.6449	0.33013	0.25569
O147	0.68773	0.33872	0.07193
O148	0.80627	0.34856	0.97877
O149	0.9137	0.32736	0.09327
O150	0.90263	0.33386	0.2919
O151	0.77107	0.36468	0.22069
O152	0.6718	0.44961	0.18019
O153	0.91661	0.44562	0.18163
O154	0.56415	0.62846	0.40149
O155	0.57495	0.49767	0.42948
O156	0.59332	0.36429	0.4319
O157	0.79673	0.62617	0.37052
O158	0.80964	0.49328	0.39107
O159	0.79379	0.36319	0.42779
O160	0.01072	0.53919	0.20689
O161	0.01841	0.36247	0.20331
O162	0.87353	0.424	0.73832
O163	0.805	0.44655	0.57455
O164	0.69369	0.44969	0.46099
O165	0.59815	0.43109	0.59864
O166	0.60142	0.43536	0.79767
O167	0.72907	0.45389	0.75464
O168	0.86042	0.68149	0.73542
O169	0.80335	0.65075	0.56445
O170	0.68566	0.64368	0.47599
O171	0.57963	0.66278	0.59196
O172	0.60406	0.66234	0.7867
O173	0.72911	0.65473	0.72333
O174	0.82187	0.55769	0.70747
O175	0.58736	0.5475	0.68968
O176	0.92745	0.36878	0.90544
O177	0.89979	0.49902	0.89934

O178	0.88576	0.63061	0.91672
O179	0.69185	0.35739	0.87822
O180	0.68254	0.48603	0.93414
O181	0.69857	0.62046	0.91027
O182	0.48916	0.45811	0.70877
O183	0.48445	0.63099	0.72089
O184	0.64067	0.92786	0.28559
O185	0.69998	0.92426	0.10971
O186	0.80211	0.94452	0.98232
O187	0.90131	0.92447	0.11191
O188	0.89604	0.94683	0.30834
O189	0.76854	0.96273	0.26663
O190	0.64555	0.16423	0.26387
O191	0.70134	0.15059	0.08935
O192	0.81235	0.13925	0.9844
O193	0.91817	0.16743	0.09631
O194	0.89736	0.15402	0.2915
O195	0.77155	0.12111	0.25487
O196	0.67327	0.04208	0.19595
O197	0.91925	0.04663	0.17874
O198	0.56683	0.87526	0.43073
O199	0.58986	0.00551	0.43129
O200	0.59467	0.13779	0.44345
O201	0.8073	0.86771	0.39431
O202	0.8147	0.99575	0.44667
O203	0.81735	0.13064	0.44326
O204	0.01125	0.95292	0.21804
O205	0.01759	0.13328	0.21625
O206	0.86025	0.04861	0.78572
O207	0.80374	0.06829	0.61142
O208	0.70355	0.06463	0.47757
O209	0.60339	0.06683	0.60805
O210	0.60469	0.04879	0.80574
O211	0.73072	0.02589	0.76467
O212	0.85898	0.83063	0.76148
O213	0.8046	0.82759	0.58373
O214	0.69092	0.85011	0.48772
O215	0.58949	0.8227	0.61059
O216	0.60531	0.84257	0.80498
O217	0.72906	0.8528	0.7425
O218	0.81678	0.94377	0.67894
O219	0.58426	0.94617	0.68135
O220	0.93336	0.12281	0.90949
O221	0.92208	0.99225	0.94228

O222	0.90333	0.86044	0.94228
O223	0.69577	0.12254	0.89401
O224	0.68272	0.99501	0.94493
O225	0.70217	0.86265	0.93825
O226	0.49168	0.04143	0.71189
O227	0.48613	0.86108	0.72326
O228	0.35892	0.43997	0.70938
O229	0.315	0.4236	0.89439
O230	0.20678	0.44535	0.00883
O231	0.10188	0.42545	0.89196
O232	0.11016	0.44666	0.69381
O233	0.23249	0.46228	0.75289
O234	0.35603	0.66172	0.72724
O235	0.30656	0.66372	0.90966
O236	0.19024	0.64656	0.00107
O237	0.08039	0.66895	0.89735
O238	0.1036	0.65327	0.70355
O239	0.22892	0.63155	0.75601
O240	0.32405	0.54723	0.81779
O241	0.0791	0.54689	0.81916
O242	0.43512	0.37227	0.58257
O243	0.41824	0.50226	0.55553
O244	0.41426	0.6362	0.55191
O245	0.20258	0.36722	0.61741
O246	0.20112	0.49433	0.56518
O247	0.19407	0.62928	0.56351
O248	0.99483	0.44633	0.78032
O249	0.98176	0.63341	0.77675
O250	0.141	0.55732	0.22052
O251	0.20119	0.56268	0.39497
O252	0.30561	0.56572	0.51804
O253	0.40455	0.56848	0.38541
O254	0.39598	0.55751	0.19005
O255	0.27036	0.52937	0.23423
O256	0.14126	0.32463	0.24758
O257	0.19712	0.33807	0.4228
O258	0.3138	0.35058	0.51156
O259	0.41883	0.33054	0.39497
O260	0.39585	0.33666	0.20006
O261	0.27145	0.35201	0.25966
O262	0.18081	0.44464	0.30634
O263	0.41767	0.44874	0.30339
O264	0.07155	0.6211	0.08209
O265	0.08841	0.48973	0.06481

O266	0.11173	0.35832	0.06009
O267	0.30132	0.62322	0.09967
O268	0.32325	0.49318	0.06001
O269	0.30127	0.35969	0.06504
O270	0.51157	0.54274	0.27147
O271	0.51651	0.36162	0.26922
O272	0.44193	0.74721	0.64514
O273	0.19731	0.74444	0.65808
O274	0.27186	0.74714	0.05481
O275	0.10817	0.74622	0.05303
O276	0.065	0.24615	0.13686
O277	0.30509	0.24328	0.15561
O278	0.23368	0.24728	0.55793
O279	0.3965	0.24848	0.54788
O280	0.56187	0.24893	0.35136
O281	0.79874	0.2404	0.33551
O282	0.72931	0.24173	0.95105
O283	0.88922	0.24552	0.94302
O284	0.93786	0.74633	0.86068
O285	0.69419	0.74697	0.85574
O286	0.76783	0.74616	0.43593
O287	0.60595	0.74968	0.44829
O288	0.94756	0.25007	0.46434
O289	0.90519	0.20071	0.62143
O290	0.86112	0.31892	0.564
O291	-0.03074	0.31057	0.63844
GA29	0.9207	0.39884	0.61373
H293	0.94493	0.28501	0.41139
H294	0.81895	0.33813	0.48717
H295	0.88116	0.16892	0.578
H296	0.99304	0.52883	0.62875
H297	0.09047	0.50025	0.51565
H298	0.07776	0.58818	0.53302
H299	0.05289	0.54869	0.42008
H300	0.94309	0.59693	0.43833
H301	0.96027	0.63549	0.55535
H302	0.89132	0.58002	0.54312
H303	0.98755	0.43628	0.35841
H304	0.06868	0.35125	0.39375
H305	0.90901	0.47523	0.47373
H306	0.11697	0.25073	0.65571
H307	0.08174	0.26385	0.65686
H308	0.05611	0.36015	0.53046
AL30	0.81643	0.32294	0.3096

AL31	0.80144	0.47435	0.69722
P311	0.92184	0.27002	0.57164
C312	0.98798	0.52997	0.54686
C313	0.05652	0.54202	0.50148
C314	0.94283	0.58887	0.51969
C315	0.9967	0.42276	0.43646
C316	0.95633	0.46214	0.51019
C317	0.04285	0.37596	0.455

### **C<sub>6</sub>H<sub>11</sub>Ga**

SI2	0.42627	0.05336	0.64322
SI3	0.3064	0.02386	0.78745
SI4	0.28203	0.05783	0.00842
SI5	0.12259	0.05995	0.01047
SI6	0.07047	0.02446	0.79877
SI7	0.18066	0.05038	0.65098
SI8	0.42257	0.82386	0.67171
SI9	0.30536	0.86658	0.8099
SI10	0.26723	0.82667	0.0293
SI11	0.11294	0.82327	0.01647
SI12	0.06619	0.86678	0.80179
SI13	0.18373	0.82458	0.67303
SI14	0.07655	0.93993	0.14934
SI15	0.19747	0.96942	0.29247
SI16	0.22013	0.93173	0.51261
SI17	0.3795	0.92963	0.51356
SI18	0.43149	0.9663	0.30378
SI19	0.32201	0.94332	0.15351
SI20	0.08267	0.16872	0.16487
SI21	0.19775	0.12597	0.30954
SI22	0.23556	0.16874	0.52618
SI23	0.38994	0.17073	0.50986
SI24	0.43651	0.12373	0.29883
SI25	0.31824	0.16343	0.17014
SI26	0.57464	0.55524	0.34783
SI27	0.68742	0.52762	0.1927
SI28	0.71384	0.55539	0.98039
SI29	0.87274	0.55889	0.97252
SI30	0.93191	0.52432	0.18358
SI31	0.8137	0.55368	0.31665
SI32	0.57918	0.32565	0.32653
SI33	0.69458	0.3711	0.18335
SI34	0.72917	0.32121	0.97171
SI35	0.88349	0.3215	0.98154

SI36	0.9368	0.36552	0.19281
SI37	0.92508	0.4344	0.83859
SI38	0.77343	0.4382	0.46937
SI39	0.61435	0.43294	0.48402
SI40	0.56842	0.46685	0.70039
SI41	0.67824	0.4341	0.84241
SI42	0.91676	0.67136	0.82245
SI43	0.80504	0.63237	0.68272
SI44	0.76337	0.6654	0.46253
SI45	0.60905	0.67025	0.48186
SI46	0.5645	0.62437	0.69808
SI47	0.68359	0.66922	0.8192
SI48	0.57772	0.93992	0.35923
SI49	0.69482	0.96334	0.21331
SI50	0.72197	0.93117	0.99266
SI51	0.8815	0.93039	0.99394
SI52	0.93194	0.96745	0.20358
SI53	0.82037	0.9423	0.35265
SI54	0.57894	0.16984	0.33249
SI55	0.69758	0.11863	0.19972
SI56	0.73472	0.1629	0.98006
SI57	0.88854	0.16806	0.98122
SI58	0.93817	0.12489	0.19366
SI59	0.81992	0.16315	0.32724
SI60	0.92549	0.04906	0.85369
SI61	0.80272	0.02034	0.70847
SI62	0.78354	0.06407	0.49126
SI63	0.62295	0.06794	0.48923
SI64	0.57141	0.0256	0.69995
SI65	0.67971	0.04761	0.85143
SI66	0.92165	0.82417	0.83593
SI67	0.80236	0.86316	0.69027
SI68	0.76768	0.82154	0.4746
SI69	0.61353	0.8235	0.49359
SI70	0.56658	0.86824	0.70413
SI71	0.683	0.82546	0.83266
SI72	0.42442	0.44279	0.6435
SI73	0.30817	0.4695	0.79683
SI74	0.28734	0.43057	0.01141
SI75	0.12866	0.43086	0.01018
SI76	0.07456	0.46721	0.79954
SI77	0.18827	0.44243	0.65871
SI78	0.42473	0.66891	0.66446
SI79	0.30428	0.62656	0.80435

SI80	0.26785	0.67069	0.01773
SI81	0.1131	0.67011	0.01128
SI82	0.06242	0.62597	0.80049
SI83	0.1819	0.666	0.67166
SI84	0.07844	0.55133	0.14712
SI85	0.19896	0.52364	0.29099
SI86	0.22626	0.56265	0.51294
SI87	0.38643	0.56681	0.50615
SI88	0.43272	0.52758	0.29142
SI89	0.32242	0.55168	0.14702
SI90	0.08428	0.3231	0.16208
SI91	0.19802	0.36505	0.31063
SI92	0.23662	0.32546	0.52828
SI93	0.39114	0.3247	0.51106
SI94	0.43711	0.36932	0.29463
SI95	0.3182	0.32208	0.17249
O96	0.36127	0.05874	0.71513
O97	0.30506	0.06438	0.89269
O98	0.20209	0.0447	0.0174
O99	0.09888	0.06511	0.89511
O100	0.10602	0.05216	0.69798
O101	0.23271	0.02708	0.7374
O102	0.36107	0.82337	0.75042
O103	0.30509	0.84135	0.92461
O104	0.18965	0.85063	0.02013
O105	0.08627	0.8261	0.90237
O106	0.10627	0.83541	0.70672
O107	0.23194	0.85466	0.76047
O108	0.32581	0.94548	0.80513
O109	0.0865	0.94515	0.81511
O110	0.43529	0.12289	0.58081
O111	0.41974	0.9917	0.56412
O112	0.40032	0.85987	0.56787
O113	0.19867	0.12527	0.61207
O114	0.1819	-0.00331	0.5593
O115	0.19742	0.86258	0.56754
O116	0.99084	0.0361	0.7849
O117	0.98633	0.85921	0.78305
O118	0.14214	0.93549	0.22004
O119	0.20069	0.92603	0.39521
O120	0.29999	0.94289	0.52704
O121	0.39906	0.92432	0.39629
O122	0.39688	0.94291	0.19983
O123	0.27021	0.96895	0.23903

O124	0.14332	0.16706	0.2447
O125	0.1977	0.15844	0.42026
O126	0.31289	0.14443	0.51555
O127	0.41508	0.16893	0.39475
O128	0.39578	0.14951	0.20064
O129	0.27136	0.13344	0.25924
O130	0.17714	0.04703	0.31564
O131	0.41833	0.04591	0.32301
O132	0.06734	0.86934	0.08956
O133	0.08275	0.00006	0.06742
O134	0.10493	0.13125	0.0625
O135	0.30343	0.86756	0.11872
O136	0.32038	0.99402	0.05821
O137	0.30157	0.12741	0.06433
O138	0.51082	0.95165	0.29341
O139	0.51613	0.13225	0.27821
O140	0.64169	0.55957	0.2806
O141	0.67778	0.56794	0.08804
O142	0.79433	0.54639	0.99331
O143	0.91354	0.55888	0.07709
O144	0.88966	0.5576	0.27474
O145	0.76531	0.53755	0.22324
O146	0.64443	0.32936	0.25628
O147	0.68858	0.33759	0.07319
O148	0.80659	0.34799	0.97821
O149	0.91263	0.3244	0.09405
O150	0.902	0.33362	0.29147
O151	0.77002	0.36676	0.22318
O152	0.66893	0.44888	0.17942
O153	0.91687	0.44431	0.17768
O154	0.56413	0.62667	0.40443
O155	0.57644	0.49598	0.43193
O156	0.59289	0.36234	0.43334
O157	0.7956	0.62435	0.36969
O158	0.80808	0.49221	0.39623
O159	0.79471	0.36119	0.42939
O160	0.01006	0.53868	0.20935
O161	0.0179	0.36115	0.20264
O162	0.87526	0.42234	0.74085
O163	0.80578	0.44215	0.57821
O164	0.69372	0.44575	0.46733
O165	0.59578	0.4282	0.60121
O166	0.60208	0.436	0.79977
O167	0.73025	0.45433	0.75744

O168	0.86168	0.68006	0.73454
O169	0.80426	0.6488	0.56365
O170	0.68578	0.64298	0.47787
O171	0.58011	0.66295	0.59403
O172	0.60573	0.6595	0.78821
O173	0.73073	0.65219	0.72382
O174	0.82454	0.55592	0.70585
O175	0.58594	0.54619	0.68784
O176	0.92886	0.3683	0.90807
O177	0.90061	0.49837	0.90173
O178	0.88605	0.62999	0.91688
O179	0.69174	0.35749	0.87959
O180	0.68288	0.48636	0.93619
O181	0.70079	0.62085	0.91228
O182	0.48849	0.45647	0.71388
O183	0.48525	0.63151	0.72397
O184	0.64012	0.9267	0.28427
O185	0.69903	0.92334	0.10806
O186	0.80191	0.9441	0.98242
O187	0.90172	0.92413	0.11088
O188	0.89546	0.94642	0.30725
O189	0.76799	0.96126	0.26479
O190	0.64429	0.1631	0.26205
O191	0.70069	0.14923	0.08786
O192	0.81253	0.13883	0.98453
O193	0.92006	0.16623	0.09266
O194	0.89655	0.15466	0.28746
O195	0.77057	0.12	0.25357
O196	0.67247	0.04093	0.19491
O197	0.91961	0.04625	0.17802
O198	0.56675	0.87414	0.42933
O199	0.59058	0.00429	0.43118
O200	0.59339	0.13691	0.44188
O201	0.80721	0.86673	0.39313
O202	0.81356	0.9951	0.44478
O203	0.81828	0.13005	0.44055
O204	0.01112	0.95226	0.21838
O205	0.01771	0.13327	0.21559
O206	0.86006	0.04732	0.78307
O207	0.8031	0.06781	0.60918
O208	0.70344	0.06591	0.47466
O209	0.60411	0.06666	0.60688
O210	0.60503	0.04889	0.80463
O211	0.73066	0.02499	0.76293

O212	0.85941	0.83053	0.75993
O213	0.80477	0.82615	0.58245
O214	0.69102	0.84862	0.48603
O215	0.58965	0.82254	0.6095
O216	0.60555	0.84201	0.8036
O217	0.72929	0.85239	0.74074
O218	0.8165	0.94307	0.67572
O219	0.58497	0.9461	0.68046
O220	0.93266	0.12256	0.90538
O221	0.92137	0.99233	0.94129
O222	0.90314	0.86038	0.94107
O223	0.69676	0.12209	0.89223
O224	0.68285	0.99468	0.94365
O225	0.70247	0.86212	0.93643
O226	0.49228	0.04149	0.71085
O227	0.48641	0.86172	0.7219
O228	0.35814	0.44044	0.71261
O229	0.31407	0.42407	0.89722
O230	0.20782	0.44713	0.01536
O231	0.10469	0.42707	0.89462
O232	0.11094	0.4451	0.69628
O233	0.23218	0.46342	0.75554
O234	0.35683	0.66192	0.72939
O235	0.30619	0.66527	0.91094
O236	0.19074	0.64581	0.00494
O237	0.08128	0.66824	0.9
O238	0.10429	0.65522	0.70549
O239	0.22947	0.63253	0.75715
O240	0.32387	0.54802	0.82112
O241	0.08114	0.54736	0.81856
O242	0.43383	0.37107	0.58744
O243	0.41917	0.50135	0.55931
O244	0.41564	0.63535	0.55468
O245	0.20358	0.36684	0.62026
O246	0.20214	0.49376	0.56715
O247	0.19441	0.62901	0.56516
O248	0.99649	0.44644	0.78426
O249	0.98291	0.63318	0.7784
O250	0.1402	0.55761	0.22478
O251	0.20302	0.56243	0.39716
O252	0.30653	0.56558	0.52245
O253	0.40493	0.567	0.38898
O254	0.39648	0.55843	0.1938
O255	0.27004	0.53034	0.23413

O256	0.14073	0.32501	0.24919
O257	0.196	0.33868	0.42512
O258	0.3135	0.34954	0.51192
O259	0.4203	0.33103	0.39876
O260	0.39561	0.33439	0.20393
O261	0.27109	0.35089	0.26217
O262	0.18174	0.4448	0.30762
O263	0.41637	0.44795	0.30387
O264	0.0716	0.62114	0.08529
O265	0.08838	0.48988	0.06817
O266	0.11275	0.35872	0.06136
O267	0.30333	0.62389	0.10035
O268	0.32569	0.49352	0.06231
O269	0.30215	0.36027	0.0681
O270	0.51181	0.54063	0.27491
O271	0.5163	0.36183	0.27045
O272	0.44249	0.74711	0.64622
O273	0.19838	0.74511	0.65758
O274	0.27133	0.74754	0.05701
O275	0.10864	0.74604	0.05488
O276	0.06609	0.24594	0.1358
O277	0.30416	0.2429	0.15567
O278	0.23237	0.24695	0.55885
O279	0.39625	0.24753	0.54924
O280	0.56094	0.24806	0.35017
O281	0.79747	0.23983	0.33203
O282	0.72931	0.24124	0.95104
O283	0.88905	0.24491	0.94071
O284	0.93749	0.74599	0.86073
O285	0.69498	0.74638	0.85313
O286	0.7684	0.74465	0.4352
O287	0.60559	0.74844	0.44812
O288	0.94913	0.25272	0.45456
O289	0.91264	0.19813	0.61086
O290	0.86367	0.31625	0.5635
O291	-0.02588	0.30957	0.631
GA29	0.92116	0.39671	0.61441
H293	0.94275	0.28773	0.40185
H294	0.82089	0.33583	0.48802
H295	0.88843	0.16738	0.566
H296	0.98603	0.53061	0.63236
H297	0.08765	0.48983	0.53112
H298	0.08278	0.57819	0.55169
H299	0.06102	0.54324	0.43391

H300	0.95351	0.59444	0.43032
H301	0.96944	0.63692	0.54474
H302	0.89595	0.58802	0.53094
H303	0.97454	0.43553	0.35769
H304	0.06339	0.35629	0.38381
H305	0.90479	0.47736	0.48193
H306	0.05875	0.36726	0.52149
AL30	0.81561	0.32274	0.30942
AL30	0.80309	0.47262	0.69953
P309	0.92636	0.26919	0.56448
C310	0.98721	0.52937	0.55011
C311	0.05904	0.53509	0.51515
C312	0.94896	0.59055	0.51203
C313	0.9903	0.42448	0.4341
C314	0.95343	0.463	0.51268
C315	0.04015	0.38081	0.4475

### 5MR-C<sub>6</sub>H<sub>10</sub>+Ga(H)

SI2	0.42639	0.05406	0.64307
SI3	0.30637	0.02374	0.78656
SI4	0.28159	0.05692	0.00786
SI5	0.12219	0.06076	0.01111
SI6	0.07039	0.02436	0.79958
SI7	0.18029	0.05145	0.65122
SI8	0.42226	0.824	0.67121
SI9	0.30569	0.8663	0.80972
SI10	0.2682	0.82754	0.02976
SI11	0.11417	0.8238	0.017
SI12	0.06686	0.86692	0.80286
SI13	0.18375	0.82525	0.67202
SI14	0.07672	0.94038	0.14961
SI15	0.19757	0.97056	0.29183
SI16	0.22002	0.93388	0.51233
SI17	0.37926	0.93042	0.51385
SI18	0.43144	0.96722	0.30474
SI19	0.32227	0.9436	0.15375
SI20	0.08261	0.16982	0.16542
SI21	0.19742	0.12739	0.30971
SI22	0.23414	0.16974	0.52717
SI23	0.38844	0.17171	0.51083
SI24	0.43584	0.12452	0.30069
SI25	0.31854	0.16315	0.16935
SI26	0.57852	0.5542	0.34767
SI27	0.68398	0.52938	0.18558

SI28	0.71586	0.55588	0.97325
SI29	0.87283	0.56068	0.97591
SI30	0.93151	0.52463	0.18407
SI31	0.8089	0.55295	0.31308
SI32	0.58125	0.32655	0.32749
SI33	0.693	0.37257	0.18189
SI34	0.73137	0.32291	0.96907
SI35	0.88573	0.3214	0.97808
SI36	0.93748	0.36625	0.18878
SI37	0.92633	0.4369	0.84248
SI38	0.78119	0.43296	0.47274
SI39	0.62361	0.4309	0.48938
SI40	0.5665	0.46712	0.69929
SI41	0.68156	0.43181	0.83033
SI42	0.91798	0.67104	0.82203
SI43	0.80514	0.63329	0.68079
SI44	0.76407	0.66485	0.46166
SI45	0.60941	0.66959	0.48254
SI46	0.5646	0.62459	0.69826
SI47	0.68456	0.67158	0.81607
SI48	0.57726	0.94003	0.3598
SI49	0.6939	0.96382	0.21348
SI50	0.72133	0.93234	0.99317
SI51	0.88102	0.93015	0.99343
SI52	0.93232	0.967	0.20239
SI53	0.82003	0.94259	0.3515
SI54	0.57859	0.17108	0.33331
SI55	0.69574	0.11872	0.1986
SI56	0.73486	0.16364	0.97994
SI57	0.88894	0.16805	0.97997
SI58	0.9386	0.1244	0.19145
SI59	0.81877	0.16275	0.32364
SI60	0.92519	0.04868	0.85234
SI61	0.80248	0.02069	0.70723
SI62	0.78279	0.06397	0.48984
SI63	0.62275	0.06808	0.48887
SI64	0.57181	0.02658	0.6996
SI65	0.68024	0.04858	0.85127
SI66	0.92168	0.82445	0.83507
SI67	0.80255	0.86387	0.68941
SI68	0.7676	0.82142	0.47371
SI69	0.61301	0.82281	0.49242
SI70	0.5663	0.86911	0.70254
SI71	0.68259	0.82724	0.83207

SI72	0.42324	0.44382	0.64571
SI73	0.30499	0.47102	0.79608
SI74	0.28838	0.43114	0.01324
SI75	0.12986	0.43163	0.01154
SI76	0.07793	0.47226	0.80338
SI77	0.18494	0.44442	0.65463
SI78	0.42504	0.66909	0.66319
SI79	0.30227	0.62782	0.80057
SI80	0.26964	0.67199	0.01559
SI81	0.11515	0.67094	0.01366
SI82	0.06515	0.62888	0.80231
SI83	0.18015	0.66732	0.66633
SI84	0.07801	0.55159	0.1471
SI85	0.20275	0.52556	0.28629
SI86	0.2257	0.56372	0.51036
SI87	0.38513	0.56713	0.50722
SI88	0.43154	0.52537	0.29452
SI89	0.32743	0.55393	0.1421
SI90	0.08406	0.32448	0.16143
SI91	0.20148	0.36526	0.30747
SI92	0.2339	0.32662	0.52797
SI93	0.38852	0.32559	0.51526
SI94	0.43609	0.36887	0.29912
SI95	0.32212	0.32081	0.17109
O96	0.3615	0.05914	0.71524
O97	0.30478	0.06365	0.89228
O98	0.20155	0.04441	0.01679
O99	0.09784	0.06564	0.89602
O100	0.10593	0.05176	0.69879
O101	0.23276	0.02712	0.73648
O102	0.36152	0.8226	0.75116
O103	0.30606	0.8428	0.92525
O104	0.19069	0.85169	0.02043
O105	0.08733	0.82574	0.9029
O106	0.10653	0.83574	0.70719
O107	0.23237	0.85306	0.76067
O108	0.32582	0.94519	0.80262
O109	0.08725	0.94521	0.81692
O110	0.43451	0.12355	0.58031
O111	0.42029	0.99193	0.56461
O112	0.39898	0.86029	0.56814
O113	0.19786	0.1268	0.61418
O114	0.18182	-0.00086	0.55775
O115	0.19705	0.86518	0.56813

O116	0.99075	0.03499	0.7846
O117	0.98693	0.85968	0.78427
O118	0.14249	0.93585	0.21984
O119	0.20076	0.92768	0.39498
O120	0.29993	0.94469	0.52694
O121	0.39901	0.9246	0.39663
O122	0.39705	0.94455	0.20026
O123	0.27042	0.96981	0.23874
O124	0.14305	0.16895	0.24553
O125	0.19669	0.1583	0.42127
O126	0.31152	0.14529	0.51654
O127	0.41356	0.17044	0.39551
O128	0.39562	0.14833	0.20108
O129	0.27103	0.13625	0.25981
O130	0.1771	0.0483	0.31323
O131	0.41862	0.04664	0.32632
O132	0.06799	0.87019	0.08871
O133	0.08207	0.00149	0.06922
O134	0.10567	0.13236	0.06326
O135	0.3044	0.86738	0.12035
O136	0.31986	0.9928	0.05683
O137	0.30145	0.12587	0.06487
O138	0.5107	0.95243	0.29362
O139	0.51527	0.13409	0.27983
O140	0.63728	0.56727	0.26682
O141	0.67334	0.56329	0.07638
O142	0.79466	0.55112	1.00044
O143	0.91468	0.56263	0.07955
O144	0.88589	0.55402	0.27474
O145	0.76161	0.54087	0.21726
O146	0.64044	0.3273	0.24586
O147	0.69098	0.34378	0.06868
O148	0.80904	0.34869	0.97502
O149	0.9152	0.32416	0.09051
O150	0.90093	0.33374	0.28593
O151	0.76697	0.36799	0.22745
O152	0.66581	0.45002	0.18343
O153	0.91731	0.44468	0.17241
O154	0.56467	0.62381	0.40759
O155	0.59921	0.49606	0.42685
O156	0.60582	0.36213	0.43067
O157	0.79427	0.6241	0.36706
O158	0.79635	0.49197	0.39292
O159	0.80457	0.35931	0.4327

O160	0.00965	0.5395	0.21053
O161	0.01808	0.36204	0.20521
O162	0.8777	0.42593	0.74386
O163	0.82798	0.44372	0.5743
O164	0.70414	0.43591	0.50615
O165	0.58756	0.42837	0.5971
O166	0.6037	0.43513	0.79522
O167	0.73018	0.44497	0.73714
O168	0.86414	0.67829	0.73185
O169	0.8072	0.64592	0.56041
O170	0.68651	0.6432	0.47918
O171	0.58054	0.66351	0.59476
O172	0.6066	0.65949	0.78775
O173	0.73151	0.65818	0.71876
O174	0.81918	0.55633	0.70855
O175	0.58553	0.54623	0.68745
O176	0.93177	0.36784	0.90552
O177	0.89623	0.49663	0.9095
O178	0.88643	0.63008	0.91599
O179	0.69467	0.35684	0.87424
O180	0.69282	0.4875	0.91809
O181	0.70464	0.62239	0.90678
O182	0.48678	0.45817	0.71737
O183	0.48541	0.63223	0.72399
O184	0.63995	0.927	0.28538
O185	0.69798	0.92379	0.1083
O186	0.80142	0.9441	0.98366
O187	0.90228	0.9234	0.10989
O188	0.89493	0.94676	0.30568
O189	0.76736	0.96196	0.26421
O190	0.64313	0.16396	0.26112
O191	0.6994	0.1487	0.08642
O192	0.81265	0.1396	0.98558
O193	0.92133	0.16647	0.09084
O194	0.89489	0.15254	0.28401
O195	0.76882	0.11932	0.25205
O196	0.67042	0.0411	0.19507
O197	0.9212	0.04563	0.17457
O198	0.56618	0.87354	0.42842
O199	0.58958	0.004	0.43285
O200	0.59331	0.13716	0.44189
O201	0.80678	0.867	0.39226
O202	0.81377	0.99546	0.44365
O203	0.81715	0.1305	0.43835

O204	0.0112	0.9512	0.21909
O205	0.01772	0.1338	0.21552
O206	0.85997	0.04779	0.78129
O207	0.80084	0.06784	0.60784
O208	0.70296	0.06563	0.47116
O209	0.6054	0.06755	0.60706
O210	0.60548	0.04929	0.80457
O211	0.73086	0.02436	0.76333
O212	0.86004	0.83083	0.7579
O213	0.80409	0.82643	0.58187
O214	0.69059	0.84745	0.4841
O215	0.58963	0.82287	0.60855
O216	0.60524	0.84333	0.80221
O217	0.72968	0.85384	0.74095
O218	0.81697	0.94357	0.67412
O219	0.58443	0.94701	0.67891
O220	0.9324	0.12203	0.90424
O221	0.92039	0.99198	0.93995
O222	0.9019	0.86004	0.94012
O223	0.69783	0.12349	0.89028
O224	0.68323	0.99674	0.94499
O225	0.70105	0.8639	0.93607
O226	0.49281	0.04318	0.71025
O227	0.48621	0.86222	0.72035
O228	0.35691	0.44249	0.71434
O229	0.30855	0.425	0.89611
O230	0.20892	0.44568	0.02841
O231	0.11309	0.43038	0.89304
O232	0.10829	0.45114	0.69485
O233	0.23055	0.46504	0.7497
O234	0.35676	0.66097	0.72663
O235	0.30238	0.66955	0.90453
O236	0.19261	0.64501	0.01147
O237	0.08495	0.6718	0.90104
O238	0.10313	0.65851	0.70392
O239	0.22861	0.633	0.74978
O240	0.31997	0.5494	0.82268
O241	0.08866	0.55198	0.82225
O242	0.43236	0.3716	0.59087
O243	0.41849	0.50156	0.55977
O244	0.41686	0.63537	0.55322
O245	0.19748	0.36818	0.61695
O246	0.19957	0.49428	0.56114
O247	0.18978	0.62899	0.56

O248	0.99893	0.45647	0.80021
O249	0.98513	0.63269	0.78212
O250	0.13987	0.55615	0.22497
O251	0.20759	0.5641	0.39264
O252	0.3055	0.56752	0.52827
O253	0.4008	0.56607	0.389
O254	0.40066	0.55776	0.19344
O255	0.27169	0.53714	0.2264
O256	0.1426	0.329	0.24474
O257	0.19642	0.33935	0.42192
O258	0.31123	0.35144	0.51778
O259	0.41692	0.3312	0.40249
O260	0.39932	0.33127	0.20598
O261	0.2743	0.34739	0.26137
O262	0.19075	0.44594	0.30351
O263	0.41094	0.44652	0.30409
O264	0.07201	0.6218	0.08568
O265	0.08752	0.49058	0.06711
O266	0.10873	0.35933	0.05778
O267	0.31256	0.62589	0.09112
O268	0.32902	0.49441	0.05932
O269	0.30815	0.36139	0.06806
O270	0.51176	0.53235	0.28832
O271	0.51634	0.36581	0.28271
O272	0.44244	0.74738	0.645
O273	0.19795	0.74611	0.65156
O274	0.27233	0.74834	0.05673
O275	0.11088	0.74689	0.05748
O276	0.06575	0.2471	0.13709
O277	0.30673	0.24246	0.14989
O278	0.23063	0.24814	0.55843
O279	0.39396	0.24816	0.55217
O280	0.56152	0.24946	0.35288
O281	0.79715	0.23959	0.32794
O282	0.72988	0.24243	0.95364
O283	0.88984	0.24459	0.93823
O284	0.93752	0.74616	0.85927
O285	0.69426	0.74821	0.853
O286	0.76966	0.74419	0.43548
O287	0.60489	0.74751	0.44744
O288	0.95052	0.24956	0.42125
O289	0.90736	0.19017	0.57239
O290	0.88612	0.31691	0.55427
O291	0.00183	0.27503	0.59712

GA29	0.91881	0.40346	0.60609
H293	0.93668	0.28489	0.37131
H294	0.84726	0.32845	0.49964
H295	0.87589	0.16941	0.52395
H296	0.97933	0.53551	0.5895
H297	0.99321	0.40868	0.63288
H298	0.09301	0.53398	0.54042
H299	0.07307	0.5497	0.41348
H300	0.97482	0.62099	0.39878
H301	0.99984	0.6485	0.5202
H302	0.91589	0.62404	0.4982
H303	0.96775	0.38998	0.38847
H304	0.09013	0.43165	0.39302
H305	0.89461	0.49193	0.43878
H306	0.07082	0.41253	0.51807
AL30	0.81456	0.32338	0.31082
AL30	0.80628	0.47197	0.69871
P309	0.94316	0.25638	0.53749
C310	0.9865	0.54091	0.50751
C311	0.05856	0.5211	0.48041
C312	0.96801	0.61283	0.47937
C313	0.98555	0.43446	0.42742
C314	0.94704	0.48677	0.45557
C315	0.05692	0.44547	0.4548

### 6MR-C<sub>6</sub>H<sub>10</sub>+Ga(H)

SI2	0.4265	0.05324	0.64283
SI3	0.30631	0.02314	0.7854
SI4	0.28207	0.0565	0.00792
SI5	0.12257	0.06032	0.01059
SI6	0.07086	0.02349	0.79867
SI7	0.18004	0.05098	0.64971
SI8	0.42297	0.82301	0.67123
SI9	0.30608	0.8654	0.80893
SI10	0.26945	0.82721	0.02968
SI11	0.11524	0.82361	0.01802
SI12	0.06737	0.86567	0.80318
SI13	0.18397	0.82328	0.67232
SI14	0.07703	0.9403	0.14985
SI15	0.19792	0.96962	0.29301
SI16	0.21987	0.9322	0.51277
SI17	0.37915	0.92906	0.51434
SI18	0.43161	0.96683	0.30563
SI19	0.32271	0.9431	0.15446

SI20	0.08299	0.16958	0.16376
SI21	0.19811	0.12624	0.30879
SI22	0.23425	0.16988	0.52591
SI23	0.38877	0.17117	0.5105
SI24	0.43619	0.12403	0.30069
SI25	0.31918	0.16208	0.16872
SI26	0.57958	0.55531	0.34466
SI27	0.68471	0.53093	0.18246
SI28	0.71746	0.55375	0.96918
SI29	0.87402	0.55925	0.97506
SI30	0.93278	0.52497	0.1834
SI31	0.80887	0.55441	0.3106
SI32	0.58089	0.32652	0.32532
SI33	0.69348	0.37316	0.18009
SI34	0.73127	0.32311	0.96853
SI35	0.88586	0.32126	0.97461
SI36	0.93915	0.36644	0.18536
SI37	0.92696	0.43685	0.83836
SI38	0.77957	0.4335	0.46903
SI39	0.62272	0.4311	0.48629
SI40	0.56715	0.46734	0.69803
SI41	0.68166	0.42957	0.82682
SI42	0.91893	0.67028	0.82198
SI43	0.80575	0.6348	0.6795
SI44	0.76618	0.66552	0.46081
SI45	0.61148	0.66938	0.48232
SI46	0.56748	0.62437	0.69913
SI47	0.68708	0.67261	0.81585
SI48	0.57749	0.9397	0.36127
SI49	0.69407	0.96351	0.21549
SI50	0.7213	0.93293	0.99462
SI51	0.88098	0.92946	0.99417
SI52	0.93246	0.96732	0.20237
SI53	0.82074	0.94333	0.35294
SI54	0.57882	0.17086	0.33374
SI55	0.69619	0.11821	0.20038
SI56	0.73448	0.16331	0.9811
SI57	0.88835	0.16767	0.98069
SI58	0.9384	0.12453	0.19178
SI59	0.81945	0.16243	0.32518
SI60	0.92568	0.04822	0.85378
SI61	0.80253	0.02084	0.7094
SI62	0.78301	0.06438	0.49162
SI63	0.623	0.06817	0.48968

SI64	0.57208	0.02589	0.70018
SI65	0.6798	0.04901	0.85298
SI66	0.92191	0.82355	0.83656
SI67	0.80261	0.86356	0.6915
SI68	0.76856	0.8221	0.47482
SI69	0.61412	0.8228	0.49351
SI70	0.56686	0.86842	0.70335
SI71	0.68255	0.82687	0.83439
SI72	0.42425	0.44375	0.64427
SI73	0.30769	0.46982	0.79794
SI74	0.29129	0.43003	0.01243
SI75	0.13274	0.43194	0.01145
SI76	0.07885	0.47232	0.80378
SI77	0.18834	0.4446	0.65808
SI78	0.42845	0.66788	0.66361
SI79	0.30435	0.62624	0.799
SI80	0.27106	0.67167	0.01286
SI81	0.11651	0.67114	0.01339
SI82	0.06631	0.62858	0.80358
SI83	0.18153	0.66542	0.66535
SI84	0.08038	0.55205	0.14807
SI85	0.20514	0.52506	0.28572
SI86	0.23042	0.56384	0.51167
SI87	0.388	0.56763	0.5071
SI88	0.43172	0.52599	0.29386
SI89	0.32911	0.55301	0.13936
SI90	0.0862	0.32436	0.16183
SI91	0.20129	0.36536	0.30926
SI92	0.23461	0.32689	0.52998
SI93	0.38961	0.32519	0.51608
SI94	0.43602	0.36914	0.2989
SI95	0.32147	0.31994	0.17279
O96	0.36182	0.05909	0.71529
O97	0.30459	0.06188	0.89199
O98	0.20201	0.04488	0.01856
O99	0.09946	0.06407	0.89493
O100	0.10575	0.05134	0.69762
O101	0.23286	0.02777	0.73516
O102	0.36208	0.82144	0.75105
O103	0.30688	0.84342	0.92512
O104	0.19183	0.85129	0.02142
O105	0.0883	0.82578	0.90406
O106	0.10679	0.8329	0.70835
O107	0.23268	0.8511	0.76081

O108	0.32555	0.94436	0.79937
O109	0.08773	0.94417	0.81439
O110	0.43478	0.12232	0.57906
O111	0.41992	0.99057	0.56548
O112	0.39937	0.85879	0.56787
O113	0.19693	0.12609	0.61095
O114	0.18166	0.99766	0.55753
O115	0.19655	0.86366	0.56865
O116	0.99116	0.03474	0.7857
O117	0.98732	0.85842	0.78569
O118	0.14254	0.93602	0.22052
O119	0.20103	0.9257	0.39526
O120	0.29976	0.94281	0.52797
O121	0.39871	0.92405	0.39698
O122	0.39751	0.94444	0.20082
O123	0.27065	0.9687	0.23954
O124	0.14376	0.1668	0.2432
O125	0.19805	0.15975	0.41872
O126	0.31169	0.14532	0.51702
O127	0.41337	0.1703	0.39489
O128	0.39634	0.14773	0.20068
O129	0.27154	0.13321	0.25764
O130	0.17789	0.04724	0.31656
O131	0.41887	0.04627	0.32714
O132	0.0688	0.8698	0.08962
O133	0.08255	0.00109	0.06895
O134	0.10472	0.1322	0.06089
O135	0.30561	0.86676	0.12055
O136	0.32	0.9925	0.05781
O137	0.30309	0.12591	0.06293
O138	0.51086	0.95182	0.29518
O139	0.51571	0.13332	0.28051
O140	0.63668	0.56943	0.26144
O141	0.67385	0.56188	0.07131
O142	0.79591	0.54752	-0.00161
O143	0.91525	0.56318	0.07934
O144	0.88657	0.55313	0.27461
O145	0.76205	0.54553	0.21354
O146	0.64072	0.32829	0.2446
O147	0.68943	0.34696	0.06547
O148	0.80908	0.34845	0.97519
O149	0.91811	0.32588	0.08524
O150	0.90227	0.33329	0.28177
O151	0.76807	0.36577	0.22224

O152	0.66833	0.45121	0.18553
O153	0.91887	0.44506	0.17136
O154	0.56667	0.62434	0.40655
O155	0.60151	0.49646	0.42178
O156	0.60366	0.36215	0.42921
O157	0.79684	0.62568	0.36569
O158	0.79162	0.49346	0.38885
O159	0.80545	0.36124	0.42757
O160	0.01112	0.53985	0.20987
O161	0.01973	0.3626	0.20263
O162	0.87767	0.42977	0.74002
O163	0.82506	0.44472	0.57155
O164	0.70296	0.4337	0.504
O165	0.58594	0.43052	0.59345
O166	0.60356	0.4323	0.79238
O167	0.72927	0.44282	0.7327
O168	0.86659	0.67741	0.73006
O169	0.80995	0.64616	0.55887
O170	0.68872	0.64324	0.47815
O171	0.58293	0.66226	0.59461
O172	0.60921	0.66014	0.7879
O173	0.73355	0.66426	0.71659
O174	0.81483	0.5574	0.70873
O175	0.58882	0.54601	0.69015
O176	0.93014	0.36608	0.89751
O177	0.89977	0.49559	0.91005
O178	0.88643	0.62864	0.91445
O179	0.69575	0.35481	0.8709
O180	0.69354	0.48576	0.91382
O181	0.70887	0.62029	0.9017
O182	0.48716	0.46058	0.716
O183	0.48855	0.63217	0.72624
O184	0.64012	0.92618	0.28683
O185	0.6985	0.92404	0.10991
O186	0.80146	0.94387	0.98391
O187	0.90187	0.92313	0.11087
O188	0.8954	0.94812	0.30636
O189	0.76751	0.96193	0.26612
O190	0.64369	0.16394	0.26222
O191	0.69993	0.14737	0.08785
O192	0.81217	0.13872	0.98417
O193	0.91891	0.1676	0.09289
O194	0.89565	0.15067	0.28663
O195	0.76926	0.11896	0.25387

O196	0.67027	0.04077	0.19811
O197	0.92176	0.04575	0.17292
O198	0.56658	0.87343	0.43044
O199	0.5899	0.0041	0.43345
O200	0.59341	0.13731	0.44277
O201	0.80823	0.8677	0.39394
O202	0.81444	0.99617	0.44507
O203	0.81716	0.13115	0.44048
O204	0.01132	0.95127	0.21879
O205	0.01765	0.13457	0.21406
O206	0.86047	0.04817	0.78264
O207	0.80064	0.06771	0.60976
O208	0.70322	0.06583	0.47205
O209	0.60585	0.06708	0.60796
O210	0.60523	0.0486	0.80557
O211	0.73111	0.02493	0.76593
O212	0.86031	0.83018	0.75931
O213	0.80446	0.82689	0.58341
O214	0.6915	0.84811	0.48467
O215	0.5908	0.82224	0.60966
O216	0.60527	0.84221	0.80326
O217	0.72986	0.85264	0.74297
O218	0.81662	0.94344	0.67732
O219	0.58526	0.94633	0.68004
O220	0.93319	0.12101	0.90751
O221	0.92086	0.9907	0.94016
O222	0.90188	0.85907	0.94157
O223	0.69618	0.1244	0.89133
O224	0.68339	0.99784	0.94753
O225	0.70006	0.8649	0.93751
O226	0.493	0.04234	0.70983
O227	0.48661	0.86191	0.72011
O228	0.3577	0.44318	0.71236
O229	0.31426	0.42269	0.89648
O230	0.21202	0.44737	0.02232
O231	0.11236	0.42957	0.89409
O232	0.11114	0.45418	0.69494
O233	0.2321	0.46276	0.75612
O234	0.35951	0.65816	0.72494
O235	0.30317	0.66993	0.9013
O236	0.19387	0.64523	0.00929
O237	0.08577	0.67284	0.90109
O238	0.10493	0.6566	0.70475
O239	0.23111	0.63017	0.74642

O240	0.32189	0.5483	0.82523
O241	0.08874	0.55174	0.82656
O242	0.43358	0.37053	0.59259
O243	0.41891	0.49947	0.55553
O244	0.42396	0.63355	0.55347
O245	0.19887	0.36806	0.6201
O246	0.20811	0.49397	0.56589
O247	0.18955	0.62745	0.55813
O248	1.00011	0.45556	0.79674
O249	0.98646	0.63254	0.78247
O250	0.14202	0.55836	0.22689
O251	0.21654	0.5617	0.39261
O252	0.30925	0.5733	0.53322
O253	0.40015	0.56655	0.38797
O254	0.40141	0.55892	0.19286
O255	0.27236	0.53486	0.22132
O256	0.14247	0.32714	0.24889
O257	0.19673	0.34184	0.42488
O258	0.31221	0.35075	0.51937
O259	0.41787	0.33221	0.40337
O260	0.39862	0.3307	0.20719
O261	0.274	0.34695	0.26325
O262	0.18946	0.44586	0.30169
O263	0.41124	0.447	0.30278
O264	0.07377	0.62162	0.08535
O265	0.09141	0.49049	0.06958
O266	0.11437	0.35963	0.06043
O267	0.31378	0.62437	0.08693
O268	0.33317	0.49243	0.05861
O269	0.30715	0.36021	0.0696
O270	0.51183	0.53345	0.28808
O271	0.51596	0.36539	0.27988
O272	0.44404	0.74655	0.64567
O273	0.19903	0.74433	0.65111
O274	0.27419	0.74777	0.05512
O275	0.1121	0.74671	0.05854
O276	0.06759	0.24726	0.13595
O277	0.30624	0.24152	0.15209
O278	0.23047	0.24808	0.55838
O279	0.39512	0.24753	0.55193
O280	0.56154	0.24937	0.35119
O281	0.79894	0.23959	0.32803
O282	0.72962	0.2424	0.9574
O283	0.88916	0.2438	0.93737

O284	0.9376	0.74523	0.86087
O285	0.69492	0.74821	0.8584
O286	0.77114	0.74506	0.43594
O287	0.60676	0.74751	0.44829
O288	0.95263	0.25115	0.4193
O289	0.90862	0.19234	0.57075
O290	0.88717	0.31885	0.55058
O291	0.00289	0.27715	0.59551
GA29	0.91794	0.40732	0.60065
H293	0.93872	0.2862	0.36895
H294	0.84888	0.32918	0.49647
H295	0.8767	0.17139	0.52313
H296	0.97223	0.53301	0.60265
H297	0.99194	0.4076	0.63198
H298	0.11491	0.52538	0.50743
H299	0.09454	0.52957	0.37955
H300	0.00783	0.6003	0.40519
H301	0.04524	0.61504	0.52302
H302	0.92035	0.58612	0.53044
H303	0.96191	0.40234	0.3804
H304	0.08174	0.41437	0.41052
H305	0.88686	0.49	0.43443
H306	0.05645	0.42698	0.53464
AL30	0.81587	0.32319	0.30766
AL30	0.80451	0.47286	0.69571
P309	0.9445	0.25842	0.53539
C310	0.9598	0.54801	0.52514
C311	0.07438	0.52081	0.45407
C312	0.02292	0.57601	0.47544
C313	0.97983	0.44203	0.42979
C314	0.9368	0.4893	0.46405
C315	0.05071	0.44686	0.45763

### C<sub>6</sub>H<sub>9</sub>Ga+H<sub>2</sub>\*

SI2	0.42534	0.0526	0.64159
SI3	0.30566	0.02051	0.78351
SI4	0.28202	0.04814	0.00789
SI5	0.12299	0.055	0.00935
SI6	0.07025	0.0215	0.79777
SI7	0.17915	0.05	0.64871
SI8	0.42262	0.82058	0.67345
SI9	0.30535	0.86263	0.80872
SI10	0.2706	0.82349	0.03114
SI11	0.11585	0.82035	0.02197

SI12	0.06669	0.86294	0.80598
SI13	0.18231	0.8202	0.67339
SI14	0.0766	0.93803	0.15092
SI15	0.19941	0.96796	0.29326
SI16	0.21846	0.92987	0.51365
SI17	0.37797	0.92738	0.51557
SI18	0.43289	0.96214	0.30786
SI19	0.32437	0.93705	0.15582
SI20	0.0855	0.16732	0.16088
SI21	0.20109	0.12623	0.30739
SI22	0.2337	0.16959	0.52451
SI23	0.38866	0.1701	0.50744
SI24	0.43875	0.11935	0.30045
SI25	0.32323	0.1569	0.16519
SI26	0.57945	0.55943	0.33646
SI27	0.68796	0.53278	0.17908
SI28	0.7143	0.55001	0.96059
SI29	0.87173	0.5554	0.97174
SI30	0.92739	0.52189	0.1835
SI31	0.8085	0.55443	0.31101
SI32	0.5737	0.32603	0.32306
SI33	0.6944	0.37403	0.1882
SI34	0.72397	0.32051	0.97381
SI35	0.87683	0.32001	0.97462
SI36	0.93269	0.36361	0.18261
SI37	0.92365	0.43356	0.83792
SI38	0.77029	0.43719	0.46739
SI39	0.61209	0.43228	0.47722
SI40	0.5631	0.46837	0.69686
SI41	0.67217	0.42367	0.82958
SI42	0.91391	0.6719	0.82722
SI43	0.80021	0.63133	0.68494
SI44	0.76631	0.66161	0.46597
SI45	0.61141	0.66789	0.48263
SI46	0.56555	0.62436	0.70186
SI47	0.68469	0.67422	0.81583
SI48	0.57921	0.93739	0.36558
SI49	0.69599	0.96186	0.22195
SI50	0.7216	0.93414	0.9979
SI51	0.88065	0.93318	1.00006
SI52	0.93241	0.96824	0.20925
SI53	0.82242	0.94044	0.36014
SI54	0.58038	0.16968	0.33536
SI55	0.69857	0.11732	0.20514

SI56	0.73239	0.16046	0.98372
SI57	0.8858	0.16673	0.98012
SI58	0.93886	0.12652	0.19359
SI59	0.82207	0.16348	0.32958
SI60	0.92527	0.04816	0.85572
SI61	0.80103	0.02061	0.71072
SI62	0.78483	0.06384	0.49425
SI63	0.62433	0.06759	0.49104
SI64	0.57087	0.02433	0.7005
SI65	0.67765	0.04829	0.85402
SI66	0.9191	0.8252	0.84442
SI67	0.80064	0.86401	0.69538
SI68	0.77101	0.81914	0.48175
SI69	0.61704	0.82178	0.50128
SI70	0.56706	0.86664	0.70878
SI71	0.68232	0.82701	0.84007
SI72	0.41896	0.44208	0.64084
SI73	0.3072	0.46608	0.80101
SI74	0.28431	0.42765	0.01434
SI75	0.12827	0.43047	0.00473
SI76	0.07163	0.4664	0.79667
SI77	0.1893	0.44359	0.66082
SI78	0.42693	0.66582	0.66245
SI79	0.30145	0.62274	0.79281
SI80	0.2716	0.66804	0.00755
SI81	0.11811	0.66641	0.01683
SI82	0.06344	0.62641	0.80462
SI83	0.17846	0.66178	0.66161
SI84	0.07615	0.54607	0.14631
SI85	0.20434	0.5209	0.28202
SI86	0.22674	0.56333	0.5087
SI87	0.38476	0.56778	0.5023
SI88	0.43392	0.5273	0.28961
SI89	0.32632	0.55306	0.13972
SI90	0.08442	0.32314	0.15503
SI91	0.19967	0.35947	0.30511
SI92	0.23394	0.32673	0.52665
SI93	0.38927	0.32449	0.50846
SI94	0.43282	0.36858	0.28969
SI95	0.31468	0.31306	0.16571
O96	0.36082	0.058	0.71463
O97	0.30478	0.05594	0.89246
O98	0.20182	0.03655	0.01743
O99	0.10039	0.06121	0.89368

O100	0.10464	0.05027	0.69664
O101	0.23189	0.02765	0.73469
O102	0.36209	0.8178	0.75401
O103	0.30561	0.84395	0.92625
O104	0.19266	0.84706	0.02783
O105	0.08974	0.82517	0.90767
O106	0.10545	0.82979	0.7109
O107	0.23206	0.84685	0.76128
O108	0.32436	0.9413	0.79294
O109	0.08602	0.94198	0.81222
O110	0.43373	0.12196	0.57849
O111	0.41807	0.99045	0.56351
O112	0.39894	0.85856	0.57206
O113	0.1958	0.125	0.60846
O114	0.18056	0.9958	0.55774
O115	0.19453	0.86161	0.5702
O116	0.99045	0.0338	0.78712
O117	0.98672	0.8537	0.7914
O118	0.14262	0.9372	0.22066
O119	0.19991	0.92405	0.39581
O120	0.29837	0.94019	0.52898
O121	0.39741	0.92042	0.39827
O122	0.39913	0.94069	0.2022
O123	0.2721	0.96344	0.24012
O124	0.14581	0.16471	0.24086
O125	0.19774	0.15988	0.4171
O126	0.31119	0.14543	0.51588
O127	0.4133	0.16675	0.39194
O128	0.39959	0.13967	0.19818
O129	0.27468	0.1372	0.2586
O130	0.18361	0.04665	0.31581
O131	0.42245	0.04185	0.32947
O132	0.06955	0.86551	0.09554
O133	0.08087	-0.00381	0.06541
O134	0.10688	0.12696	0.06062
O135	0.30814	0.86008	0.12376
O136	0.32013	0.98387	0.05641
O137	0.30286	0.11615	0.06549
O138	0.51182	0.94519	0.29956
O139	0.51832	0.1301	0.28219
O140	0.63926	0.57155	0.25706
O141	0.67717	0.56213	0.06731
O142	0.79371	0.53474	-0.023
O143	0.90416	0.56052	0.08224

O144	0.88678	0.55019	0.27989
O145	0.76498	0.54975	0.20918
O146	0.64148	0.33427	0.25933
O147	0.68861	0.34163	0.07744
O148	0.80094	0.34889	0.96603
O149	0.90158	0.322	0.0894
O150	0.90357	0.3324	0.28613
O151	0.76904	0.36582	0.22974
O152	0.67235	0.45289	0.1842
O153	0.91295	0.44227	0.16907
O154	0.56756	0.62834	0.39906
O155	0.59584	0.49998	0.41526
O156	0.57731	0.36676	0.42828
O157	0.79709	0.62497	0.36829
O158	0.78644	0.49228	0.38249
O159	0.80524	0.36433	0.4317
O160	0.00596	0.53642	0.20427
O161	0.01354	0.35818	0.17963
O162	0.8721	0.42772	0.74165
O163	0.80475	0.45525	0.57102
O164	0.692	0.42188	0.47636
O165	0.58444	0.43831	0.5894
O166	0.59596	0.42522	0.78634
O167	0.72608	0.43047	0.74221
O168	0.86233	0.67349	0.73395
O169	0.80823	0.63731	0.56365
O170	0.68817	0.64033	0.48035
O171	0.57977	0.65579	0.59223
O172	0.60651	0.6654	0.78644
O173	0.7301	0.66882	0.71491
O174	0.79992	0.55486	0.72373
O175	0.58798	0.54608	0.70436
O176	0.92509	0.36544	0.90325
O177	0.91135	0.49759	0.90821
O178	0.88348	0.62696	0.91753
O179	0.67983	0.35098	0.88391
O180	0.67989	0.48502	0.91006
O181	0.707	0.61832	0.8964
O182	0.48242	0.46428	0.70791
O183	0.48647	0.63202	0.72821
O184	0.64155	0.923	0.2908
O185	0.6994	0.92601	0.11347
O186	0.80139	0.94788	0.98654
O187	0.89948	0.92641	0.11728

O188	0.89724	0.94691	0.31387
O189	0.76947	0.95768	0.27212
O190	0.64626	0.16431	0.26542
O191	0.69884	0.14155	0.08991
O192	0.81032	0.13601	0.98444
O193	0.91814	0.16536	0.09126
O194	0.89873	0.15787	0.2879
O195	0.77309	0.12197	0.25321
O196	0.67315	0.03985	0.21083
O197	0.9213	0.04726	0.18442
O198	0.56967	0.87357	0.44006
O199	0.59112	0.00452	0.43224
O200	0.59506	0.13727	0.44514
O201	0.81141	0.86441	0.401
O202	0.81437	0.99333	0.45184
O203	0.82076	0.1276	0.44028
O204	0.01146	0.95094	0.22027
O205	0.01872	0.13587	0.21179
O206	0.85987	0.04397	0.78543
O207	0.8022	0.06931	0.61289
O208	0.70474	0.06572	0.47545
O209	0.60579	0.06503	0.60886
O210	0.60316	0.04717	0.80647
O211	0.72969	0.02593	0.767
O212	0.85821	0.83592	0.76777
O213	0.80646	0.82376	0.59068
O214	0.69441	0.84669	0.49124
O215	0.59396	0.81969	0.61763
O216	0.60479	0.84374	0.81119
O217	0.7279	0.85213	0.74622
O218	0.81176	0.94361	0.67472
O219	0.58331	0.94454	0.68179
O220	0.93129	0.12291	0.90367
O221	0.92178	0.99428	0.94728
O222	0.90307	0.86302	0.9488
O223	0.6933	0.12369	0.89287
O224	0.68157	0.99685	0.94824
O225	0.70266	0.86479	0.94234
O226	0.49179	0.04117	0.70831
O227	0.48688	0.85764	0.72353
O228	0.35541	0.43605	0.71523
O229	0.31689	0.423	0.90313
O230	0.20655	0.4517	0.00655
O231	0.10156	0.42464	0.89028

O232	0.11105	0.45221	0.69289
O233	0.23059	0.45671	0.76325
O234	0.3569	0.65579	0.72069
O235	0.2954	0.66937	0.89164
O236	0.19528	0.64036	0.01782
O237	0.09172	0.66511	0.9022
O238	0.1032	0.65023	0.70458
O239	0.2294	0.62269	0.73674
O240	0.32116	0.54571	0.82193
O241	0.07168	0.54585	0.82242
O242	0.43212	0.37045	0.58582
O243	0.40504	0.49692	0.5536
O244	0.42404	0.62983	0.5537
O245	0.20044	0.36827	0.61819
O246	0.21113	0.49661	0.57496
O247	0.18538	0.62801	0.55118
O248	0.99464	0.44018	0.77607
O249	0.98561	0.64386	0.78839
O250	0.13524	0.54341	0.22878
O251	0.20502	0.55038	0.3943
O252	0.30541	0.58029	0.5156
O253	0.40505	0.56693	0.38599
O254	0.39875	0.5586	0.19159
O255	0.26704	0.55285	0.22256
O256	0.13126	0.33339	0.25306
O257	0.19397	0.3433	0.42356
O258	0.31151	0.34908	0.51208
O259	0.41595	0.33099	0.39455
O260	0.38814	0.33853	0.19909
O261	0.26382	0.31998	0.2602
O262	0.21023	0.43933	0.28338
O263	0.41658	0.44803	0.30228
O264	0.0746	0.61809	0.08912
O265	0.08481	0.48705	0.06296
O266	0.11872	0.35778	0.05764
O267	0.32001	0.61826	0.06871
O268	0.32515	0.48349	0.07701
O269	0.28878	0.35522	0.06918
O270	0.51302	0.53925	0.27482
O271	0.51046	0.35568	0.25979
O272	0.44211	0.74447	0.64319
O273	0.19603	0.74099	0.65245
O274	0.27657	0.74351	0.05165
O275	0.11189	0.74265	0.05858

O276	0.07289	0.24477	0.12928
O277	0.31688	0.23502	0.13406
O278	0.22877	0.24798	0.55634
O279	0.39593	0.24715	0.54526
O280	0.56099	0.2478	0.35043
O281	0.79944	0.23996	0.33929
O282	0.72676	0.23984	0.96373
O283	0.88335	0.24291	0.93688
O284	0.9264	0.74647	0.87157
O285	0.69397	0.74817	0.86422
O286	0.77277	0.74167	0.44552
O287	0.60905	0.74712	0.45481
O288	0.96143	0.27072	0.44643
O289	0.94147	0.21897	0.61166
O290	0.87898	0.33036	0.56708
O291	-0.00536	0.33449	0.61371
GA29	0.93276	0.41445	0.62136
H293	0.94578	0.29994	0.38933
H294	0.83521	0.3449	0.49117
H295	0.91851	0.18401	0.57326
H296	0.94343	0.55522	0.7052
H297	0.90709	0.54693	0.7057
H298	0.10675	0.54663	0.51765
H299	0.05872	0.55534	0.4084
H300	-0.0152	0.59052	0.53637
H301	0.01928	0.5349	0.62322
H302	0.89675	0.5158	0.52879
H303	1.01713	0.39805	0.33245
H304	0.11724	0.44457	0.40797
H305	0.90606	0.43622	0.39061
H306	0.07867	0.4223	0.52095
AL30	0.81745	0.32216	0.31275
AL30	0.79531	0.46978	0.69765
P309	0.94515	0.28922	0.55755
C310	0.94501	0.49043	0.523
C311	0.06339	0.52691	0.47838
C312	0.00309	0.53868	0.54505
C313	1.01151	0.42948	0.39816
C314	0.95142	0.45038	0.42989
C315	0.07215	0.45259	0.45242
<b>C<sub>6</sub>H<sub>9</sub>Ga</b>			
SI2	0.42584	0.05274	0.64216
SI3	0.30521	0.02004	0.78165

SI4	0.28271	0.0489	0.00733
SI5	0.12321	0.05713	0.00909
SI6	0.07093	0.02309	0.79689
SI7	0.17882	0.04962	0.64581
SI8	0.42183	0.81974	0.67134
SI9	0.30507	0.86236	0.80728
SI10	0.26996	0.82362	0.02888
SI11	0.11528	0.82131	0.01833
SI12	0.06606	0.86473	0.80302
SI13	0.18197	0.82052	0.67297
SI14	0.07715	0.93868	0.14907
SI15	0.19947	0.96721	0.29265
SI16	0.21877	0.92919	0.51236
SI17	0.37817	0.92821	0.51474
SI18	0.43271	0.96207	0.30584
SI19	0.32382	0.93658	0.15467
SI20	0.08455	0.16721	0.16131
SI21	0.2021	0.12475	0.30476
SI22	0.23451	0.1694	0.52177
SI23	0.38963	0.16997	0.50743
SI24	0.43983	0.1195	0.29974
SI25	0.32463	0.15658	0.16372
SI26	0.57762	0.55935	0.33611
SI27	0.68836	0.53123	0.17983
SI28	0.71212	0.55117	0.96322
SI29	0.86976	0.55703	0.96989
SI30	0.92687	0.5243	0.18159
SI31	0.80914	0.55568	0.31017
SI32	0.57348	0.32495	0.32194
SI33	0.69476	0.37265	0.18735
SI34	0.72456	0.31922	0.97278
SI35	0.87821	0.32002	0.97594
SI36	0.93253	0.36593	0.18425
SI37	0.92332	0.4344	0.83848
SI38	0.76902	0.43817	0.46547
SI39	0.61009	0.43244	0.47481
SI40	0.56464	0.46799	0.69513
SI41	0.67179	0.42567	0.83351
SI42	0.91468	0.66928	0.82227
SI43	0.80319	0.6302	0.68197
SI44	0.76583	0.66187	0.46465
SI45	0.61112	0.66847	0.47977
SI46	0.5651	0.62429	0.69803
SI47	0.68474	0.67272	0.8121

SI48	0.57884	0.93762	0.36421
SI49	0.69684	0.96182	0.22151
SI50	0.7224	0.93086	0.99797
SI51	0.88195	0.92843	0.99785
SI52	0.93277	0.96736	0.20726
SI53	0.82338	0.94008	0.35999
SI54	0.58165	0.16879	0.33587
SI55	0.69954	0.11745	0.20395
SI56	0.73293	0.16005	0.98236
SI57	0.8869	0.16678	0.98488
SI58	0.93886	0.12531	0.19675
SI59	0.82228	0.16271	0.33105
SI60	0.92611	0.04809	0.8582
SI61	0.80368	0.02065	0.71347
SI62	0.78505	0.06224	0.49545
SI63	0.62453	0.06629	0.49142
SI64	0.57093	0.02312	0.70079
SI65	0.67914	0.04563	0.85401
SI66	0.92142	0.82213	0.84268
SI67	0.80269	0.86431	0.6986
SI68	0.77098	0.82005	0.48303
SI69	0.61705	0.82209	0.49985
SI70	0.56648	0.86528	0.70755
SI71	0.68267	0.82668	0.83863
SI72	0.41899	0.44146	0.64123
SI73	0.30798	0.46574	0.80258
SI74	0.28258	0.42753	0.01616
SI75	0.12675	0.42927	0.00552
SI76	0.07245	0.4652	0.79784
SI77	0.18999	0.44273	0.66225
SI78	0.42611	0.66492	0.65875
SI79	0.3021	0.62266	0.79236
SI80	0.27006	0.66851	0.0039
SI81	0.11543	0.66762	0.01104
SI82	0.06104	0.62327	0.80277
SI83	0.17775	0.66173	0.66442
SI84	0.07583	0.5468	0.14414
SI85	0.20226	0.52157	0.28419
SI86	0.22537	0.56302	0.50942
SI87	0.38385	0.56617	0.50011
SI88	0.43414	0.52761	0.28536
SI89	0.32332	0.55361	0.1423
SI90	0.08332	0.32357	0.15857
SI91	0.19868	0.36029	0.30729

SI92	0.23434	0.3266	0.52696
SI93	0.38972	0.32466	0.50705
SI94	0.43314	0.3679	0.28675
SI95	0.31296	0.31277	0.16682
O96	0.36109	0.05803	0.71471
O97	0.30287	0.05491	0.89077
O98	0.20237	0.04145	0.02174
O99	0.10294	0.06184	0.89234
O100	0.10467	0.05144	0.69498
O101	0.23202	0.02736	0.73118
O102	0.3609	0.817	0.7513
O103	0.3064	0.84375	0.92489
O104	0.19224	0.84778	0.02337
O105	0.08863	0.82621	0.90433
O106	0.10476	0.83179	0.70771
O107	0.23108	0.8472	0.76174
O108	0.32433	0.9409	0.79075
O109	0.08612	0.94344	0.81054
O110	0.43445	0.12233	0.57961
O111	0.41848	0.99096	0.56333
O112	0.39893	0.85917	0.57083
O113	0.19562	0.12407	0.60369
O114	0.17932	0.9943	0.55627
O115	0.19635	0.86047	0.5691
O116	0.99119	0.03643	0.7881
O117	0.9859	0.85656	0.78833
O118	0.14303	0.93677	0.2191
O119	0.20013	0.92267	0.39461
O120	0.2985	0.94132	0.52751
O121	0.39774	0.92127	0.39753
O122	0.39874	0.93968	0.20068
O123	0.27222	0.96329	0.23964
O124	0.147	0.16293	0.23743
O125	0.20015	0.16075	0.41296
O126	0.31212	0.14535	0.51544
O127	0.41475	0.16597	0.39235
O128	0.4014	0.14276	0.19825
O129	0.27563	0.1327	0.25445
O130	0.18334	0.04566	0.31689
O131	0.42191	0.04192	0.32561
O132	0.0696	0.86673	0.09233
O133	0.0818	-0.00245	0.06464
O134	0.1037	0.129	0.05811
O135	0.30685	0.85978	0.12247

O136	0.31911	0.9834	0.05526
O137	0.30849	0.11638	0.06178
O138	0.51168	0.94512	0.29757
O139	0.51974	0.12874	0.28307
O140	0.64123	0.56706	0.26265
O141	0.67661	0.56485	0.0708
O142	0.79187	0.53605	-0.02321
O143	0.90323	0.5621	0.07978
O144	0.88722	0.55407	0.27778
O145	0.76565	0.54718	0.20893
O146	0.64151	0.33403	0.25923
O147	0.69014	0.33755	0.07826
O148	0.80177	0.347	0.96577
O149	0.90219	0.32364	0.09105
O150	0.90358	0.33491	0.28803
O151	0.76902	0.36585	0.23093
O152	0.67265	0.45132	0.17844
O153	0.91233	0.44439	0.16955
O154	0.56745	0.62983	0.39516
O155	0.5863	0.50049	0.41897
O156	0.57562	0.36643	0.4267
O157	0.79516	0.62682	0.36466
O158	0.7908	0.49388	0.38434
O159	0.80427	0.3646	0.43285
O160	0.00546	0.53855	0.20174
O161	0.01343	0.36072	0.18301
O162	0.87284	0.42658	0.74146
O163	0.79874	0.45421	0.57242
O164	0.68997	0.42564	0.46196
O165	0.58879	0.43526	0.59048
O166	0.59635	0.42659	0.78734
O167	0.72718	0.43614	0.74942
O168	0.86284	0.67642	0.72978
O169	0.80881	0.63579	0.56029
O170	0.68774	0.64047	0.47946
O171	0.57825	0.65616	0.58844
O172	0.60647	0.66578	0.78181
O173	0.73075	0.66275	0.71272
O174	0.81096	0.55466	0.72202
O175	0.58843	0.54621	0.69993
O176	0.92579	0.36668	0.90483
O177	0.90939	0.49901	0.90666
O178	0.88067	0.62865	0.91475
O179	0.68027	0.35215	0.88501

O180	0.67653	0.48532	0.91712
O181	0.70388	0.6181	0.89632
O182	0.4839	0.46415	0.70445
O183	0.48597	0.63169	0.72481
O184	0.64163	0.92383	0.29005
O185	0.70136	0.92447	0.11423
O186	0.80245	0.94176	0.98379
O187	0.9007	0.92467	0.11543
O188	0.89776	0.94576	0.31191
O189	0.76977	0.95819	0.27334
O190	0.64726	0.16373	0.26544
O191	0.69934	0.143	0.0893
O192	0.81113	0.13685	0.98538
O193	0.91642	0.16721	0.09784
O194	0.89976	0.15419	0.29376
O195	0.77402	0.12224	0.25235
O196	0.67452	0.03976	0.20777
O197	0.92097	0.04636	0.18222
O198	0.56953	0.87375	0.43868
O199	0.58968	0.00476	0.43123
O200	0.59726	0.13689	0.44572
O201	0.81173	0.86424	0.40127
O202	0.81683	0.99299	0.45199
O203	0.81818	0.12764	0.44204
O204	0.01204	0.95126	0.2186
O205	0.01896	0.13414	0.21367
O206	0.8603	0.04948	0.78814
O207	0.80303	0.06744	0.61375
O208	0.7049	0.06133	0.47707
O209	0.60554	0.06394	0.60907
O210	0.60459	0.04445	0.8065
O211	0.73123	0.02315	0.76709
O212	0.85751	0.83034	0.7706
O213	0.80619	0.82622	0.59192
O214	0.69432	0.84765	0.49131
O215	0.59352	0.81885	0.61593
O216	0.60506	0.84251	0.80924
O217	0.72891	0.85643	0.74829
O218	0.81992	0.94343	0.68278
O219	0.58185	0.94332	0.68048
O220	0.93371	0.12022	0.91404
O221	0.92212	0.98907	0.94232
O222	0.90527	0.8573	0.94958
O223	0.69479	0.12097	0.89282

O224	0.68351	0.99439	0.94843
O225	0.70048	0.86159	0.94434
O226	0.49207	0.0411	0.70953
O227	0.48643	0.8554	0.72291
O228	0.35714	0.43457	0.71878
O229	0.31699	0.42409	0.90613
O230	0.20485	0.45091	0.00564
O231	0.09942	0.42151	0.89153
O232	0.11157	0.44956	0.69442
O233	0.23144	0.45626	0.76443
O234	0.35575	0.65441	0.71604
O235	0.30033	0.66953	0.89132
O236	0.1928	0.64267	0.00292
O237	0.08238	0.66648	0.90028
O238	0.1018	0.64966	0.7049
O239	0.22824	0.6236	0.74143
O240	0.32188	0.5456	0.821
O241	0.07718	0.54436	0.82473
O242	0.43212	0.37011	0.58554
O243	0.40235	0.49607	0.55488
O244	0.42322	0.62863	0.55028
O245	0.20252	0.36751	0.62034
O246	0.21075	0.49645	0.57668
O247	0.18645	0.62829	0.55428
O248	0.99416	0.44297	0.77599
O249	0.98161	0.63079	0.78242
O250	0.13472	0.54389	0.22678
O251	0.1994	0.55059	0.39675
O252	0.30434	0.57884	0.50989
O253	0.40602	0.56398	0.38477
O254	0.39694	0.5605	0.1901
O255	0.26654	0.55399	0.22907
O256	0.13048	0.33317	0.25615
O257	0.19288	0.34502	0.42594
O258	0.31179	0.3486	0.51024
O259	0.41662	0.33259	0.39351
O260	0.3872	0.33684	0.19841
O261	0.26311	0.32111	0.26234
O262	0.20836	0.44008	0.28492
O263	0.41855	0.44785	0.29459
O264	0.07562	0.61861	0.08682
O265	0.08353	0.48686	0.06198
O266	0.11805	0.35726	0.06073
O267	0.31391	0.61757	0.07013

O268	0.32144	0.48314	0.08199
O269	0.28682	0.35482	0.07028
O270	0.51282	0.54202	0.26865
O271	0.51041	0.35299	0.25669
O272	0.44041	0.74372	0.63925
O273	0.19476	0.74096	0.65491
O274	0.27474	0.74354	0.04968
O275	0.11095	0.74355	0.05455
O276	0.0704	0.2452	0.13436
O277	0.31387	0.23466	0.13551
O278	0.22899	0.24755	0.55478
O279	0.39676	0.24733	0.54362
O280	0.56175	0.2468	0.35069
O281	0.80157	0.23983	0.3391
O282	0.72625	0.23884	0.95773
O283	0.8866	0.24264	0.93959
O284	0.93582	0.74317	0.86284
O285	0.69622	0.74746	0.85657
O286	0.77258	0.7423	0.44826
O287	0.60977	0.74773	0.45221
O288	0.96474	0.27465	0.44365
O289	0.94537	0.22031	0.60779
O290	0.88152	0.33158	0.56582
O291	-0.00273	0.33592	0.61285
GA29	0.93558	0.41478	0.62383
H293	0.94687	0.30341	0.38715
H294	0.83537	0.3466	0.49148
H295	0.92303	0.18524	0.56878
H296	0.10166	0.55124	0.5389
H297	0.05823	0.56539	0.42664
H298	-0.02396	0.59502	0.54234
H299	0.00749	0.54288	0.63575
H300	0.89143	0.51561	0.53783
H301	1.01765	0.41067	0.3334
H302	0.11564	0.45489	0.41881
H303	0.9048	0.44301	0.3921
H304	0.07447	0.42771	0.52711
AL30	0.81766	0.32258	0.31401
AL30	0.79705	0.4704	0.69878
P307	0.94791	0.29116	0.55508
C308	0.94106	0.49329	0.52999
C309	0.05956	0.53395	0.49416
C310	-0.00397	0.54425	0.55552
C311	1.01028	0.43907	0.40187

C312	0.94928	0.45692	0.43368
C313	0.06929	0.46079	0.46123
<b>C<sub>6</sub>H<sub>8</sub>+Ga(H)</b>			
SI2	0.42584	0.05297	0.64273
SI3	0.30507	0.02037	0.78246
SI4	0.28247	0.04969	0.00795
SI5	0.12282	0.05752	0.01005
SI6	0.07097	0.02334	0.79747
SI7	0.17874	0.04986	0.64621
SI8	0.42197	0.82027	0.6709
SI9	0.30519	0.86252	0.80773
SI10	0.27029	0.82368	0.02906
SI11	0.1156	0.82113	0.01776
SI12	0.06604	0.8651	0.80289
SI13	0.18211	0.82065	0.67354
SI14	0.07749	0.93823	0.14947
SI15	0.19955	0.96736	0.29324
SI16	0.21884	0.92935	0.51294
SI17	0.37825	0.92876	0.51459
SI18	0.43262	0.96301	0.30559
SI19	0.3237	0.93704	0.15479
SI20	0.08427	0.16767	0.16216
SI21	0.20202	0.1248	0.30523
SI22	0.23446	0.16958	0.52218
SI23	0.38934	0.17023	0.5086
SI24	0.4396	0.12066	0.30041
SI25	0.32432	0.15715	0.16464
SI26	0.57737	0.55912	0.33716
SI27	0.68612	0.53066	0.17857
SI28	0.71235	0.55149	0.96313
SI29	0.87025	0.55753	0.9676
SI30	0.92774	0.5246	0.17872
SI31	0.80764	0.55702	0.30603
SI32	0.57515	0.3258	0.32327
SI33	0.69434	0.37162	0.18527
SI34	0.72453	0.31887	0.97251
SI35	0.87816	0.31897	0.98179
SI36	0.9338	0.36654	0.18736
SI37	0.92406	0.43153	0.84095
SI38	0.77264	0.44045	0.46589
SI39	0.61299	0.43399	0.478
SI40	0.56537	0.46822	0.69668
SI41	0.67674	0.42527	0.82859

SI42	0.9156	0.66919	0.81934
SI43	0.80394	0.62858	0.68113
SI44	0.76491	0.66205	0.46357
SI45	0.61009	0.66926	0.47825
SI46	0.56472	0.62477	0.69654
SI47	0.68446	0.67226	0.81134
SI48	0.57878	0.9384	0.3645
SI49	0.69673	0.96186	0.22184
SI50	0.72235	0.93001	0.99834
SI51	0.88201	0.92771	0.99802
SI52	0.93304	0.96651	0.2076
SI53	0.82329	0.94033	0.3603
SI54	0.58135	0.16986	0.33723
SI55	0.6992	0.11762	0.20567
SI56	0.73272	0.15967	0.98367
SI57	0.88657	0.16593	0.98672
SI58	0.93917	0.12459	0.1981
SI59	0.82254	0.16263	0.33246
SI60	0.92607	0.04784	0.85898
SI61	0.80374	0.02063	0.71421
SI62	0.78514	0.06276	0.49634
SI63	0.62465	0.06711	0.49192
SI64	0.57108	0.02302	0.70099
SI65	0.67905	0.04507	0.85477
SI66	0.92168	0.82213	0.84207
SI67	0.80262	0.86459	0.69888
SI68	0.77073	0.82017	0.48329
SI69	0.61667	0.82257	0.49959
SI70	0.56661	0.86529	0.70752
SI71	0.68275	0.82658	0.83848
SI72	0.42105	0.44199	0.64248
SI73	0.30634	0.46819	0.79872
SI74	0.28503	0.42809	0.01446
SI75	0.1295	0.4298	0.00805
SI76	0.07471	0.46405	0.80054
SI77	0.18717	0.44397	0.65697
SI78	0.42549	0.66553	0.65757
SI79	0.30185	0.6237	0.79235
SI80	0.27042	0.66903	0.00364
SI81	0.11597	0.6673	0.00858
SI82	0.06201	0.6225	0.80006
SI83	0.1784	0.66165	0.66287
SI84	0.07578	0.54732	0.14175
SI85	0.2032	0.52317	0.28015

SI86	0.22464	0.56306	0.50608
SI87	0.3842	0.5651	0.50087
SI88	0.43265	0.52671	0.28615
SI89	0.32651	0.55311	0.13672
SI90	0.08368	0.324	0.16003
SI91	0.1992	0.36156	0.3079
SI92	0.23472	0.32678	0.52726
SI93	0.38995	0.32499	0.50896
SI94	0.43373	0.36776	0.28856
SI95	0.31495	0.31349	0.16698
O96	0.36126	0.05798	0.71564
O97	0.30232	0.05569	0.89127
O98	0.20214	0.04295	0.02322
O99	0.10292	0.06191	0.89312
O100	0.10469	0.05185	0.69566
O101	0.23209	0.02764	0.73136
O102	0.36087	0.81768	0.75052
O103	0.30713	0.84326	0.92512
O104	0.19255	0.84768	0.02263
O105	0.08838	0.82661	0.90422
O106	0.10481	0.83191	0.70783
O107	0.2311	0.84737	0.76246
O108	0.32409	0.94125	0.79235
O109	0.08638	0.94371	0.8105
O110	0.43436	0.12282	0.5808
O111	0.41837	0.99163	0.56321
O112	0.39954	0.85974	0.5702
O113	0.19537	0.12432	0.60394
O114	0.17926	0.9944	0.55684
O115	0.19659	0.8606	0.56972
O116	0.9912	0.03648	0.78904
O117	0.98585	0.8573	0.78794
O118	0.14329	0.9367	0.2196
O119	0.20025	0.9228	0.39518
O120	0.29858	0.94146	0.52804
O121	0.39758	0.9222	0.39723
O122	0.39878	0.94051	0.20034
O123	0.27232	0.96352	0.24024
O124	0.14728	0.16307	0.23726
O125	0.20009	0.16109	0.41328
O126	0.31196	0.14511	0.51595
O127	0.41462	0.16661	0.39361
O128	0.4013	0.14468	0.19921
O129	0.27572	0.13216	0.25521

O130	0.18313	0.04575	0.31767
O131	0.42175	0.04288	0.32506
O132	0.07027	0.8663	0.09261
O133	0.08193	0.99744	0.06546
O134	0.10243	0.1293	0.05869
O135	0.3069	0.8602	0.1226
O136	0.31846	0.98378	0.05538
O137	0.30914	0.11684	0.06246
O138	0.51167	0.94618	0.29784
O139	0.51952	0.13003	0.284
O140	0.63897	0.56738	0.2603
O141	0.67276	0.5617	0.06837
O142	0.79201	0.54101	0.98242
O143	0.90824	0.56089	0.07412
O144	0.88478	0.55692	0.26942
O145	0.76307	0.54884	0.20602
O146	0.64244	0.33191	0.25798
O147	0.68673	0.33868	0.07499
O148	0.80186	0.34609	0.97287
O149	0.90352	0.32188	0.09641
O150	0.90408	0.33609	0.29155
O151	0.76934	0.3634	0.22579
O152	0.67221	0.45042	0.18132
O153	0.9127	0.44448	0.16988
O154	0.56631	0.63035	0.39395
O155	0.59017	0.50194	0.42125
O156	0.58155	0.36749	0.42712
O157	0.79396	0.62729	0.36314
O158	0.78962	0.49431	0.37947
O159	0.80328	0.36539	0.43015
O160	0.00619	0.53867	0.20186
O161	0.01465	0.36174	0.1882
O162	0.87637	0.42057	0.74102
O163	0.81069	0.45538	0.56797
O164	0.69352	0.43001	0.47515
O165	0.5868	0.43508	0.59127
O166	0.60026	0.42747	0.78665
O167	0.73107	0.43494	0.74223
O168	0.86338	0.67609	0.72712
O169	0.80717	0.63507	0.55929
O170	0.68667	0.64131	0.47773
O171	0.57742	0.65673	0.58694
O172	0.60625	0.66661	0.77975
O173	0.73122	0.6597	0.71363

O174	0.81388	0.55314	0.72076
O175	0.58828	0.54676	0.69897
O176	0.92528	0.36591	0.91164
O177	0.90433	0.49786	0.90161
O178	0.88175	0.6288	0.91193
O179	0.68461	0.35158	0.88006
O180	0.6829	0.48422	0.91273
O181	0.70164	0.6186	0.89766
O182	0.48488	0.46255	0.70995
O183	0.48542	0.6315	0.72267
O184	0.6415	0.92396	0.29046
O185	0.70131	0.92436	0.11471
O186	0.80243	0.94074	0.98408
O187	0.90068	0.92413	0.1157
O188	0.89771	0.94552	0.31228
O189	0.76971	0.95826	0.27359
O190	0.64703	0.16414	0.26696
O191	0.69956	0.14348	0.09125
O192	0.81079	0.13604	0.9867
O193	0.91604	0.16631	0.09961
O194	0.89975	0.15309	0.29511
O195	0.77338	0.12199	0.25551
O196	0.67436	0.03988	0.20848
O197	0.92192	0.04564	0.18283
O198	0.56923	0.87485	0.43948
O199	0.59023	0.00562	0.43113
O200	0.59686	0.13771	0.44699
O201	0.81166	0.86467	0.40214
O202	0.81671	0.9938	0.45167
O203	0.81938	0.12863	0.44471
O204	0.01221	0.95005	0.21903
O205	0.01905	0.13448	0.21552
O206	0.86025	0.04942	0.78897
O207	0.80288	0.06752	0.61458
O208	0.70512	0.06297	0.47714
O209	0.60592	0.06405	0.60961
O210	0.60457	0.04404	0.80697
O211	0.73128	0.02311	0.76775
O212	0.85743	0.8305	0.77068
O213	0.80562	0.82622	0.5924
O214	0.69405	0.84771	0.49102
O215	0.59357	0.81882	0.61585
O216	0.60512	0.84248	0.80927
O217	0.72889	0.85746	0.74887

O218	0.82016	0.94362	0.6827
O219	0.58205	0.94329	0.68026
O220	0.93348	0.11975	0.91554
O221	0.92198	0.98848	0.94258
O222	0.90557	0.85667	0.94956
O223	0.69437	0.12023	0.8947
O224	0.68345	0.99339	0.94854
O225	0.70028	0.86062	0.94505
O226	0.49223	0.04102	0.70961
O227	0.48656	0.85562	0.72292
O228	0.35689	0.43813	0.716
O229	0.31119	0.42304	0.89966
O230	0.2072	0.45218	0.01824
O231	0.10991	0.42295	0.89087
O232	0.10943	0.44801	0.69333
O233	0.23096	0.46321	0.7547
O234	0.35561	0.65535	0.71618
O235	0.29895	0.6717	0.89007
O236	0.19349	0.64207	0.00467
O237	0.08518	0.66649	0.89624
O238	0.10217	0.64797	0.70092
O239	0.22839	0.62341	0.74027
O240	0.3219	0.54704	0.82342
O241	0.07764	0.54386	0.82385
O242	0.43236	0.36983	0.58819
O243	0.40987	0.49672	0.55408
O244	0.42082	0.63023	0.54841
O245	0.20258	0.36812	0.61991
O246	0.20095	0.49588	0.56575
O247	0.18851	0.62957	0.55203
O248	0.9979	0.43764	0.79038
O249	0.98271	0.63101	0.7797
O250	0.13601	0.54633	0.22251
O251	0.20336	0.5572	0.38998
O252	0.30442	0.57162	0.51727
O253	0.40261	0.56384	0.38391
O254	0.39869	0.56085	0.18908
O255	0.26817	0.5495	0.22062
O256	0.13228	0.3322	0.25612
O257	0.19339	0.34458	0.42598
O258	0.31211	0.34934	0.511
O259	0.41782	0.33312	0.39597
O260	0.39022	0.33328	0.20015
O261	0.26525	0.32602	0.26162

O262	0.20507	0.4419	0.28919
O263	0.41519	0.44713	0.29386
O264	0.0743	0.61838	0.08234
O265	0.08312	0.48664	0.0606
O266	0.11753	0.35751	0.06131
O267	0.31626	0.61835	0.06732
O268	0.32882	0.48428	0.07198
O269	0.29247	0.35568	0.06865
O270	0.5119	0.53864	0.27363
O271	0.51187	0.35592	0.2607
O272	0.44049	0.74425	0.63877
O273	0.19481	0.74109	0.65547
O274	0.27484	0.7437	0.0508
O275	0.11121	0.74312	0.05262
O276	0.06983	0.24571	0.13566
O277	0.31178	0.23513	0.13724
O278	0.22961	0.24776	0.55542
O279	0.39606	0.24752	0.54516
O280	0.56163	0.24794	0.35254
O281	0.80278	0.24	0.34029
O282	0.72593	0.23835	0.95843
O283	0.88605	0.24207	0.94306
O284	0.93658	0.7431	0.86026
O285	0.69682	0.7473	0.85413
O286	0.77253	0.74249	0.44829
O287	0.60873	0.74856	0.45088
O288	0.96533	0.27057	0.43876
O289	0.93076	0.20954	0.59356
O290	0.88332	0.33009	0.55904
O291	0.99564	0.31787	0.61731
GA29	0.94046	0.40214	0.6256
H293	0.94514	0.2992	0.3831
H294	0.83509	0.34697	0.48675
H295	0.90553	0.17939	0.54935
H296	0.08838	0.57854	0.51848
H297	0.06428	0.5844	0.39288
H298	0.97495	0.62384	0.53343
H299	-0.03114	0.47245	0.6057
H300	0.8817	0.54959	0.4945
H301	0.01305	0.39876	0.37162
H302	0.10834	0.47103	0.41004
H303	0.9005	0.44535	0.38935
H304	0.07236	0.45981	0.52763
AL30	0.81745	0.32264	0.31217

AL30	0.80325	0.46848	0.69568
P307	0.94497	0.28154	0.5501
C308	0.9321	0.53562	0.47241
C309	0.05309	0.55826	0.46386
C310	0.98361	0.57614	0.49511
C311	0.0047	0.44657	0.40934
C312	0.94292	0.4723	0.42005
C313	0.06321	0.48213	0.4532

### **C<sub>6</sub>H<sub>7</sub>Ga+H<sub>2</sub>\***

SI2	0.4268	0.05242	0.64324
SI3	0.30591	0.02034	0.7829
SI4	0.28301	0.05118	0.00803
SI5	0.12331	0.05914	0.01035
SI6	0.07163	0.02249	0.79775
SI7	0.17943	0.04921	0.64664
SI8	0.42272	0.81969	0.67023
SI9	0.30619	0.86258	0.80757
SI10	0.27081	0.82463	0.02909
SI11	0.11667	0.82277	0.01693
SI12	0.06768	0.86405	0.8017
SI13	0.1839	0.82061	0.67211
SI14	0.07776	0.93926	0.14911
SI15	0.1994	0.96729	0.29256
SI16	0.21984	0.92964	0.51232
SI17	0.37907	0.92855	0.51459
SI18	0.43301	0.96389	0.30585
SI19	0.32405	0.9382	0.15462
SI20	0.0838	0.1679	0.16237
SI21	0.20139	0.12434	0.30492
SI22	0.23521	0.16825	0.52244
SI23	0.38983	0.16981	0.51007
SI24	0.43966	0.1216	0.30154
SI25	0.32406	0.15763	0.16575
SI26	0.57592	0.55793	0.33859
SI27	0.68748	0.5266	0.18526
SI28	0.71009	0.54911	0.96619
SI29	0.86828	0.55577	0.96639
SI30	0.92671	0.52284	0.17757
SI31	0.81294	0.55259	0.31379
SI32	0.57996	0.32486	0.32399
SI33	0.69373	0.36904	0.18055
SI34	0.72781	0.31902	0.96792
SI35	0.88199	0.31853	0.98171

SI36	0.93354	0.36507	0.19168
SI37	0.92597	0.43101	0.8411
SI38	0.77661	0.43779	0.47163
SI39	0.617	0.43595	0.48027
SI40	0.56483	0.46686	0.6959
SI41	0.67368	0.42602	0.83061
SI42	0.91615	0.66743	0.82009
SI43	0.80427	0.62873	0.68157
SI44	0.76531	0.6613	0.46307
SI45	0.61041	0.66881	0.47724
SI46	0.56456	0.62296	0.69458
SI47	0.68289	0.66985	0.81344
SI48	0.57891	0.93831	0.3644
SI49	0.69677	0.96132	0.2206
SI50	0.7228	0.92826	0.99825
SI51	0.88254	0.92622	0.99714
SI52	0.93324	0.96568	0.20657
SI53	0.82335	0.93948	0.35895
SI54	0.5817	0.16978	0.33932
SI55	0.69965	0.11695	0.20678
SI56	0.73395	0.16001	0.98486
SI57	0.88792	0.1653	0.98592
SI58	0.93946	0.12335	0.19737
SI59	0.82285	0.16103	0.33302
SI60	0.92662	0.04649	0.85821
SI61	0.80352	0.0191	0.71455
SI62	0.78487	0.06115	0.49612
SI63	0.62477	0.06655	0.4927
SI64	0.57204	0.02242	0.70223
SI65	0.67934	0.04442	0.85677
SI66	0.9229	0.82049	0.84105
SI67	0.80306	0.86226	0.69808
SI68	0.77117	0.81905	0.48156
SI69	0.61707	0.82215	0.4988
SI70	0.5675	0.86452	0.70752
SI71	0.68298	0.82406	0.83896
SI72	0.41967	0.44208	0.64215
SI73	0.30553	0.46793	0.79772
SI74	0.28519	0.42719	0.01429
SI75	0.12816	0.42931	0.0066
SI76	0.0756	0.46474	0.79924
SI77	0.18656	0.44225	0.65471
SI78	0.42461	0.66493	0.65698
SI79	0.30187	0.62362	0.79373

SI80	0.26934	0.66949	0.00587
SI81	0.11494	0.66943	0.01127
SI82	0.06258	0.62331	0.80258
SI83	0.17806	0.6631	0.66463
SI84	0.07585	0.54821	0.13768
SI85	0.20035	0.52284	0.28204
SI86	0.21921	0.56258	0.5059
SI87	0.37938	0.56487	0.50094
SI88	0.431	0.52604	0.28748
SI89	0.32448	0.55247	0.13882
SI90	0.08219	0.32375	0.1625
SI91	0.20013	0.36129	0.30852
SI92	0.23548	0.32504	0.52678
SI93	0.3904	0.32408	0.51018
SI94	0.43611	0.36727	0.29185
SI95	0.31839	0.31466	0.16925
O96	0.36219	0.05784	0.71601
O97	0.30269	0.05641	0.89118
O98	0.20268	0.04487	0.02364
O99	0.10311	0.06143	0.89345
O100	0.10546	0.05107	0.69613
O101	0.23299	0.02682	0.7314
O102	0.36188	0.81779	0.75028
O103	0.30783	0.84299	0.92483
O104	0.1934	0.84993	0.02299
O105	0.09099	0.82544	0.90241
O106	0.10647	0.83165	0.70612
O107	0.23226	0.84778	0.76162
O108	0.32536	0.94138	0.7934
O109	0.08716	0.94287	0.81067
O110	0.43543	0.1222	0.58114
O111	0.41955	0.99089	0.56403
O112	0.40013	0.85912	0.56945
O113	0.19594	0.12369	0.60466
O114	0.17995	0.99435	0.55653
O115	0.19799	0.86079	0.56853
O116	0.99188	0.03518	0.7887
O117	0.98749	0.85529	0.78768
O118	0.14346	0.93547	0.21935
O119	0.20104	0.92313	0.39471
O120	0.29952	0.94198	0.52782
O121	0.39824	0.92252	0.39712
O122	0.399	0.94223	0.20045
O123	0.27222	0.9643	0.23967

O124	0.14689	0.16365	0.23765
O125	0.20073	0.15982	0.41359
O126	0.31276	0.1437	0.51668
O127	0.41486	0.16748	0.39486
O128	0.40104	0.14536	0.20057
O129	0.27509	0.13071	0.25457
O130	0.18153	0.04547	0.31619
O131	0.4225	0.0437	0.32647
O132	0.06994	0.86884	0.08848
O133	0.08246	1.00017	0.06817
O134	0.10287	0.13138	0.05761
O135	0.30808	0.86125	0.12202
O136	0.31876	0.98517	0.05549
O137	0.30996	0.11855	0.062
O138	0.51197	0.94668	0.29766
O139	0.5195	0.13148	0.28483
O140	0.63943	0.56429	0.26475
O141	0.67763	0.5607	0.07621
O142	0.79011	0.53732	0.97543
O143	0.90187	0.55926	0.07582
O144	0.88879	0.55605	0.27263
O145	0.76458	0.53799	0.2191
O146	0.64237	0.32464	0.24787
O147	0.68775	0.34122	0.06725
O148	0.80542	0.34547	0.9711
O149	0.90714	0.32132	0.09657
O150	0.90115	0.33453	0.2936
O151	0.76875	0.36105	0.22099
O152	0.66909	0.44719	0.18429
O153	0.91156	0.44274	0.17266
O154	0.56621	0.62989	0.39369
O155	0.58551	0.50011	0.42303
O156	0.59867	0.36619	0.42494
O157	0.79529	0.62384	0.3655
O158	0.8061	0.49097	0.39322
O159	0.79317	0.36031	0.42909
O160	0.00538	0.53653	0.19222
O161	0.01459	0.3612	0.19932
O162	0.87309	0.41821	0.74672
O163	0.815	0.43967	0.57788
O164	0.69743	0.44644	0.48427
O165	0.58719	0.4319	0.59169
O166	0.59725	0.42591	0.78831
O167	0.72556	0.44307	0.74334

O168	0.86401	0.67536	0.72773
O169	0.80689	0.63641	0.56032
O170	0.68698	0.64091	0.47633
O171	0.57808	0.65566	0.58583
O172	0.6053	0.66509	0.77843
O173	0.73144	0.65713	0.71766
O174	0.81607	0.55236	0.7162
O175	0.58911	0.54512	0.69712
O176	0.92977	0.3652	0.91163
O177	0.90381	0.49629	0.90257
O178	0.88052	0.62739	0.91188
O179	0.68915	0.35105	0.87335
O180	0.67693	0.48178	0.92015
O181	0.69679	0.61581	0.90072
O182	0.48425	0.4637	0.70712
O183	0.48504	0.62888	0.71868
O184	0.64157	0.92429	0.2902
O185	0.7016	0.92251	0.11456
O186	0.80285	0.93916	0.98385
O187	0.90138	0.92272	0.11483
O188	0.89776	0.94491	0.31127
O189	0.76964	0.95787	0.27275
O190	0.64738	0.16249	0.26941
O191	0.70213	0.14648	0.09429
O192	0.81186	0.13604	0.9862
O193	0.91711	0.16547	0.09895
O194	0.89952	0.15173	0.29405
O195	0.77317	0.11857	0.25931
O196	0.67457	0.03923	0.20437
O197	0.92149	0.04464	0.18128
O198	0.56955	0.87444	0.43884
O199	0.59029	0.00516	0.43193
O200	0.59631	0.13719	0.44908
O201	0.81207	0.86377	0.40068
O202	0.81656	0.99268	0.45078
O203	0.82069	0.12763	0.44681
O204	0.01244	0.94987	0.21904
O205	0.01937	0.1326	0.21521
O206	0.86101	0.04749	0.78777
O207	0.80206	0.06563	0.61442
O208	0.70517	0.06295	0.47551
O209	0.60747	0.063	0.61078
O210	0.60506	0.04395	0.80832
O211	0.73169	0.02323	0.76952

O212	0.85935	0.82906	0.76818
O213	0.80592	0.82458	0.59089
O214	0.69457	0.84684	0.48945
O215	0.59462	0.81862	0.6153
O216	0.60566	0.84086	0.80913
O217	0.72982	0.85301	0.74887
O218	0.8184	0.94185	0.68276
O219	0.58342	0.9427	0.68209
O220	0.93398	0.11841	0.91469
O221	0.9223	0.98717	0.94189
O222	0.90595	0.8553	0.94812
O223	0.69416	0.11913	0.89888
O224	0.68355	0.9916	0.94904
O225	0.70096	0.85887	0.94477
O226	0.49322	0.04048	0.71008
O227	0.48741	0.85511	0.72191
O228	0.35693	0.4362	0.71767
O229	0.30901	0.42263	0.89854
O230	0.20653	0.44714	0.02121
O231	0.10983	0.42229	0.88919
O232	0.10958	0.44346	0.6936
O233	0.23102	0.46429	0.75057
O234	0.35618	0.65639	0.71952
O235	0.29947	0.66991	0.89328
O236	0.19211	0.6435	0.0042
O237	0.08076	0.66632	0.90188
O238	0.10294	0.65704	0.70977
O239	0.22886	0.62435	0.74053
O240	0.32202	0.54653	0.82245
O241	0.08315	0.54489	0.81974
O242	0.43248	0.37003	0.58827
O243	0.40528	0.49678	0.555
O244	0.4161	0.63026	0.5479
O245	0.2038	0.36646	0.61945
O246	0.19704	0.4932	0.56129
O247	0.18262	0.62747	0.55548
O248	0.99756	0.44332	0.78875
O249	0.98274	0.62777	0.78172
O250	0.13536	0.54551	0.21902
O251	0.19774	0.5598	0.38956
O252	0.29945	0.57131	0.51636
O253	0.39917	0.56277	0.38435
O254	0.39725	0.55916	0.18959
O255	0.26754	0.54547	0.22436

O256	0.13636	0.32904	0.25202
O257	0.19365	0.34092	0.42537
O258	0.31261	0.34823	0.5097
O259	0.4197	0.33146	0.39804
O260	0.39483	0.33109	0.20208
O261	0.2696	0.33221	0.26316
O262	0.19982	0.44208	0.29578
O263	0.41527	0.44604	0.29578
O264	0.0738	0.62208	0.08747
O265	0.08451	0.49061	0.05252
O266	0.11092	0.35882	0.06153
O267	0.31302	0.61969	0.07418
O268	0.32703	0.48605	0.06893
O269	0.29793	0.35576	0.06902
O270	0.5101	0.53958	0.27471
O271	0.51548	0.35908	0.26956
O272	0.4413	0.74349	0.63874
O273	0.19823	0.74155	0.65223
O274	0.27412	0.74469	0.05109
O275	0.11207	0.74545	0.05457
O276	0.06695	0.24573	0.1375
O277	0.3108	0.23606	0.14245
O278	0.23099	0.24626	0.55607
O279	0.39621	0.24689	0.54804
O280	0.56325	0.24814	0.35628
O281	0.80127	0.23795	0.33949
O282	0.72786	0.23831	0.95624
O283	0.88861	0.24152	0.94271
O284	0.93725	0.74144	0.86044
O285	0.69561	0.74467	0.85681
O286	0.77298	0.74154	0.44507
O287	0.60884	0.74813	0.4502
O288	0.95022	0.25227	0.45242
O289	0.90623	0.1883	0.59774
O290	0.85908	0.30828	0.56089
O291	0.96774	0.29829	0.63519
GA29	0.91212	0.38679	0.61778
H293	0.93899	0.28564	0.39925
H294	0.81716	0.33177	0.48648
H295	0.87957	0.16194	0.54885
H296	0.05249	0.56758	0.60114
H297	0.01414	0.45258	0.60795
H298	0.90689	0.53623	0.59932
H299	0.08154	0.54397	0.60155

H300	0.9451	0.61334	0.46958
H301	0.07714	0.46261	0.34777
H302	0.03452	0.38037	0.46971
H303	1.04486	0.58156	0.36485
H304	0.96131	0.40437	0.40501
AL30	0.81493	0.32086	0.31017
AL30	0.80147	0.46798	0.70133
P307	0.92265	0.2612	0.56197
C308	0.96532	0.56243	0.47386
C309	-0.02666	0.45087	0.55276
C310	0.94307	0.51938	0.54401
C311	0.03815	0.47791	0.39969
C312	1.01965	0.54268	0.40802
C313	0.00136	0.42339	0.45453

### C<sub>6</sub>H<sub>7</sub>Ga

SI2	0.42598	0.05233	0.64336
SI3	0.3044	0.02053	0.78237
SI4	0.28247	0.05173	0.00818
SI5	0.12256	0.05737	0.00964
SI6	0.07098	0.02302	0.796
SI7	0.17826	0.05052	0.64547
SI8	0.42162	0.81943	0.6696
SI9	0.30437	0.86197	0.80646
SI10	0.26992	0.82435	0.02823
SI11	0.11537	0.82171	0.01648
SI12	0.06591	0.86477	0.8006
SI13	0.18164	0.81931	0.67179
SI14	0.07737	0.93761	0.14937
SI15	0.19881	0.96679	0.29345
SI16	0.21875	0.92944	0.51327
SI17	0.37799	0.9286	0.51473
SI18	0.43221	0.96379	0.30567
SI19	0.32321	0.93815	0.15469
SI20	0.08217	0.16589	0.16201
SI21	0.20068	0.12367	0.3039
SI22	0.23408	0.16928	0.52034
SI23	0.38874	0.16976	0.50978
SI24	0.43899	0.12195	0.30094
SI25	0.32305	0.15806	0.16557
SI26	0.57743	0.55755	0.33677
SI27	0.68911	0.52675	0.18448
SI28	0.71135	0.5487	0.96458
SI29	0.86961	0.55579	0.96718

SI30	0.92883	0.52395	0.17915
SI31	0.81406	0.55353	0.31306
SI32	0.58143	0.32473	0.32449
SI33	0.69439	0.36889	0.18017
SI34	0.72831	0.31926	0.96794
SI35	0.88249	0.31852	0.98328
SI36	0.93541	0.3653	0.19307
SI37	0.92659	0.43072	0.84189
SI38	0.77836	0.43871	0.4717
SI39	0.61911	0.43619	0.48012
SI40	0.56521	0.46611	0.69537
SI41	0.67559	0.42534	0.82774
SI42	0.91663	0.66778	0.8207
SI43	0.8046	0.62895	0.68175
SI44	0.76559	0.66125	0.4632
SI45	0.61063	0.66807	0.47666
SI46	0.56413	0.62249	0.69392
SI47	0.6828	0.66972	0.81292
SI48	0.57832	0.93776	0.36413
SI49	0.69644	0.96115	0.22056
SI50	0.72225	0.92835	0.99795
SI51	0.88194	0.92613	0.99714
SI52	0.93249	0.96511	0.2066
SI53	0.823	0.93935	0.35925
SI54	0.58141	0.16977	0.33958
SI55	0.6993	0.11686	0.20691
SI56	0.73366	0.16004	0.98509
SI57	0.8876	0.16503	0.98732
SI58	0.93845	0.12246	0.19877
SI59	0.82228	0.16113	0.33388
SI60	0.92613	0.04656	0.8588
SI61	0.80309	0.01902	0.71517
SI62	0.78439	0.061	0.49656
SI63	0.62426	0.06583	0.49264
SI64	0.57135	0.0222	0.70229
SI65	0.67876	0.04467	0.85689
SI66	0.92203	0.82075	0.84094
SI67	0.80217	0.86208	0.69853
SI68	0.77067	0.81897	0.48211
SI69	0.61658	0.82159	0.49875
SI70	0.56643	0.86413	0.70733
SI71	0.68198	0.82398	0.83867
SI72	0.42114	0.44205	0.64071
SI73	0.30464	0.46828	0.79379

SI74	0.28635	0.42606	0.01021
SI75	0.12889	0.42635	0.00685
SI76	0.07601	0.46452	0.80009
SI77	0.18498	0.44356	0.65071
SI78	0.42366	0.66462	0.65556
SI79	0.30051	0.62349	0.79196
SI80	0.26993	0.669	0.00531
SI81	0.11608	0.66837	0.00312
SI82	0.06356	0.6221	0.7971
SI83	0.17738	0.66065	0.65858
SI84	0.07641	0.54895	0.13288
SI85	0.20002	0.52346	0.27501
SI86	0.22069	0.56101	0.50021
SI87	0.38138	0.56348	0.49822
SI88	0.43249	0.52509	0.28517
SI89	0.3263	0.55106	0.13445
SI90	0.0825	0.32104	0.16115
SI91	0.19947	0.36261	0.3037
SI92	0.23473	0.32655	0.52409
SI93	0.38984	0.32404	0.51043
SI94	0.43672	0.36657	0.2923
SI95	0.31975	0.31566	0.16781
O96	0.36153	0.0574	0.71638
O97	0.30212	0.05584	0.89124
O98	0.20218	0.04526	0.02412
O99	0.10325	0.06034	0.89247
O100	0.10423	0.05288	0.69479
O101	0.23171	0.02932	0.73104
O102	0.36067	0.81779	0.74947
O103	0.30675	0.84335	0.92406
O104	0.19221	0.84856	0.02205
O105	0.08817	0.828	0.90321
O106	0.10434	0.83025	0.7064
O107	0.2306	0.84502	0.76152
O108	0.32188	0.94102	0.79101
O109	0.0867	0.94329	0.80575
O110	0.4341	0.12212	0.58114
O111	0.41871	0.9908	0.56415
O112	0.39933	0.85897	0.56878
O113	0.19434	0.12476	0.6021
O114	0.17906	0.99444	0.55698
O115	0.1964	0.86065	0.56941
O116	0.99117	0.03566	0.78873
O117	0.98563	0.85667	0.78648

O118	0.14274	0.93528	0.2203
O119	0.20045	0.92254	0.39552
O120	0.29846	0.94171	0.52907
O121	0.39678	0.92316	0.39709
O122	0.39822	0.94144	0.20053
O123	0.27152	0.96384	0.24021
O124	0.14624	0.16192	0.23533
O125	0.20003	0.16088	0.41124
O126	0.31148	0.14417	0.51589
O127	0.41405	0.16732	0.39475
O128	0.40014	0.14599	0.20021
O129	0.27441	0.12935	0.25352
O130	0.18115	0.04493	0.31784
O131	0.42222	0.04383	0.32501
O132	0.06973	0.86581	0.09231
O133	0.0829	0.99662	0.06536
O134	0.09983	0.12872	0.05732
O135	0.30676	0.86149	0.12105
O136	0.31837	0.9861	0.05659
O137	0.30927	0.11981	0.06085
O138	0.5111	0.94611	0.29796
O139	0.51877	0.1325	0.28457
O140	0.64081	0.56525	0.26283
O141	0.6784	0.55908	0.07447
O142	0.79137	0.53759	0.97504
O143	0.90273	0.55905	0.077
O144	0.89062	0.55667	0.27446
O145	0.76635	0.53924	0.21739
O146	0.64259	0.32405	0.2461
O147	0.6876	0.34275	0.06601
O148	0.80594	0.34535	0.97319
O149	0.90856	0.32228	0.09755
O150	0.90205	0.3348	0.29433
O151	0.76946	0.35991	0.21996
O152	0.67094	0.44731	0.1866
O153	0.91515	0.44354	0.17518
O154	0.56675	0.62921	0.39251
O155	0.58847	0.49979	0.42076
O156	0.60256	0.36615	0.42427
O157	0.79579	0.62443	0.36522
O158	0.80634	0.49164	0.3918
O159	0.79424	0.36116	0.42909
O160	0.0074	0.5398	0.19307
O161	0.01646	0.36013	0.20089

O162	0.87417	0.41867	0.74678
O163	0.81922	0.44204	0.57603
O164	0.69942	0.44705	0.4887
O165	0.58647	0.43232	0.58981
O166	0.599	0.42489	0.78629
O167	0.72719	0.44157	0.73961
O168	0.86439	0.67538	0.72842
O169	0.80728	0.63651	0.56048
O170	0.68731	0.64042	0.47617
O171	0.57788	0.65471	0.58493
O172	0.60521	0.66433	0.77778
O173	0.73172	0.65769	0.71735
O174	0.81627	0.55276	0.71723
O175	0.58847	0.54462	0.69716
O176	0.92978	0.36487	0.91214
O177	0.90537	0.49636	0.90339
O178	0.88182	0.62751	0.91286
O179	0.69109	0.35071	0.8717
O180	0.67923	0.48161	0.91644
O181	0.69749	0.61578	0.90011
O182	0.4848	0.46169	0.70901
O183	0.4844	0.6287	0.71696
O184	0.6409	0.92411	0.28959
O185	0.70143	0.92244	0.11442
O186	0.80231	0.93917	0.98328
O187	0.90065	0.92223	0.11483
O188	0.89741	0.944	0.31141
O189	0.76918	0.95764	0.27312
O190	0.64685	0.16224	0.26932
O191	0.70177	0.14626	0.09439
O192	0.8115	0.13584	0.98637
O193	0.91622	0.165	0.10068
O194	0.89902	0.15089	0.29579
O195	0.77267	0.11888	0.25983
O196	0.67439	0.0391	0.20448
O197	0.91984	0.04399	0.18182
O198	0.56917	0.87366	0.43818
O199	0.5897	0.00447	0.43195
O200	0.59583	0.13642	0.44884
O201	0.81144	0.86385	0.40139
O202	0.81669	0.99302	0.45055
O203	0.81949	0.12803	0.44781
O204	0.01184	0.9499	0.21821
O205	0.01841	0.13076	0.21679

O206	0.86041	0.04758	0.78855
O207	0.80172	0.06526	0.61481
O208	0.70468	0.06199	0.47592
O209	0.60684	0.0625	0.61069
O210	0.60449	0.04389	0.80827
O211	0.73111	0.02335	0.76972
O212	0.85775	0.82825	0.7693
O213	0.80558	0.8246	0.59129
O214	0.69403	0.84659	0.49024
O215	0.59351	0.81828	0.61501
O216	0.60455	0.84047	0.80898
O217	0.72862	0.85295	0.74833
O218	0.81802	0.94164	0.68398
O219	0.58234	0.94239	0.68232
O220	0.93369	0.11823	0.91596
O221	0.92203	0.98698	0.94212
O222	0.90536	0.85521	0.94826
O223	0.69367	0.11941	0.89892
O224	0.68304	0.9919	0.94926
O225	0.70008	0.85913	0.94423
O226	0.49257	0.04062	0.70994
O227	0.48631	0.85469	0.72158
O228	0.3565	0.43855	0.71282
O229	0.30712	0.42135	0.89309
O230	0.20735	0.4436	0.02262
O231	0.11164	0.42179	0.88857
O232	0.10874	0.44663	0.6923
O233	0.23062	0.46542	0.74523
O234	0.35519	0.65601	0.71808
O235	0.29815	0.66976	0.89158
O236	0.1931	0.64186	0.00576
O237	0.08901	0.66937	0.88872
O238	0.10095	0.64697	0.69554
O239	0.22767	0.6242	0.73791
O240	0.32061	0.54653	0.82157
O241	0.08194	0.54434	0.82348
O242	0.43272	0.36931	0.58836
O243	0.41128	0.49691	0.55212
O244	0.4145	0.63049	0.54622
O245	0.20107	0.36734	0.61594
O246	0.19402	0.49361	0.55618
O247	0.18714	0.62794	0.54832
O248	0.99841	0.44181	0.78979
O249	0.98338	0.6285	0.78245

O250	0.13787	0.55335	0.21137
O251	0.20004	0.55891	0.38364
O252	0.30116	0.56494	0.51304
O253	0.40127	0.56309	0.38152
O254	0.39897	0.55681	0.18599
O255	0.26961	0.54092	0.2197
O256	0.13856	0.32413	0.24845
O257	0.1949	0.34399	0.42139
O258	0.31234	0.3493	0.51079
O259	0.41894	0.33113	0.3982
O260	0.39643	0.32962	0.20206
O261	0.27106	0.3385	0.25929
O262	0.19171	0.44277	0.28601
O263	0.41578	0.44536	0.29516
O264	0.07082	0.61832	0.06994
O265	0.08481	0.48593	0.05661
O266	0.11059	0.35501	0.05877
O267	0.31469	0.61993	0.07346
O268	0.32841	0.48659	0.06052
O269	0.30266	0.35525	0.06477
O270	0.51177	0.53816	0.27295
O271	0.51631	0.35898	0.27198
O272	0.44011	0.74327	0.63786
O273	0.19398	0.74014	0.65051
O274	0.27428	0.74439	0.05005
O275	0.11116	0.74342	0.04981
O276	0.06463	0.24348	0.13679
O277	0.3086	0.23677	0.14547
O278	0.22969	0.2476	0.55238
O279	0.39499	0.24677	0.54797
O280	0.5642	0.24829	0.35773
O281	0.80163	0.23829	0.34011
O282	0.72784	0.23848	0.95733
O283	0.88884	0.24141	0.94485
O284	0.93777	0.74193	0.86041
O285	0.69474	0.74462	0.85666
O286	0.77269	0.74157	0.44543
O287	0.60889	0.74749	0.45023
O288	0.95076	0.25294	0.45232
O289	0.90523	0.18912	0.59718
O290	0.86042	0.30999	0.56069
O291	0.96871	0.29782	0.63543
GA29	0.91418	0.38786	0.61796
H293	0.93929	0.28633	0.39919

H294	0.81881	0.33277	0.4867
H295	0.87835	0.16322	0.54802
H296	0.02224	0.44171	0.60706
H297	0.92652	0.53772	0.62527
H298	0.96646	0.61941	0.50313
H299	0.07129	0.46571	0.33812
H300	0.03075	0.38056	0.45718
H301	1.05247	0.58536	0.37565
H302	0.95671	0.41321	0.40495
AL30	0.8157	0.32106	0.31035
AL30	0.80313	0.46844	0.69994
P305	0.92322	0.26178	0.56188
C306	0.98081	0.56664	0.49692
C307	-0.02038	0.44939	0.55659
C308	0.95767	0.52125	0.56305
C309	0.03839	0.48105	0.39871
C310	1.02751	0.54634	0.41908
C311	0.00035	0.42662	0.45169

### C<sub>6</sub>H<sub>6</sub>\*

SI2	0.42584	0.05278	0.64195
SI3	0.30374	0.02069	0.78001
SI4	0.28221	0.05124	0.00691
SI5	0.12198	0.05829	0.00816
SI6	0.07099	0.02349	0.79366
SI7	0.17752	0.05125	0.64269
SI8	0.42229	0.82	0.66866
SI9	0.30458	0.86153	0.80592
SI10	0.27133	0.82423	0.02751
SI11	0.11665	0.82303	0.01665
SI12	0.06679	0.86543	0.79989
SI13	0.18204	0.81721	0.6733
SI14	0.07765	0.93835	0.14933
SI15	0.19874	0.96548	0.29546
SI16	0.21844	0.92797	0.5143
SI17	0.37774	0.92887	0.51357
SI18	0.43157	0.96423	0.30462
SI19	0.32242	0.93722	0.15504
SI20	0.08206	0.16567	0.16072
SI21	0.20199	0.12188	0.30116
SI22	0.23305	0.17139	0.51697
SI23	0.38952	0.172	0.50975
SI24	0.43865	0.12199	0.3009
SI25	0.32394	0.15633	0.1631

SI26	0.57933	0.55534	0.33766
SI27	0.69435	0.52485	0.18777
SI28	0.71338	0.5522	0.96835
SI29	0.86995	0.55857	0.96991
SI30	0.9246	0.52681	0.17904
SI31	0.81714	0.5481	0.32584
SI32	0.5782	0.3257	0.32852
SI33	0.69669	0.37009	0.18731
SI34	0.72765	0.31897	0.9725
SI35	0.88163	0.32093	0.98143
SI36	0.9352	0.36772	0.18798
SI37	0.92823	0.4371	0.85112
SI38	0.78096	0.43331	0.47938
SI39	0.62116	0.43402	0.47923
SI40	0.57219	0.47097	0.69378
SI41	0.66972	0.43136	0.84426
SI42	0.91667	0.66988	0.82217
SI43	0.80447	0.63247	0.68238
SI44	0.76529	0.66226	0.46315
SI45	0.61022	0.66859	0.47543
SI46	0.56584	0.62608	0.69416
SI47	0.6832	0.67232	0.81507
SI48	0.57723	0.93847	0.36222
SI49	0.69547	0.9631	0.21826
SI50	0.722	0.93109	0.99657
SI51	0.88147	0.92855	0.99462
SI52	0.9325	0.9658	0.2038
SI53	0.82234	0.93999	0.3559
SI54	0.58155	0.16993	0.33673
SI55	0.69665	0.11849	0.19824
SI56	0.73332	0.16151	0.97836
SI57	0.88777	0.16725	0.98317
SI58	0.93863	0.12308	0.19462
SI59	0.81963	0.16158	0.3247
SI60	0.92534	0.04774	0.85467
SI61	0.80272	0.01835	0.70954
SI62	0.78342	0.06029	0.49215
SI63	0.62383	0.06551	0.49017
SI64	0.57155	0.02274	0.69955
SI65	0.67961	0.04493	0.85239
SI66	0.92207	0.82246	0.83785
SI67	0.80261	0.8618	0.69306
SI68	0.76971	0.81884	0.47667
SI69	0.61584	0.82162	0.49493

SI70	0.56714	0.86479	0.70426
SI71	0.683	0.82565	0.83685
SI72	0.42194	0.44293	0.64294
SI73	0.31573	0.46496	0.80463
SI74	0.28744	0.42908	0.0227
SI75	0.13126	0.42738	0.01178
SI76	0.07669	0.46691	0.80872
SI77	0.19293	0.44367	0.66335
SI78	0.42509	0.66532	0.65606
SI79	0.3032	0.62216	0.79094
SI80	0.27103	0.66821	0.00448
SI81	0.11713	0.67065	0.00121
SI82	0.06289	0.6232	0.80121
SI83	0.1777	0.65828	0.66112
SI84	0.07544	0.55108	0.13169
SI85	0.19566	0.52387	0.27888
SI86	0.22104	0.56083	0.50213
SI87	0.37921	0.56443	0.50058
SI88	0.43587	0.52431	0.28686
SI89	0.32353	0.55521	0.14979
SI90	0.08423	0.32142	0.16323
SI91	0.19889	0.3636	0.30452
SI92	0.23308	0.32906	0.52656
SI93	0.38997	0.32595	0.50925
SI94	0.43463	0.36598	0.28748
SI95	0.31652	0.31292	0.16967
O96	0.36179	0.05742	0.71574
O97	0.30182	0.05393	0.89007
O98	0.2018	0.04888	0.0234
O99	0.10298	0.06009	0.89089
O100	0.10385	0.05493	0.69308
O101	0.23166	0.0329	0.72848
O102	0.36161	0.81831	0.74907
O103	0.30852	0.84461	0.92407
O104	0.19376	0.84923	0.02181
O105	0.08911	0.83042	0.90378
O106	0.10468	0.82883	0.70694
O107	0.23068	0.84197	0.76394
O108	0.3192	0.94074	0.78641
O109	0.08821	0.94396	0.80119
O110	0.43368	0.12293	0.58047
O111	0.41799	0.99168	0.56221
O112	0.39945	0.85963	0.56818
O113	0.19214	0.12473	0.59488

O114	0.17815	0.99268	0.55797
O115	0.19784	0.85902	0.57155
O116	0.99115	0.03581	0.78648
O117	0.98655	0.85835	0.78595
O118	0.14241	0.93594	0.22125
O119	0.19915	0.9205	0.3969
O120	0.2981	0.94169	0.52788
O121	0.39659	0.92303	0.39593
O122	0.39769	0.94269	0.1991
O123	0.27133	0.96122	0.24232
O124	0.14709	0.15841	0.23148
O125	0.20272	0.16265	0.40563
O126	0.3113	0.14979	0.51882
O127	0.41298	0.16768	0.39398
O128	0.40086	0.14642	0.19954
O129	0.27524	0.12518	0.24915
O130	0.18257	0.04377	0.32165
O131	0.42121	0.04408	0.32531
O132	0.07068	0.86643	0.09277
O133	0.08397	0.99693	0.0648
O134	0.09687	0.12933	0.05435
O135	0.30794	0.86012	0.12164
O136	0.31491	0.98455	0.05676
O137	0.31274	0.11831	0.05763
O138	0.51036	0.9467	0.29533
O139	0.51848	0.1316	0.28482
O140	0.64413	0.56069	0.26626
O141	0.69405	0.56754	0.08428
O142	0.79289	0.53469	0.95727
O143	0.88838	0.56567	0.08726
O144	0.89266	0.55382	0.283
O145	0.76918	0.52654	0.23397
O146	0.64353	0.33165	0.25919
O147	0.696	0.32958	0.08233
O148	0.80483	0.34674	0.96823
O149	0.9035	0.32275	0.0982
O150	0.90507	0.33756	0.29211
O151	0.76984	0.36888	0.23651
O152	0.67178	0.44736	0.16936
O153	0.91531	0.44583	0.16891
O154	0.56806	0.62778	0.39121
O155	0.58851	0.49925	0.42532
O156	0.58927	0.36581	0.43326
O157	0.79532	0.62057	0.36958

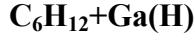
O158	0.81662	0.49003	0.41166
O159	0.80755	0.35708	0.44012
O160	0.00286	0.54612	0.18258
O161	0.01624	0.36156	0.19122
O162	0.86958	0.43104	0.76856
O163	0.80645	0.43684	0.59246
O164	0.70145	0.43556	0.46078
O165	0.60576	0.43488	0.59728
O166	0.59499	0.43188	0.79435
O167	0.72401	0.44917	0.76139
O168	0.86411	0.67824	0.73098
O169	0.80783	0.64316	0.56184
O170	0.68711	0.64165	0.47839
O171	0.57675	0.65788	0.58397
O172	0.60574	0.66903	0.7781
O173	0.73167	0.66081	0.71916
O174	0.8155	0.55615	0.71386
O175	0.59435	0.54969	0.69716
O176	0.93176	0.36871	0.91763
O177	0.91959	0.50209	0.92275
O178	0.88279	0.63035	0.91576
O179	0.68195	0.35675	0.89068
O180	0.67041	0.48719	0.93418
O181	0.69683	0.61844	0.90298
O182	0.49173	0.46969	0.68639
O183	0.48597	0.63038	0.71843
O184	0.64048	0.92629	0.28844
O185	0.70082	0.92357	0.11277
O186	0.80198	0.94278	0.98335
O187	0.90166	0.92269	0.11159
O188	0.89666	0.94454	0.3078
O189	0.76824	0.9609	0.27124
O190	0.64544	0.16408	0.26281
O191	0.69748	0.14694	0.08502
O192	0.81145	0.13875	0.98684
O193	0.91935	0.16519	0.09481
O194	0.89713	0.15162	0.2897
O195	0.77096	0.12123	0.24801
O196	0.67238	0.04051	0.19949
O197	0.91999	0.04459	0.17825
O198	0.56817	0.87369	0.4348
O199	0.58674	0.0048	0.43155
O200	0.59813	0.13673	0.44529
O201	0.81018	0.86416	0.39608

O202	0.81756	0.99235	0.44904
O203	0.81656	0.12641	0.43746
O204	0.01178	0.95095	0.21715
O205	0.01815	0.13169	0.21674
O206	0.86016	0.0464	0.78334
O207	0.80058	0.06612	0.61043
O208	0.70382	0.0585	0.4716
O209	0.60691	0.06383	0.60846
O210	0.60486	0.04426	0.80545
O211	0.731	0.02045	0.76558
O212	0.85971	0.829	0.76231
O213	0.8045	0.82357	0.58615
O214	0.69319	0.84667	0.48551
O215	0.59351	0.81885	0.6116
O216	0.60573	0.84159	0.80562
O217	0.72997	0.85286	0.74571
O218	0.81792	0.94138	0.6764
O219	0.58266	0.94309	0.67859
O220	0.93156	0.12084	0.90793
O221	0.92157	0.98995	0.94082
O222	0.90302	0.85799	0.94333
O223	0.69705	0.12027	0.88926
O224	0.68304	0.99497	0.94832
O225	0.70048	0.86255	0.9411
O226	0.49273	0.04089	0.70767
O227	0.48708	0.85547	0.71997
O228	0.37177	0.42933	0.73566
O229	0.31995	0.42822	0.91219
O230	0.20892	0.4499	0.01796
O231	0.10881	0.42072	0.89606
O232	0.11815	0.4541	0.70679
O233	0.24228	0.45292	0.75773
O234	0.35576	0.65784	0.71693
O235	0.30161	0.66676	0.89227
O236	0.19367	0.64328	0.00042
O237	0.08799	0.67433	0.88816
O238	0.1017	0.64358	0.6988
O239	0.22947	0.62169	0.73871
O240	0.32711	0.54578	0.81566
O241	0.08009	0.54655	0.83632
O242	0.43458	0.37379	0.58117
O243	0.38819	0.49846	0.57024
O244	0.41601	0.62942	0.54816
O245	0.19816	0.3676	0.61965

O246	0.21048	0.49593	0.57431
O247	0.18497	0.62639	0.55007
O248	0.99943	0.44356	0.79113
O249	0.98306	0.63001	0.78272
O250	0.13431	0.55556	0.21488
O251	0.18798	0.5468	0.39405
O252	0.29981	0.57716	0.48829
O253	0.41435	0.55359	0.39423
O254	0.39622	0.56531	0.20067
O255	0.26567	0.55264	0.2351
O256	0.13476	0.32437	0.2583
O257	0.196	0.3531	0.42454
O258	0.3118	0.34803	0.51911
O259	0.41367	0.33372	0.39442
O260	0.39385	0.32732	0.19953
O261	0.26884	0.33212	0.26431
O262	0.19467	0.44214	0.27156
O263	0.41578	0.44519	0.28345
O264	0.07275	0.61912	0.06605
O265	0.08552	0.48481	0.06314
O266	0.11977	0.35545	0.06624
O267	0.31258	0.6182	0.07569
O268	0.3258	0.48451	0.08965
O269	0.29542	0.35484	0.07075
O270	0.5152	0.53564	0.26949
O271	0.51409	0.35634	0.26891
O272	0.44086	0.74396	0.63649
O273	0.1938	0.73789	0.65279
O274	0.27578	0.74406	0.04739
O275	0.11275	0.74484	0.05055
O276	0.06672	0.24404	0.13767
O277	0.30667	0.23444	0.14347
O278	0.22243	0.24945	0.54829
O279	0.39955	0.24897	0.54653
O280	0.56348	0.24789	0.35642
O281	0.80128	0.2392	0.33184
O282	0.72755	0.23947	0.94734
O283	0.88938	0.24397	0.94196
O284	0.93849	0.7442	0.86068
O285	0.69573	0.74696	0.85957
O286	0.77152	0.74186	0.43762
O287	0.60769	0.74763	0.44611
O288	0.97591	0.26348	0.41288
O289	0.93804	0.16375	0.52021

O290	0.87927	0.2774	0.54016
O291	0.99811	0.25944	0.5977
GA29	0.9164	0.38823	0.6247
H293	0.94901	0.29349	0.36517
H294	0.83356	0.32542	0.48851
H295	0.89518	0.14623	0.49265
H296	0.0427	0.40412	0.59752
H297	0.00663	0.51987	0.64865
H298	0.99894	0.61016	0.52272
H299	0.04652	0.46608	0.2927
H300	0.05703	0.37662	0.41836
H301	0.0207	0.58412	0.34438
H302	0.04423	0.24992	0.57891
AL30	0.81915	0.32274	0.31451
AL30	0.79957	0.4715	0.71367
P305	0.9438	0.24225	0.51459
C306	0.01146	0.55906	0.49982
C307	0.03403	0.44287	0.54163
C308	0.01646	0.50823	0.57056
C309	0.03858	0.47856	0.37075
C310	0.02359	0.54431	0.39976
C311	0.04422	0.42758	0.44132

**c) structures associated with the three H<sub>2</sub> formation steps over P/Ga/ZSM-5 in the absence of CO<sub>2</sub> (states shown in Fig. 6)**



find above

**TS1**

SI2	0.4253	0.05402	0.64365
SI3	0.30488	0.02309	0.78585
SI4	0.28158	0.05695	0.00832
SI5	0.12212	0.05996	0.01122
SI6	0.07045	0.02503	0.79872
SI7	0.17927	0.05156	0.64962
SI8	0.42105	0.82389	0.66912
SI9	0.30454	0.86564	0.80841
SI10	0.26818	0.8262	0.02882
SI11	0.11353	0.823	0.01667
SI12	0.06586	0.86727	0.80197
SI13	0.18241	0.82475	0.67176
SI14	0.07628	0.93968	0.14922
SI15	0.19753	0.97007	0.2915
SI16	0.21861	0.93351	0.5121

SI17	0.37776	0.93106	0.51331
SI18	0.43077	0.96728	0.30381
SI19	0.3222	0.94281	0.1529
SI20	0.08111	0.16907	0.16471
SI21	0.19724	0.12713	0.30848
SI22	0.23451	0.16998	0.52594
SI23	0.38902	0.17167	0.51072
SI24	0.4362	0.12512	0.29937
SI25	0.31842	0.16416	0.16803
SI26	0.57592	0.55634	0.34566
SI27	0.68665	0.53144	0.1879
SI28	0.71408	0.5562	0.97338
SI29	0.87259	0.56137	0.97621
SI30	0.9329	0.52657	0.185
SI31	0.81263	0.55716	0.31367
SI32	0.57818	0.32746	0.33042
SI33	0.69526	0.3736	0.18959
SI34	0.72819	0.32122	0.97734
SI35	0.88265	0.32184	0.97635
SI36	0.93892	0.36805	0.18681
SI37	0.92389	0.43827	0.84024
SI38	0.77897	0.43822	0.46843
SI39	0.61858	0.43342	0.48668
SI40	0.56878	0.46823	0.70332
SI41	0.67999	0.42872	0.83772
SI42	0.91884	0.67048	0.82
SI43	0.79858	0.63622	0.686
SI44	0.76246	0.66619	0.46318
SI45	0.60779	0.6702	0.47903
SI46	0.56224	0.62571	0.69706
SI47	0.67837	0.67491	0.8199
SI48	0.57625	0.93988	0.36264
SI49	0.69337	0.96405	0.21978
SI50	0.72093	0.93452	0.997
SI51	0.88068	0.92869	0.99464
SI52	0.9315	0.96647	0.20325
SI53	0.82077	0.94346	0.35595
SI54	0.57883	0.17162	0.33431
SI55	0.69556	0.11849	0.20327
SI56	0.73296	0.16177	0.98217
SI57	0.88634	0.16731	0.98316
SI58	0.93632	0.12376	0.19429
SI59	0.81894	0.16313	0.32873
SI60	0.92528	0.04813	0.85609

SI61	0.80154	0.02059	0.71188
SI62	0.78317	0.06462	0.4944
SI63	0.62277	0.06803	0.49082
SI64	0.57049	0.02613	0.70041
SI65	0.6782	0.04952	0.85391
SI66	0.9213	0.8239	0.83603
SI67	0.79989	0.86269	0.69468
SI68	0.76604	0.82261	0.47738
SI69	0.6121	0.82368	0.49545
SI70	0.56497	0.86919	0.70409
SI71	0.67896	0.8278	0.83945
SI72	0.42647	0.44388	0.63986
SI73	0.30681	0.47121	0.78757
SI74	0.28931	0.43055	0.00424
SI75	0.13113	0.42994	0.00925
SI76	0.07662	0.47141	0.80292
SI77	0.18322	0.44539	0.65034
SI78	0.42223	0.66962	0.65849
SI79	0.30331	0.62764	0.79985
SI80	0.26965	0.67055	0.01455
SI81	0.11488	0.67043	0.00706
SI82	0.06544	0.62803	0.79716
SI83	0.18234	0.66644	0.66514
SI84	0.08	0.55105	0.14351
SI85	0.20223	0.52369	0.28441
SI86	0.22633	0.56208	0.50736
SI87	0.38471	0.56509	0.50434
SI88	0.43052	0.52522	0.29126
SI89	0.32554	0.54993	0.13876
SI90	0.08499	0.32356	0.15909
SI91	0.19989	0.36578	0.30511
SI92	0.2355	0.32636	0.52577
SI93	0.38991	0.32531	0.51061
SI94	0.43517	0.36784	0.29342
SI95	0.31979	0.32234	0.16479
O96	0.36029	0.05902	0.71556
O97	0.3025	0.06273	0.89172
O98	0.20162	0.04527	0.02098
O99	0.10006	0.06474	0.89516
O100	0.105	0.05353	0.69771
O101	0.23161	0.02646	0.73461
O102	0.36	0.82215	0.74862
O103	0.30534	0.84163	0.92375
O104	0.19043	0.84976	0.0207

O105	0.08652	0.82742	0.90294
O106	0.10504	0.83443	0.70698
O107	0.23082	0.8529	0.76043
O108	0.32463	0.9446	0.80172
O109	0.08689	0.94556	0.8128
O110	0.43424	0.12378	0.58178
O111	0.41879	0.9925	0.56424
O112	0.39799	0.86075	0.56646
O113	0.19779	0.12656	0.61198
O114	0.17976	0.99875	0.55669
O115	0.19549	0.86489	0.56795
O116	0.99072	0.03667	0.78707
O117	0.9857	0.8606	0.78502
O118	0.14197	0.93615	0.21961
O119	0.20034	0.92689	0.39444
O120	0.2984	0.94477	0.52772
O121	0.39693	0.92602	0.39588
O122	0.39701	0.94347	0.19943
O123	0.27025	0.96869	0.23803
O124	0.14155	0.16744	0.24486
O125	0.19747	0.15909	0.41951
O126	0.31193	0.14572	0.51597
O127	0.41442	0.16953	0.39582
O128	0.39565	0.15118	0.20123
O129	0.27038	0.1359	0.25699
O130	0.1778	0.04788	0.31396
O131	0.41825	0.04706	0.32199
O132	0.06795	0.86863	0.09039
O133	0.08187	0.99974	0.06699
O134	0.10343	0.13128	0.06257
O135	0.30445	0.8667	0.11866
O136	0.31996	0.99268	0.05668
O137	0.30337	0.12617	0.06324
O138	0.51008	0.95195	0.29543
O139	0.51587	0.1344	0.27996
O140	0.63828	0.56616	0.27005
O141	0.67383	0.56437	0.07853
O142	0.79357	0.55702	0.99662
O143	0.91301	0.56306	0.08082
O144	0.89003	0.55843	0.27691
O145	0.76399	0.54696	0.21831
O146	0.64423	0.33252	0.26198
O147	0.68968	0.34015	0.07956
O148	0.80561	0.3482	0.97857

O149	0.91583	0.32927	0.0859
O150	0.90424	0.33293	0.28364
O151	0.77036	0.36901	0.23052
O152	0.67099	0.45163	0.18534
O153	0.91751	0.44666	0.17786
O154	0.56221	0.62773	0.40096
O155	0.5904	0.49975	0.43055
O156	0.58992	0.36525	0.43679
O157	0.79759	0.62702	0.37094
O158	0.8021	0.49407	0.38917
O159	0.8088	0.3636	0.43264
O160	0.01155	0.5407	0.20691
O161	0.01969	0.36399	0.19842
O162	0.87803	0.43531	0.73747
O163	0.81603	0.45071	0.57416
O164	0.69948	0.43437	0.47804
O165	0.5967	0.43281	0.60238
O166	0.60263	0.43575	0.80149
O167	0.72996	0.43658	0.74502
O168	0.86218	0.67644	0.73393
O169	0.80111	0.64745	0.56558
O170	0.68458	0.64304	0.47297
O171	0.57905	0.66014	0.59057
O172	0.60115	0.66616	0.78459
O173	0.72817	0.66896	0.72415
O174	0.80387	0.55875	0.71728
O175	0.58605	0.54795	0.69704
O176	0.92483	0.36599	0.89526
O177	0.89487	0.49497	0.91365
O178	0.89109	0.6291	0.91572
O179	0.68781	0.35408	0.88526
O180	0.69439	0.48484	0.92394
O181	0.69564	0.61916	0.90309
O182	0.48898	0.45585	0.71416
O183	0.48221	0.63086	0.71733
O184	0.63915	0.92515	0.28895
O185	0.69896	0.92672	0.11272
O186	0.80122	0.94371	0.98394
O187	0.90107	0.92238	0.11155
O188	0.89498	0.94631	0.3073
O189	0.76672	0.96237	0.2705
O190	0.64343	0.16672	0.26168
O191	0.69955	0.14368	0.08881
O192	0.81064	0.13715	0.98274

O193	0.91493	0.16729	0.09661
O194	0.89508	0.14998	0.29073
O195	0.76863	0.12035	0.25673
O196	0.6687	0.04141	0.20637
O197	0.91956	0.04503	0.17519
O198	0.56416	0.87462	0.43353
O199	0.58906	0.00461	0.43393
O200	0.59465	0.13722	0.44224
O201	0.80729	0.86846	0.39861
O202	0.8165	0.99774	0.44653
O203	0.81513	0.1329	0.44442
O204	0.01068	0.95137	0.21826
O205	0.01583	0.13364	0.21441
O206	0.85981	0.04676	0.78548
O207	0.80131	0.06761	0.61237
O208	0.7032	0.06388	0.47589
O209	0.60403	0.06809	0.60871
O210	0.60369	0.04736	0.80647
O211	0.72983	0.02622	0.76706
O212	0.85901	0.83006	0.76023
O213	0.80097	0.82618	0.58662
O214	0.68922	0.84957	0.48582
O215	0.58995	0.82183	0.61221
O216	0.60263	0.84565	0.80598
O217	0.72812	0.85008	0.7482
O218	0.81302	0.94272	0.68018
O219	0.58305	0.94679	0.67775
O220	0.93218	0.12066	0.91114
O221	0.92155	0.98957	0.94112
O222	0.90126	0.85809	0.94218
O223	0.69337	0.12535	0.89144
O224	0.68344	0.99957	0.94969
O225	0.69757	0.86676	0.94125
O226	0.49144	0.04247	0.71114
O227	0.4847	0.86188	0.71953
O228	0.35877	0.44266	0.70576
O229	0.30949	0.42436	0.88699
O230	0.2101	0.44651	0.01862
O231	0.1102	0.42831	0.89226
O232	0.10759	0.44906	0.69546
O233	0.23218	0.46758	0.74075
O234	0.35485	0.66381	0.72444
O235	0.30636	0.66618	0.90643
O236	0.19245	0.64577	0.00316

O237	0.08506	0.67283	0.89417
O238	0.1046	0.65442	0.69765
O239	0.22844	0.6337	0.75303
O240	0.32297	0.54904	0.81582
O241	0.08753	0.55108	0.82171
O242	0.43529	0.37252	0.58243
O243	0.42517	0.50346	0.55633
O244	0.41035	0.63638	0.54889
O245	0.19769	0.36967	0.61164
O246	0.18996	0.49652	0.55604
O247	0.19768	0.63039	0.55848
O248	0.99724	0.45679	0.79904
O249	0.98557	0.6331	0.77641
O250	0.14226	0.558	0.22055
O251	0.21207	0.56486	0.38823
O252	0.30584	0.55544	0.52879
O253	0.39875	0.56558	0.38554
O254	0.39858	0.5558	0.1899
O255	0.27122	0.52628	0.2217
O256	0.1415	0.32628	0.24563
O257	0.20015	0.33647	0.41784
O258	0.31275	0.35136	0.51685
O259	0.41566	0.32899	0.39604
O260	0.39683	0.33293	0.19972
O261	0.27164	0.35314	0.25167
O262	0.18393	0.44575	0.30755
O263	0.41241	0.44594	0.30314
O264	0.07297	0.61909	0.07712
O265	0.08921	0.48748	0.06807
O266	0.11405	0.35684	0.05667
O267	0.30696	0.62303	0.09459
O268	0.33018	0.49355	0.05121
O269	0.30749	0.36013	0.05877
O270	0.51045	0.5352	0.28246
O271	0.51497	0.36201	0.2731
O272	0.44153	0.74757	0.64091
O273	0.19745	0.74583	0.65166
O274	0.2732	0.74695	0.05557
O275	0.10935	0.74543	0.05406
O276	0.06466	0.24644	0.1359
O277	0.30436	0.24329	0.14925
O278	0.23115	0.24828	0.55868
O279	0.39535	0.24849	0.55028
O280	0.56114	0.24965	0.35484

O281	0.79925	0.24064	0.33112
O282	0.72849	0.24104	0.96145
O283	0.88729	0.24389	0.94141
O284	0.93857	0.74558	0.85702
O285	0.68679	0.74912	0.86777
O286	0.76744	0.74574	0.43791
O287	0.60412	0.74897	0.44879
O288	0.94589	0.25264	0.42973
O289	0.8919	0.20665	0.58271
O290	0.89244	0.33362	0.55531
O291	0.99839	0.27398	0.60485
GA29	0.92316	0.42398	0.60432
H293	0.93737	0.28722	0.37606
H294	0.84466	0.34538	0.48978
H295	0.86494	0.18208	0.53207
H296	0.02935	0.53882	0.60121
H297	0.09263	0.52704	0.4419
H298	0.08	0.61341	0.47097
H299	0.03079	0.57318	0.37784
H300	0.93305	0.62036	0.47035
H301	0.98385	0.6526	0.56806
H302	0.91639	0.5981	0.59651
H303	0.96046	0.4026	0.39241
H304	0.07311	0.3609	0.41488
H305	0.91752	0.50227	0.45875
H306	0.99782	0.38556	0.65235
H307	1.00072	0.34144	0.63344
H308	0.09222	0.43027	0.50302
AL30	0.81854	0.32344	0.31108
AL31	0.79966	0.47384	0.69901
P311	0.93562	0.26674	0.54411
C312	0.00308	0.548	0.53008
C313	0.0549	0.56626	0.45073
C314	0.95632	0.60799	0.54264
C315	0.99448	0.42974	0.44204
C316	0.96256	0.48546	0.49822
C317	0.05643	0.40572	0.45398

### **C<sub>6</sub>H<sub>11</sub>Ga+H<sub>2</sub>**

find above

### **C<sub>6</sub>H<sub>10</sub>+Ga(H)**

find above

**TS2**

SI2	0.42576	0.05254	0.64286
SI3	0.30489	0.02161	0.78317
SI4	0.28201	0.05304	0.00747
SI5	0.12246	0.05779	0.00958
SI6	0.07078	0.02312	0.79677
SI7	0.17877	0.05046	0.64663
SI8	0.42221	0.82149	0.66987
SI9	0.30532	0.86369	0.80779
SI10	0.26931	0.82543	0.02913
SI11	0.11488	0.82209	0.0183
SI12	0.06618	0.86481	0.80265
SI13	0.18262	0.82092	0.67281
SI14	0.07657	0.93864	0.14973
SI15	0.1981	0.96759	0.29344
SI16	0.21855	0.93021	0.51309
SI17	0.37766	0.92886	0.51439
SI18	0.4309	0.96557	0.30556
SI19	0.32263	0.9401	0.15415
SI20	0.08243	0.16743	0.16168
SI21	0.19895	0.1241	0.3064
SI22	0.23448	0.16932	0.52241
SI23	0.38908	0.17008	0.50967
SI24	0.43713	0.12327	0.29972
SI25	0.32005	0.15952	0.16628
SI26	0.5778	0.55832	0.33627
SI27	0.68231	0.53207	0.17415
SI28	0.71464	0.5511	0.95892
SI29	0.87126	0.55651	0.9665
SI30	0.92994	0.5251	0.17684
SI31	0.8064	0.55614	0.30288
SI32	0.5765	0.32703	0.32151
SI33	0.69231	0.37362	0.17981
SI34	0.72649	0.32041	0.97089
SI35	0.88105	0.31973	0.9683
SI36	0.93868	0.36646	0.17743
SI37	0.92255	0.43472	0.82651
SI38	0.7758	0.43412	0.45747
SI39	0.61799	0.43435	0.47754
SI40	0.56662	0.46789	0.69664
SI41	0.67989	0.42368	0.82171
SI42	0.91806	0.66778	0.81742
SI43	0.80298	0.63463	0.67608

SI44	0.76508	0.66515	0.45743
SI45	0.60994	0.66927	0.47672
SI46	0.5659	0.62464	0.69639
SI47	0.68555	0.67466	0.81077
SI48	0.57716	0.93899	0.36353
SI49	0.69383	0.96233	0.22033
SI50	0.72163	0.93211	0.99723
SI51	0.88118	0.9263	0.99527
SI52	0.93176	0.96721	0.20302
SI53	0.82164	0.94375	0.35746
SI54	0.57942	0.17103	0.33538
SI55	0.69653	0.1168	0.20478
SI56	0.73187	0.16045	0.98362
SI57	0.88554	0.16588	0.984
SI58	0.93696	0.1243	0.19398
SI59	0.81996	0.16214	0.32847
SI60	0.92572	0.04622	0.85719
SI61	0.80269	0.02028	0.71165
SI62	0.78396	0.06589	0.49493
SI63	0.62332	0.06818	0.49099
SI64	0.57099	0.02395	0.70054
SI65	0.67886	0.04735	0.85369
SI66	0.92115	0.82139	0.83804
SI67	0.80123	0.8632	0.69504
SI68	0.76898	0.82175	0.47794
SI69	0.6148	0.82296	0.49667
SI70	0.56683	0.86652	0.70554
SI71	0.68156	0.82675	0.83892
SI72	0.42377	0.44187	0.64326
SI73	0.30846	0.46929	0.79839
SI74	0.2893	0.42929	0.01253
SI75	0.13272	0.43037	0.01355
SI76	0.07672	0.46553	0.80507
SI77	0.18859	0.44151	0.66113
SI78	0.42615	0.66673	0.65941
SI79	0.30363	0.62493	0.79649
SI80	0.27073	0.67017	0.00934
SI81	0.11652	0.66861	0.01012
SI82	0.06585	0.62342	0.80146
SI83	0.18066	0.66248	0.66386
SI84	0.07815	0.55079	0.14635
SI85	0.20227	0.52404	0.28292
SI86	0.22678	0.56006	0.51168
SI87	0.38484	0.56404	0.50591

SI88	0.42919	0.52421	0.29229
SI89	0.32758	0.55255	0.13861
SI90	0.08661	0.32232	0.16242
SI91	0.19803	0.36355	0.31009
SI92	0.2364	0.32704	0.52856
SI93	0.3913	0.32407	0.51193
SI94	0.43401	0.36674	0.29228
SI95	0.31606	0.31646	0.17078
O96	0.361	0.05839	0.71515
O97	0.30247	0.05858	0.89089
O98	0.2019	0.04384	0.02171
O99	0.10195	0.06171	0.89293
O100	0.10464	0.05207	0.69546
O101	0.23187	0.02771	0.73195
O102	0.36164	0.8198	0.75036
O103	0.30634	0.84309	0.92464
O104	0.19158	0.84952	0.02241
O105	0.08757	0.8268	0.9048
O106	0.10544	0.83066	0.70879
O107	0.23171	0.8484	0.76105
O108	0.32394	0.94267	0.79533
O109	0.08657	0.94346	0.80933
O110	0.43465	0.12185	0.57978
O111	0.4186	0.99069	0.56424
O112	0.39892	0.85897	0.56781
O113	0.19568	0.12518	0.60574
O114	0.17944	0.99572	0.55622
O115	0.1954	0.8617	0.56939
O116	0.99109	0.03611	0.78745
O117	0.98601	0.85722	0.78702
O118	0.14187	0.93574	0.22082
O119	0.20078	0.92298	0.39518
O120	0.29823	0.94185	0.52972
O121	0.39598	0.92406	0.39657
O122	0.39748	0.94282	0.20034
O123	0.27051	0.96592	0.23905
O124	0.14394	0.16266	0.23948
O125	0.19909	0.16034	0.41441
O126	0.31187	0.14435	0.51606
O127	0.41381	0.16875	0.39434
O128	0.39734	0.14798	0.20013
O129	0.27228	0.13026	0.25482
O130	0.17942	0.04527	0.31895
O131	0.41937	0.04543	0.32462

O132	0.06883	0.86685	0.09264
O133	0.08239	0.99757	0.06568
O134	0.10207	0.12938	0.05855
O135	0.30599	0.86346	0.1211
O136	0.31907	0.98808	0.05593
O137	0.30623	0.12156	0.06144
O138	0.51001	0.94935	0.29792
O139	0.51684	0.13284	0.28132
O140	0.63163	0.5715	0.24823
O141	0.67094	0.55895	0.06091
O142	0.79299	0.54517	0.9891
O143	0.91289	0.56001	0.0703
O144	0.88358	0.55534	0.26572
O145	0.75869	0.55033	0.20598
O146	0.64169	0.33079	0.25091
O147	0.68391	0.34603	0.06628
O148	0.8042	0.34536	0.97857
O149	0.91943	0.3294	0.0737
O150	0.90279	0.33139	0.27323
O151	0.76799	0.3648	0.21691
O152	0.66866	0.45205	0.18394
O153	0.91688	0.44487	0.16948
O154	0.56573	0.62879	0.3947
O155	0.6038	0.50265	0.41567
O156	0.58693	0.36841	0.42496
O157	0.79515	0.6265	0.361
O158	0.79016	0.49312	0.37734
O159	0.80728	0.36229	0.42067
O160	0.0076	0.54085	0.20482
O161	0.01919	0.36259	0.19298
O162	0.87727	0.43539	0.72382
O163	0.81514	0.45076	0.56217
O164	0.69832	0.42622	0.48419
O165	0.5861	0.4385	0.58762
O166	0.60231	0.42605	0.78512
O167	0.7289	0.43322	0.72826
O168	0.86785	0.67341	0.72263
O169	0.80789	0.64243	0.55487
O170	0.68725	0.64351	0.47302
O171	0.57944	0.65535	0.58634
O172	0.60777	0.6673	0.7781
O173	0.73373	0.671	0.71251
O174	0.80369	0.55746	0.70977
O175	0.58886	0.54654	0.7018

O176	0.91773	0.36217	0.88044
O177	0.8976	0.4935	0.90048
O178	0.883	0.6269	0.90827
O179	0.69192	0.35024	0.87137
O180	0.69158	0.4827	0.90434
O181	0.70456	0.6171	0.89053
O182	0.48669	0.46017	0.71389
O183	0.48672	0.63189	0.72213
O184	0.63902	0.9233	0.28834
O185	0.69994	0.9253	0.11312
O186	0.80186	0.94162	0.98343
O187	0.90101	0.92216	0.11258
O188	0.8955	0.94859	0.30784
O189	0.76674	0.96011	0.2722
O190	0.64497	0.16459	0.26503
O191	0.69861	0.14243	0.09035
O192	0.80971	0.13627	0.98501
O193	0.91425	0.16859	0.0975
O194	0.8969	0.14939	0.29228
O195	0.77029	0.11832	0.25622
O196	0.66955	0.03976	0.20723
O197	0.92045	0.0456	0.173
O198	0.56648	0.87482	0.43718
O199	0.59078	0.00515	0.43149
O200	0.59407	0.13778	0.44467
O201	0.81089	0.8685	0.40119
O202	0.8161	0.99805	0.44767
O203	0.81683	0.13294	0.44413
O204	0.01085	0.95147	0.21792
O205	0.01659	0.13418	0.21292
O206	0.86028	0.04672	0.78639
O207	0.80259	0.06828	0.61309
O208	0.70386	0.06574	0.47708
O209	0.60441	0.06567	0.60868
O210	0.60431	0.04556	0.80632
O211	0.73074	0.02476	0.76654
O212	0.85867	0.82966	0.76299
O213	0.80234	0.8247	0.58844
O214	0.69196	0.84833	0.48517
O215	0.59343	0.82004	0.61367
O216	0.60434	0.84237	0.80735
O217	0.72884	0.8541	0.74836
O218	0.81616	0.94284	0.67853
O219	0.58379	0.94444	0.67972

O220	0.93208	0.11765	0.9153
O221	0.92239	0.98594	0.93937
O222	0.90208	0.85485	0.94524
O223	0.69348	0.12294	0.89269
O224	0.68389	0.99647	0.94838
O225	0.69856	0.86351	0.94324
O226	0.49189	0.04053	0.71024
O227	0.48657	0.85837	0.72001
O228	0.35751	0.44116	0.71231
O229	0.31483	0.42251	0.89753
O230	0.21099	0.45144	0.0171
O231	0.10833	0.42453	0.89844
O232	0.11161	0.44306	0.70027
O233	0.23251	0.46411	0.75702
O234	0.35757	0.65785	0.72164
O235	0.30126	0.67036	0.89691
O236	0.19388	0.6429	0.00826
O237	0.08699	0.66866	0.89716
O238	0.10423	0.65097	0.70221
O239	0.23025	0.62634	0.74412
O240	0.32386	0.54784	0.82464
O241	0.08602	0.54573	0.82363
O242	0.43361	0.36886	0.5912
O243	0.41819	0.49716	0.55408
O244	0.41948	0.6313	0.55035
O245	0.20585	0.36604	0.62457
O246	0.2003	0.4924	0.56758
O247	0.19025	0.62708	0.55514
O248	0.99876	0.44736	0.79376
O249	0.98598	0.62912	0.7821
O250	0.13826	0.55767	0.22732
O251	0.21115	0.55625	0.39334
O252	0.30606	0.56572	0.5329
O253	0.39619	0.56296	0.38679
O254	0.39942	0.55927	0.19277
O255	0.26936	0.5399	0.2206
O256	0.13653	0.32396	0.25793
O257	0.19466	0.34763	0.42879
O258	0.3138	0.34933	0.51146
O259	0.42104	0.33139	0.39996
O260	0.39289	0.32867	0.20439
O261	0.26886	0.3384	0.26442
O262	0.19024	0.44349	0.28924
O263	0.40996	0.44479	0.29768

O264	0.07311	0.61926	0.08099
O265	0.08941	0.48721	0.07172
O266	0.12198	0.35765	0.06627
O267	0.31508	0.62185	0.07929
O268	0.33259	0.48855	0.06406
O269	0.29928	0.35832	0.06974
O270	0.50906	0.53235	0.28726
O271	0.51256	0.35976	0.26358
O272	0.44183	0.74526	0.64016
O273	0.19706	0.74182	0.65241
O274	0.2739	0.74581	0.05317
O275	0.11154	0.74429	0.05451
O276	0.06854	0.24548	0.13403
O277	0.30413	0.23801	0.14606
O278	0.23077	0.24776	0.55365
O279	0.39586	0.24673	0.54929
O280	0.56153	0.24954	0.35157
O281	0.79999	0.23945	0.32646
O282	0.72547	0.23965	0.96312
O283	0.88574	0.24104	0.93713
O284	0.93684	0.74246	0.85704
O285	0.69436	0.74789	0.86168
O286	0.77151	0.74519	0.43688
O287	0.60613	0.74851	0.44954
O288	0.96078	0.26628	0.42055
O289	0.93745	0.20322	0.57836
O290	0.87933	0.31675	0.54968
O291	1.00134	0.31183	0.59308
GA29	0.91178	0.4216	0.57735
H293	0.94157	0.29589	0.36525
H294	0.84411	0.33116	0.48808
H295	0.90587	0.17519	0.54042
H296	0.98978	0.45595	0.61462
H297	0.98888	0.38103	0.60437
H298	0.11653	0.48045	0.42784
H299	0.05738	0.53276	0.36739
H300	0.06875	0.59294	0.51354
H301	0.08914	0.52318	0.58686
H302	0.97111	0.57593	0.61999
H303	0.91093	0.44949	0.37622
H304	0.02419	0.41505	0.34947
H305	0.88582	0.54367	0.49687
H306	0.03349	0.40168	0.47752
AL30	0.81664	0.32232	0.30142

AL30	0.79901	0.47293	0.68909
P309	0.94712	0.27597	0.5344
C310	0.98448	0.53929	0.56261
C311	0.06545	0.49961	0.43154
C312	0.05588	0.53989	0.52749
C313	0.94616	0.46181	0.43547
C314	0.93535	0.52092	0.49337
C315	0.01804	0.43964	0.42229

### **C<sub>6</sub>H<sub>9</sub>Ga+H<sub>2</sub>**

find above

### **C<sub>6</sub>H<sub>8</sub>+Ga(H)**

find above

### **TS3**

SI2	0.4259	0.05134	0.64438
SI3	0.30391	0.02083	0.78324
SI4	0.28178	0.05287	0.00864
SI5	0.12169	0.05739	0.00996
SI6	0.07058	0.01989	0.79658
SI7	0.17752	0.04933	0.64493
SI8	0.42046	0.82033	0.66919
SI9	0.30351	0.86224	0.80819
SI10	0.26959	0.82443	0.02995
SI11	0.11527	0.82078	0.01776
SI12	0.06526	0.86117	0.80176
SI13	0.18199	0.81865	0.67409
SI14	0.07724	0.93698	0.15009
SI15	0.19838	0.96487	0.29511
SI16	0.21877	0.92799	0.51378
SI17	0.37802	0.92792	0.51418
SI18	0.43214	0.96663	0.30557
SI19	0.32278	0.93899	0.15527
SI20	0.0811	0.16367	0.16273
SI21	0.20052	0.12089	0.30448
SI22	0.23285	0.16854	0.52051
SI23	0.3874	0.16938	0.51242
SI24	0.43804	0.12489	0.30299
SI25	0.3218	0.1572	0.16727
SI26	0.57223	0.56122	0.32724
SI27	0.67304	0.53154	0.16649
SI28	0.71377	0.54917	0.95117
SI29	0.86802	0.54671	0.95056

SI30	0.92637	0.52106	0.16159
SI31	0.80243	0.55669	0.29393
SI32	0.5809	0.32841	0.31888
SI33	0.68776	0.37449	0.17113
SI34	0.73167	0.32152	0.96534
SI35	0.88496	0.31477	0.99346
SI36	0.93367	0.36358	0.19244
SI37	0.92492	0.41456	0.84769
SI38	0.77773	0.44155	0.45996
SI39	0.62333	0.4427	0.46954
SI40	0.57214	0.46543	0.68651
SI41	0.69355	0.42234	0.8085
SI42	0.91615	0.66435	0.80891
SI43	0.79899	0.64361	0.6673
SI44	0.76201	0.6688	0.44574
SI45	0.6071	0.67012	0.46863
SI46	0.5668	0.62209	0.68968
SI47	0.68396	0.67625	0.8093
SI48	0.57734	0.94054	0.36515
SI49	0.69489	0.96297	0.22342
SI50	0.72127	0.93152	0.99983
SI51	0.88132	0.92305	0.99711
SI52	0.9322	0.96267	0.2061
SI53	0.82281	0.94423	0.36016
SI54	0.58144	0.17359	0.34139
SI55	0.69712	0.11772	0.20789
SI56	0.7321	0.1614	0.9864
SI57	0.88693	0.16291	0.98518
SI58	0.93768	0.11992	0.19778
SI59	0.82074	0.16364	0.32999
SI60	0.92484	0.04185	0.85706
SI61	0.80061	0.01702	0.70997
SI62	0.78529	0.06754	0.49533
SI63	0.62464	0.06862	0.49359
SI64	0.57155	0.02387	0.70295
SI65	0.67916	0.04804	0.85615
SI66	0.91887	0.81807	0.83812
SI67	0.79669	0.85974	0.69556
SI68	0.76522	0.82171	0.47893
SI69	0.61139	0.82387	0.49847
SI70	0.56403	0.8665	0.70744
SI71	0.67712	0.82575	0.84388
SI72	0.42798	0.43992	0.65366
SI73	0.31044	0.46807	0.806

SI74	0.28899	0.42655	0.02083
SI75	0.13124	0.4278	0.02637
SI76	0.07387	0.46151	0.81715
SI77	0.18664	0.43855	0.67098
SI78	0.4251	0.66541	0.65912
SI79	0.30435	0.62382	0.80016
SI80	0.2689	0.6695	0.01024
SI81	0.11466	0.66719	0.01134
SI82	0.06411	0.6207	0.80275
SI83	0.18139	0.66027	0.66627
SI84	0.07461	0.55091	0.1542
SI85	0.19536	0.52165	0.28914
SI86	0.22228	0.55506	0.51986
SI87	0.38093	0.55947	0.5152
SI88	0.42263	0.52148	0.29785
SI89	0.32106	0.55215	0.14493
SI90	0.08243	0.31857	0.17288
SI91	0.19538	0.36179	0.3132
SI92	0.23536	0.32664	0.53248
SI93	0.39021	0.32336	0.51977
SI94	0.43279	0.36492	0.29956
SI95	0.31623	0.31344	0.17681
O96	0.36164	0.05696	0.71763
O97	0.30075	0.05688	0.89149
O98	0.20151	0.04798	0.0258
O99	0.10312	0.0576	0.89249
O100	0.10379	0.04967	0.69528
O101	0.23188	0.02962	0.72995
O102	0.35881	0.81866	0.74792
O103	0.30664	0.84166	0.92512
O104	0.19185	0.84872	0.02289
O105	0.08853	0.82427	0.90385
O106	0.10407	0.82749	0.70702
O107	0.22915	0.84645	0.76452
O108	0.32103	0.9414	0.7946
O109	0.08523	0.93997	0.80729
O110	0.4336	0.1202	0.5799
O111	0.41894	0.98856	0.56736
O112	0.39818	0.85696	0.56581
O113	0.19146	0.12378	0.60033
O114	0.17897	0.99312	0.55671
O115	0.19689	0.85961	0.57147
O116	0.99093	0.03274	0.78875
O117	0.98523	0.85154	0.7877

O118	0.14253	0.93376	0.22116
O119	0.20014	0.91969	0.39631
O120	0.29846	0.94117	0.52816
O121	0.39762	0.92482	0.39667
O122	0.39786	0.9443	0.20054
O123	0.27102	0.963	0.24166
O124	0.1462	0.15733	0.23367
O125	0.2007	0.16081	0.40986
O126	0.31028	0.14336	0.51916
O127	0.41145	0.16957	0.39666
O128	0.3993	0.14821	0.20177
O129	0.27418	0.12444	0.25335
O130	0.18059	0.0426	0.32238
O131	0.42192	0.04647	0.32645
O132	0.06901	0.86597	0.09116
O133	0.08334	0.99669	0.06752
O134	0.09658	0.12873	0.0554
O135	0.30728	0.86217	0.12146
O136	0.3165	0.98659	0.05698
O137	0.31043	0.12041	0.06074
O138	0.51131	0.9505	0.29673
O139	0.51757	0.13745	0.28784
O140	0.61813	0.57385	0.22954
O141	0.6677	0.55528	0.05096
O142	0.7912	0.54389	0.98766
O143	0.91702	0.54725	0.04751
O144	0.87431	0.55611	0.23858
O145	0.74657	0.55039	0.20856
O146	0.63509	0.32556	0.22938
O147	0.68695	0.35311	0.05447
O148	0.8097	0.34377	0.97926
O149	0.90376	0.31048	0.11164
O150	0.8963	0.34385	0.29675
O151	0.7616	0.36687	0.21744
O152	0.66001	0.45151	0.18105
O153	0.91535	0.44012	0.16081
O154	0.56142	0.63198	0.38569
O155	0.60707	0.50756	0.40172
O156	0.61045	0.37277	0.41113
O157	0.79591	0.62704	0.35461
O158	0.79651	0.49292	0.37129
O159	0.78923	0.36224	0.42336
O160	0.00047	0.54144	0.20077
O161	0.014	0.35681	0.20513

O162	0.88774	0.36744	0.76598
O163	0.82727	0.44848	0.55613
O164	0.7021	0.44989	0.49874
O165	0.57888	0.44288	0.56993
O166	0.61996	0.4206	0.75621
O167	0.75214	0.43311	0.72907
O168	0.86861	0.67382	0.7118
O169	0.803	0.65322	0.54709
O170	0.68443	0.64531	0.4573
O171	0.58015	0.65138	0.57869
O172	0.6076	0.66598	0.77104
O173	0.73426	0.68325	0.71347
O174	0.7907	0.56597	0.69432
O175	0.59148	0.54458	0.69713
O176	0.9382	0.3678	0.94596
O177	0.8815	0.48165	0.87898
O178	0.88045	0.61663	0.89117
O179	0.7023	0.34915	0.86105
O180	0.69224	0.48185	0.89255
O181	0.70506	0.61597	0.88345
O182	0.49478	0.45302	0.71931
O183	0.4874	0.62815	0.71439
O184	0.64043	0.92416	0.29254
O185	0.70001	0.9261	0.11604
O186	0.8018	0.93739	0.98541
O187	0.90165	0.91871	0.11425
O188	0.89672	0.94173	0.31049
O189	0.76824	0.95995	0.27403
O190	0.64605	0.16531	0.26946
O191	0.69892	0.14378	0.0936
O192	0.80982	0.13686	0.98763
O193	0.91801	0.16027	0.09684
O194	0.8973	0.1499	0.29302
O195	0.77094	0.11905	0.25921
O196	0.67063	0.04048	0.21043
O197	0.91875	0.04142	0.18173
O198	0.56433	0.8773	0.4398
O199	0.59037	0.00721	0.43245
O200	0.59605	0.13935	0.45005
O201	0.80918	0.87205	0.41129
O202	0.82062	1.0028	0.44435
O203	0.81668	0.13643	0.44707
O204	0.01168	0.94864	0.219
O205	0.01755	0.12843	0.21797

O206	0.86039	0.03683	0.78511
O207	0.80349	0.06733	0.61383
O208	0.70512	0.06495	0.47764
O209	0.6067	0.06477	0.61157
O210	0.60431	0.04503	0.80951
O211	0.73006	0.02632	0.76729
O212	0.85713	0.83115	0.76291
O213	0.79652	0.81773	0.59124
O214	0.68863	0.84894	0.48797
O215	0.5901	0.81968	0.61545
O216	0.60056	0.84251	0.81
O217	0.7261	0.85026	0.75366
O218	0.80738	0.93952	0.67214
O219	0.58251	0.94411	0.68197
O220	0.92897	0.11513	0.90997
O221	0.92234	0.98371	0.94282
O222	0.9021	0.8519	0.94599
O223	0.69313	0.12366	0.89598
O224	0.68613	0.99722	0.95061
O225	0.69441	0.86392	0.94695
O226	0.49266	0.04157	0.71108
O227	0.48357	0.85876	0.72058
O228	0.3639	0.43943	0.72677
O229	0.31438	0.42212	0.90592
O230	0.21017	0.44531	0.02775
O231	0.10582	0.4235	0.91229
O232	0.11222	0.43507	0.71791
O233	0.23606	0.46137	0.76006
O234	0.35938	0.6568	0.72757
O235	0.30117	0.67055	0.89909
O236	0.19213	0.64245	1.00467
O237	0.08178	0.6658	0.90033
O238	0.10574	0.64713	0.70596
O239	0.2318	0.62432	0.74547
O240	0.32409	0.54712	0.83099
O241	0.08188	0.54272	0.82799
O242	0.43336	0.36748	0.59841
O243	0.42092	0.49848	0.56917
O244	0.41129	0.63131	0.55055
O245	0.20413	0.36433	0.62891
O246	0.18932	0.49291	0.58043
O247	0.19034	0.62585	0.55669
O248	0.99608	0.44215	0.80561
O249	0.98578	0.629	0.77417

O250	0.12869	0.55743	0.24443
O251	0.20749	0.54757	0.40207
O252	0.3023	0.55425	0.54355
O253	0.39008	0.55508	0.39623
O254	0.39099	0.56088	0.20359
O255	0.25951	0.54147	0.22213
O256	0.13317	0.31927	0.26774
O257	0.19501	0.34958	0.43283
O258	0.31298	0.34916	0.51948
O259	0.42022	0.33172	0.40842
O260	0.39294	0.32258	0.21443
O261	0.26621	0.33737	0.2662
O262	0.18412	0.44078	0.28779
O263	0.40488	0.44171	0.29676
O264	0.07416	0.61856	0.08666
O265	0.09086	0.48631	0.08435
O266	0.11784	0.3555	0.07853
O267	0.31109	0.61988	0.08094
O268	0.32997	0.48659	0.0744
O269	0.30301	0.35519	0.07471
O270	0.50206	0.53051	0.29169
O271	0.51232	0.36233	0.27674
O272	0.44156	0.74402	0.64138
O273	0.19726	0.73967	0.65477
O274	0.27273	0.74484	0.0551
O275	0.11106	0.74323	0.05474
O276	0.06498	0.24215	0.14156
O277	0.30282	0.23538	0.15121
O278	0.22853	0.2468	0.55298
O279	0.39399	0.24545	0.55479
O280	0.56647	0.25281	0.35947
O281	0.80023	0.24095	0.32559
O282	0.72662	0.24065	0.9659
O283	0.89136	0.23999	0.94551
O284	0.93024	0.73819	0.85677
O285	0.68652	0.74679	0.86976
O286	0.76659	0.74896	0.42371
O287	0.60163	0.75022	0.44897
O288	0.94767	0.26739	0.42682
O289	0.92987	0.20467	0.58483
O290	0.85912	0.31206	0.55328
O291	0.97495	0.32486	0.59805
GA29	0.90197	0.38956	0.63293
H293	0.92988	0.30126	0.3737

H294	0.81618	0.33529	0.48067
H295	0.90172	0.17285	0.54731
H296	0.98112	0.46925	0.62369
H297	0.05282	0.51904	0.63704
H298	0.97626	0.60393	0.56993
H299	0.89481	0.47593	0.68578
H300	0.92249	0.58195	0.40555
H301	0.00946	0.38444	0.3911
H302	0.09511	0.47584	0.4718
H303	0.91989	0.46206	0.34301
H304	0.07003	0.40748	0.54733
AL30	0.80953	0.32496	0.30272
AL30	0.81059	0.48452	0.67735
P307	0.92923	0.27728	0.5384
C308	0.95059	0.54299	0.44421
C309	0.01836	0.50008	0.58057
C310	0.98102	0.55566	0.53202
C311	0.00261	0.43213	0.42971
C312	0.95476	0.4761	0.40139
C313	0.05155	0.45204	0.50778

### **C<sub>6</sub>H<sub>7</sub>Ga+H<sub>2</sub>**

find above

### **d) structures associated with the two H<sub>2</sub> formation steps over P/Ga/ZSM-5 in the presence of CO<sub>2</sub> (states shown in Fig. 7 and Fig. S6)**

### **C<sub>6</sub>H<sub>10</sub>+Ga(H)+CO<sub>2</sub>**

SI2	0.42718	0.05284	0.64293
SI3	0.30655	0.02354	0.78477
SI4	0.2824	0.05678	0.00778
SI5	0.1227	0.06001	0.01012
SI6	0.07108	0.02504	0.79698
SI7	0.1806	0.0531	0.64886
SI8	0.42303	0.82281	0.67008
SI9	0.30626	0.86538	0.80838
SI10	0.2695	0.82707	0.02884
SI11	0.11509	0.82363	0.01743
SI12	0.0667	0.86674	0.80208
SI13	0.18369	0.82332	0.67294
SI14	0.07757	0.94019	0.1499
SI15	0.19832	0.96993	0.29435
SI16	0.21959	0.93291	0.51372
SI17	0.37881	0.92927	0.5141
SI18	0.4316	0.96593	0.30461

SI19	0.32225	0.94287	0.15445
SI20	0.08327	0.16919	0.16417
SI21	0.19946	0.12642	0.30875
SI22	0.2374	0.17089	0.52452
SI23	0.39122	0.17058	0.51009
SI24	0.43772	0.12363	0.2994
SI25	0.32017	0.16215	0.16795
SI26	0.57958	0.55673	0.34117
SI27	0.68607	0.53131	0.1808
SI28	0.71766	0.55302	0.96605
SI29	0.87482	0.55837	0.97254
SI30	0.93289	0.52423	0.18262
SI31	0.80959	0.55563	0.30879
SI32	0.58178	0.32676	0.32368
SI33	0.69528	0.37308	0.17985
SI34	0.73111	0.32329	0.96856
SI35	0.88555	0.32111	0.97565
SI36	0.9394	0.36551	0.18733
SI37	0.92768	0.4356	0.83614
SI38	0.77777	0.43621	0.46788
SI39	0.62089	0.43272	0.48405
SI40	0.56708	0.46808	0.69789
SI41	0.6814	0.42861	0.82474
SI42	0.91994	0.66992	0.82118
SI43	0.80576	0.63525	0.68014
SI44	0.76662	0.66508	0.46099
SI45	0.61224	0.66907	0.48082
SI46	0.56803	0.62483	0.69884
SI47	0.68734	0.67377	0.81562
SI48	0.57666	0.9391	0.36139
SI49	0.69423	0.96389	0.21642
SI50	0.72127	0.93375	0.99543
SI51	0.88112	0.9291	0.99312
SI52	0.93285	0.96759	0.20197
SI53	0.8213	0.94188	0.35222
SI54	0.57989	0.17112	0.33329
SI55	0.69614	0.11882	0.19816
SI56	0.73369	0.16341	0.98002
SI57	0.88758	0.16755	0.98254
SI58	0.93846	0.12498	0.19349
SI59	0.81912	0.1623	0.32361
SI60	0.92545	0.04885	0.85265
SI61	0.80258	0.02076	0.70907
SI62	0.78086	0.06107	0.49012

SI63	0.62142	0.06704	0.48888
SI64	0.57238	0.02504	0.70013
SI65	0.68022	0.0491	0.85288
SI66	0.92201	0.82307	0.83655
SI67	0.80294	0.86342	0.69213
SI68	0.76914	0.82199	0.47513
SI69	0.61524	0.82267	0.49392
SI70	0.56726	0.86776	0.70309
SI71	0.68264	0.82733	0.83492
SI72	0.42538	0.4436	0.64329
SI73	0.30906	0.47134	0.79606
SI74	0.29241	0.42935	0.00988
SI75	0.1337	0.43122	0.01164
SI76	0.07961	0.469	0.80189
SI77	0.19068	0.445	0.65688
SI78	0.42871	0.66787	0.66207
SI79	0.30502	0.62683	0.79765
SI80	0.27118	0.67166	0.01143
SI81	0.11667	0.67026	0.011
SI82	0.06698	0.62646	0.80045
SI83	0.18236	0.66522	0.66356
SI84	0.08054	0.55215	0.14697
SI85	0.20478	0.52562	0.28365
SI86	0.23061	0.56366	0.50972
SI87	0.38839	0.56629	0.50602
SI88	0.432	0.52613	0.29228
SI89	0.329	0.5525	0.13692
SI90	0.08686	0.32403	0.16322
SI91	0.20177	0.3664	0.30821
SI92	0.2404	0.3282	0.52746
SI93	0.39456	0.32492	0.51432
SI94	0.43856	0.36899	0.29662
SI95	0.32203	0.32031	0.17089
O96	0.3624	0.05936	0.71509
O97	0.305	0.06152	0.89188
O98	0.20232	0.04588	0.01893
O99	0.10026	0.06392	0.89428
O100	0.10629	0.05452	0.69698
O101	0.23322	0.02976	0.73447
O102	0.36229	0.82149	0.75027
O103	0.30751	0.84377	0.92483
O104	0.19185	0.8508	0.01988
O105	0.08702	0.8283	0.90438
O106	0.10644	0.83232	0.70885

O107	0.23255	0.85072	0.76152
O108	0.32501	0.94447	0.79774
O109	0.08735	0.94533	0.80948
O110	0.43692	0.12188	0.57935
O111	0.41993	0.99057	0.56508
O112	0.39917	0.85886	0.5671
O113	0.19796	0.12804	0.60888
O114	0.18183	0.99897	0.55758
O115	0.19602	0.86462	0.57002
O116	0.99141	0.03683	0.78488
O117	0.98662	0.85917	0.78511
O118	0.14278	0.9374	0.22119
O119	0.20078	0.92559	0.39624
O120	0.29954	0.94316	0.52871
O121	0.39784	0.92444	0.39655
O122	0.3972	0.94378	0.20006
O123	0.27088	0.96843	0.24048
O124	0.14436	0.16565	0.24292
O125	0.20097	0.16202	0.41729
O126	0.31422	0.14422	0.51695
O127	0.41533	0.16938	0.39433
O128	0.39734	0.14792	0.20013
O129	0.27245	0.13233	0.25603
O130	0.17936	0.04756	0.31973
O131	0.42072	0.04575	0.32508
O132	0.06983	0.86867	0.0923
O133	0.08319	-0.00038	0.06676
O134	0.10358	0.13125	0.06122
O135	0.30484	0.86664	0.12039
O136	0.3196	0.99257	0.05821
O137	0.30436	0.12625	0.06185
O138	0.51038	0.94868	0.29368
O139	0.51726	0.13327	0.27916
O140	0.63733	0.56997	0.25868
O141	0.67481	0.5607	0.06895
O142	0.79642	0.54558	0.99287
O143	0.91456	0.56141	0.07807
O144	0.8873	0.55369	0.2737
O145	0.76316	0.54795	0.21103
O146	0.64374	0.32831	0.24661
O147	0.68888	0.34772	0.06501
O148	0.8088	0.34852	0.97639
O149	0.91811	0.3259	0.08615
O150	0.9035	0.33243	0.2844

O151	0.77035	0.36424	0.21944
O152	0.67112	0.45138	0.18704
O153	0.91899	0.44428	0.17333
O154	0.56727	0.62587	0.403
O155	0.60004	0.49761	0.4186
O156	0.60147	0.36339	0.42828
O157	0.79813	0.62639	0.36548
O158	0.79078	0.49417	0.38544
O159	0.80289	0.3629	0.4263
O160	0.0112	0.53961	0.20812
O161	0.0202	0.36223	0.20289
O162	0.87781	0.43023	0.73766
O163	0.82328	0.44763	0.56969
O164	0.70113	0.43557	0.50161
O165	0.58432	0.43329	0.59122
O166	0.60345	0.42998	0.78952
O167	0.72932	0.44169	0.73094
O168	0.86752	0.67719	0.72934
O169	0.80993	0.6452	0.55922
O170	0.68922	0.64205	0.47706
O171	0.58305	0.66047	0.59248
O172	0.6095	0.6626	0.78609
O173	0.73419	0.66656	0.71649
O174	0.81322	0.55801	0.71146
O175	0.59017	0.54648	0.69421
O176	0.92896	0.36567	0.89718
O177	0.90283	0.4961	0.90655
O178	0.88736	0.62861	0.91403
O179	0.69612	0.35443	0.87022
O180	0.69209	0.4858	0.91054
O181	0.70867	0.62021	0.90003
O182	0.48704	0.46239	0.71648
O183	0.48895	0.6326	0.725
O184	0.64045	0.92708	0.28858
O185	0.69822	0.92454	0.11065
O186	0.80155	0.94359	0.98469
O187	0.90288	0.92394	0.10957
O188	0.89584	0.94712	0.30552
O189	0.76795	0.96195	0.26626
O190	0.64524	0.16472	0.26256
O191	0.69677	0.14661	0.0848
O192	0.81128	0.13874	0.98611
O193	0.91797	0.1679	0.09499
O194	0.89649	0.1514	0.28944

O195	0.77079	0.12158	0.24652
O196	0.67082	0.04126	0.19953
O197	0.92145	0.04626	0.17467
O198	0.56715	0.87298	0.43132
O199	0.58533	0.00445	0.43303
O200	0.59436	0.13742	0.44238
O201	0.80881	0.86608	0.39236
O202	0.81492	0.99368	0.44567
O203	0.81287	0.12806	0.43654
O204	0.01178	0.95211	0.21826
O205	0.01772	0.13496	0.21523
O206	0.86076	0.05015	0.7802
O207	0.79796	0.06619	0.60813
O208	0.70126	0.06026	0.46942
O209	0.60536	0.06667	0.60756
O210	0.60568	0.04769	0.8054
O211	0.7316	0.02368	0.76691
O212	0.85997	0.82893	0.75996
O213	0.80519	0.82756	0.58343
O214	0.69232	0.84878	0.48498
O215	0.59189	0.82134	0.61004
O216	0.60526	0.84192	0.80351
O217	0.72997	0.85269	0.74314
O218	0.81798	0.9432	0.67916
O219	0.58591	0.94559	0.67942
O220	0.93238	0.12031	0.91016
O221	0.92039	0.98951	0.93627
O222	0.90165	0.85805	0.94193
O223	0.69674	0.12513	0.88835
O224	0.68411	0.99945	0.94926
O225	0.69935	0.86634	0.93744
O226	0.49323	0.04086	0.71053
O227	0.48696	0.86129	0.71895
O228	0.35782	0.44369	0.70937
O229	0.31488	0.42313	0.89353
O230	0.21315	0.44629	0.02071
O231	0.11244	0.42842	0.89474
O232	0.11311	0.44851	0.69465
O233	0.23317	0.46741	0.75422
O234	0.3598	0.65933	0.72367
O235	0.30259	0.67095	0.89943
O236	0.19416	0.64472	0.00903
O237	0.0873	0.67042	0.8979
O238	0.10563	0.65461	0.70164

O239	0.23186	0.62964	0.74454
O240	0.32472	0.54942	0.82439
O241	0.08834	0.54904	0.82129
O242	0.43652	0.36983	0.59399
O243	0.42063	0.49824	0.55288
O244	0.42359	0.63257	0.55269
O245	0.20812	0.3694	0.62065
O246	0.20478	0.49466	0.56287
O247	0.19184	0.62881	0.55541
O248	0.00112	0.45132	0.79284
O249	0.98703	0.63174	0.78094
O250	0.1414	0.55999	0.22689
O251	0.2177	0.56188	0.39043
O252	0.30961	0.57008	0.53301
O253	0.4002	0.56615	0.38677
O254	0.4007	0.55853	0.19179
O255	0.27138	0.53463	0.21759
O256	0.14243	0.32644	0.25151
O257	0.20076	0.34424	0.42447
O258	0.31765	0.35163	0.51279
O259	0.425	0.33222	0.40289
O260	0.39882	0.33039	0.20743
O261	0.27378	0.34939	0.25876
O262	0.18804	0.44661	0.29943
O263	0.41344	0.44669	0.30174
O264	0.07341	0.62118	0.08292
O265	0.0931	0.49036	0.06955
O266	0.11587	0.35942	0.06248
O267	0.31452	0.62378	0.08374
O268	0.33405	0.49171	0.05669
O269	0.30943	0.35929	0.06599
O270	0.5118	0.53562	0.28427
O271	0.51804	0.36485	0.27291
O272	0.44413	0.74652	0.64317
O273	0.19892	0.74448	0.65117
O274	0.27435	0.7476	0.05439
O275	0.11166	0.74609	0.05475
O276	0.06865	0.24697	0.13638
O277	0.30648	0.24161	0.15268
O278	0.23746	0.24931	0.55663
O279	0.39831	0.24718	0.55027
O280	0.56242	0.24966	0.35023
O281	0.80022	0.23974	0.33255
O282	0.72921	0.24261	0.95782

O283	0.8885	0.24352	0.93901
O284	0.93892	0.74485	0.85996
O285	0.69541	0.74885	0.86028
O286	0.77107	0.74472	0.43763
O287	0.60865	0.74748	0.44834
O288	0.95616	0.25027	0.45137
O289	0.87911	0.19356	0.57761
O290	0.87552	0.32124	0.55467
O291	-0.02881	0.26689	0.6439
O292	0.0963	0.28199	0.56052
O293	0.10172	0.27409	0.73568
GA29	0.9159	0.40582	0.6003
H295	0.9404	0.27929	0.39603
H296	0.83796	0.33439	0.49226
H297	0.85657	0.17175	0.5195
H298	0.97394	0.53178	0.60449
H299	0.99114	0.40269	0.62519
H300	0.10911	0.53653	0.51685
H301	0.09539	0.54098	0.38654
H302	-0.00216	0.60086	0.40373
H303	0.03532	0.62365	0.51907
H304	0.91559	0.58322	0.5406
H305	0.96654	0.40631	0.37732
H306	0.08561	0.42396	0.41262
H307	0.88658	0.48936	0.43465
H308	0.05705	0.4344	0.53573
AL30	0.81728	0.32287	0.30715
AL31	0.80398	0.47361	0.69498
P311	0.92504	0.25578	0.56014
C312	0.95703	0.54801	0.52938
C313	0.07201	0.52983	0.4583
C314	0.01614	0.58099	0.47542
C315	0.98186	0.44603	0.42858
C316	0.9362	0.48965	0.46557
C317	0.052	0.45445	0.45859
C318	0.09716	0.27764	0.64834
<b>TS<sub>COOH</sub></b>			
SI2	0.42669	0.0529	0.64292
SI3	0.30656	0.02299	0.78508
SI4	0.28206	0.05646	0.0078
SI5	0.12203	0.05992	0.0097
SI6	0.0709	0.02567	0.79609
SI7	0.18109	0.05123	0.64885

SI8	0.423	0.82262	0.66939
SI9	0.30672	0.86523	0.80858
SI10	0.26984	0.82664	0.02849
SI11	0.11546	0.82345	0.0177
SI12	0.06655	0.86728	0.80236
SI13	0.18389	0.82233	0.67465
SI14	0.07797	0.94012	0.15
SI15	0.19877	0.96971	0.29577
SI16	0.21935	0.93077	0.51426
SI17	0.37857	0.92933	0.51364
SI18	0.43178	0.96531	0.30348
SI19	0.32174	0.94225	0.15457
SI20	0.08286	0.1688	0.16467
SI21	0.20008	0.12638	0.30919
SI22	0.23851	0.17005	0.52357
SI23	0.39236	0.17038	0.50835
SI24	0.43958	0.12328	0.29812
SI25	0.32091	0.16185	0.16796
SI26	0.58196	0.55517	0.34215
SI27	0.68943	0.53131	0.18326
SI28	0.71975	0.55397	0.9662
SI29	0.87764	0.55983	0.9787
SI30	0.93165	0.52466	0.18894
SI31	0.8109	0.55234	0.31919
SI32	0.58171	0.32683	0.32689
SI33	0.69639	0.3737	0.18285
SI34	0.7318	0.32342	0.97125
SI35	0.88626	0.32173	0.98047
SI36	0.93984	0.36623	0.19032
SI37	0.92957	0.43841	0.84676
SI38	0.77934	0.43252	0.47773
SI39	0.62176	0.43127	0.48689
SI40	0.56656	0.46824	0.70093
SI41	0.67951	0.43055	0.82929
SI42	0.91974	0.67101	0.82494
SI43	0.80502	0.63649	0.68271
SI44	0.76732	0.66521	0.46352
SI45	0.61295	0.66761	0.48406
SI46	0.56798	0.62533	0.70309
SI47	0.68765	0.67509	0.81768
SI48	0.57573	0.93794	0.3608
SI49	0.69394	0.96518	0.21652
SI50	0.72071	0.93571	0.99551
SI51	0.88051	0.93072	0.99201

SI52	0.93327	0.9672	0.20128
SI53	0.82129	0.94136	0.35064
SI54	0.58135	0.17119	0.33057
SI55	0.69561	0.11997	0.1932
SI56	0.73399	0.16377	0.97612
SI57	0.88785	0.16815	0.98269
SI58	0.93812	0.12477	0.19454
SI59	0.81742	0.16271	0.32018
SI60	0.92497	0.05029	0.85062
SI61	0.80269	0.02088	0.70711
SI62	0.77871	0.05874	0.48775
SI63	0.62	0.06499	0.4868
SI64	0.57178	0.02531	0.69869
SI65	0.68067	0.04946	0.8506
SI66	0.92172	0.82389	0.83581
SI67	0.80357	0.86378	0.69066
SI68	0.76873	0.82176	0.47378
SI69	0.61505	0.82152	0.49365
SI70	0.56714	0.868	0.7024
SI71	0.68318	0.82872	0.8344
SI72	0.42611	0.44218	0.64357
SI73	0.31015	0.46942	0.79582
SI74	0.29176	0.42996	0.01066
SI75	0.13331	0.43131	0.01236
SI76	0.07833	0.46945	0.80382
SI77	0.19011	0.44496	0.657
SI78	0.42861	0.66769	0.6629
SI79	0.30604	0.62528	0.79882
SI80	0.27197	0.67087	0.01227
SI81	0.11736	0.66997	0.0116
SI82	0.06602	0.62639	0.80262
SI83	0.18314	0.66356	0.66695
SI84	0.08021	0.55145	0.14857
SI85	0.20528	0.52428	0.28522
SI86	0.23141	0.56274	0.51063
SI87	0.38955	0.56492	0.50659
SI88	0.43365	0.52586	0.29287
SI89	0.3295	0.55225	0.13874
SI90	0.08737	0.32384	0.16398
SI91	0.20232	0.36444	0.31047
SI92	0.23979	0.32719	0.53003
SI93	0.3939	0.32472	0.51444
SI94	0.43837	0.36868	0.29636
SI95	0.32189	0.3198	0.17169

O96	0.36168	0.0595	0.71474
O97	0.30491	0.06128	0.89199
O98	0.20179	0.04701	0.01861
O99	0.09975	0.06453	0.89379
O100	0.10674	0.05569	0.69679
O101	0.23285	0.02781	0.7356
O102	0.36215	0.82127	0.74944
O103	0.30842	0.84358	0.92502
O104	0.19228	0.8505	0.01865
O105	0.08643	0.82939	0.90533
O106	0.1066	0.83244	0.70977
O107	0.23271	0.85095	0.76249
O108	0.32602	0.94422	0.79819
O109	0.08711	0.94601	0.80849
O110	0.43686	0.12198	0.57964
O111	0.41925	0.99089	0.56472
O112	0.39953	0.85908	0.56648
O113	0.20157	0.12482	0.60734
O114	0.18045	0.99577	0.55954
O115	0.19696	0.86191	0.57021
O116	0.99131	0.03808	0.78359
O117	0.98653	0.86006	0.78503
O118	0.14309	0.93891	0.2214
O119	0.20032	0.92426	0.39668
O120	0.29916	0.94262	0.52866
O121	0.39733	0.92489	0.39595
O122	0.39692	0.94378	0.19903
O123	0.27122	0.9678	0.24171
O124	0.1446	0.16409	0.24213
O125	0.20052	0.16336	0.41698
O126	0.31522	0.14424	0.51166
O127	0.41864	0.16906	0.39379
O128	0.3981	0.14778	0.20002
O129	0.27307	0.13283	0.2566
O130	0.18126	0.04744	0.32307
O131	0.42283	0.04539	0.32373
O132	0.07086	0.86806	0.09401
O133	0.08317	0.99876	0.06543
O134	0.10177	0.13074	0.06124
O135	0.30447	0.86594	0.12094
O136	0.31803	0.99154	0.05796
O137	0.30495	0.12539	0.06239
O138	0.50997	0.94587	0.29148
O139	0.51891	0.13302	0.27633

O140	0.63901	0.56993	0.25906
O141	0.68295	0.565	0.07336
O142	0.79929	0.54003	0.98135
O143	0.90704	0.5666	0.09124
O144	0.88905	0.54897	0.28603
O145	0.7661	0.54295	0.21973
O146	0.64517	0.33087	0.25299
O147	0.69045	0.34323	0.07069
O148	0.80951	0.34892	0.97866
O149	0.91637	0.32387	0.09271
O150	0.90468	0.33436	0.28913
O151	0.7715	0.36702	0.22329
O152	0.67137	0.45185	0.18202
O153	0.91987	0.44467	0.17219
O154	0.56887	0.62313	0.40661
O155	0.60465	0.49521	0.41662
O156	0.59803	0.36219	0.43358
O157	0.7989	0.6253	0.3694
O158	0.79106	0.49393	0.39946
O159	0.80494	0.36143	0.43078
O160	0.01059	0.54047	0.20898
O161	0.02085	0.36226	0.20335
O162	0.87394	0.43496	0.75831
O163	0.82331	0.44215	0.58037
O164	0.70143	0.42965	0.50692
O165	0.58346	0.43618	0.59249
O166	0.60197	0.42846	0.79172
O167	0.72743	0.44517	0.73657
O168	0.86578	0.67797	0.73551
O169	0.81105	0.64843	0.56242
O170	0.69019	0.6417	0.48094
O171	0.58356	0.65955	0.59576
O172	0.60946	0.66353	0.79004
O173	0.73304	0.66813	0.71713
O174	0.81173	0.55919	0.71194
O175	0.58914	0.54677	0.70119
O176	0.9322	0.36778	0.90729
O177	0.91883	0.50025	0.92301
O178	0.88963	0.63031	0.92027
O179	0.69554	0.35712	0.87627
O180	0.6863	0.48864	0.91502
O181	0.7111	0.62212	0.90186
O182	0.48643	0.46159	0.71844
O183	0.48875	0.63415	0.72795

O184	0.64082	0.92851	0.28985
O185	0.69699	0.92607	0.11043
O186	0.80102	0.94599	0.98665
O187	0.90404	0.9245	0.10754
O188	0.89581	0.94551	0.30377
O189	0.76804	0.96333	0.26538
O190	0.64605	0.1671	0.25804
O191	0.69476	0.1454	0.07864
O192	0.81157	0.13936	0.98535
O193	0.91804	0.16703	0.09526
O194	0.89569	0.15058	0.2907
O195	0.77106	0.12412	0.23855
O196	0.67039	0.04254	0.19985
O197	0.92177	0.04604	0.17551
O198	0.56712	0.87133	0.42979
O199	0.58066	0.00361	0.43294
O200	0.59737	0.13619	0.43822
O201	0.80753	0.86566	0.38978
O202	0.8165	0.99297	0.44472
O203	0.80695	0.12673	0.43172
O204	0.0122	0.95215	0.21826
O205	0.01725	0.13563	0.21704
O206	0.86068	0.05226	0.77707
O207	0.79611	0.06594	0.60565
O208	0.69936	0.05287	0.46781
O209	0.60373	0.06713	0.60542
O210	0.60612	0.0481	0.80315
O211	0.73196	0.02184	0.76589
O212	0.86055	0.8284	0.75752
O213	0.80528	0.82859	0.58153
O214	0.69187	0.8482	0.48438
O215	0.59165	0.82132	0.60972
O216	0.60578	0.84312	0.80273
O217	0.73068	0.85354	0.74235
O218	0.81983	0.94351	0.6784
O219	0.58499	0.9459	0.67752
O220	0.93227	0.1218	0.90826
O221	0.91925	0.99117	0.93439
O222	0.89984	0.8599	0.93965
O223	0.69872	0.1259	0.88254
O224	0.68384	0.00159	0.9491
O225	0.69957	0.8686	0.93633
O226	0.49262	0.04085	0.71079
O227	0.48693	0.86077	0.71887

O228	0.35837	0.44069	0.70936
O229	0.31508	0.42231	0.89476
O230	0.21257	0.448	0.01933
O231	0.11112	0.4274	0.89563
O232	0.11371	0.45323	0.6968
O233	0.2345	0.46507	0.75334
O234	0.35921	0.6591	0.72348
O235	0.30515	0.66844	0.90152
O236	0.19483	0.64439	0.0081
O237	0.08719	0.67114	0.89892
O238	0.10619	0.65135	0.70314
O239	0.23187	0.62804	0.74896
O240	0.32634	0.5476	0.82268
O241	0.08466	0.54889	0.82838
O242	0.43751	0.36877	0.593
O243	0.4217	0.49678	0.55316
O244	0.42418	0.63105	0.55449
O245	0.20321	0.36786	0.62068
O246	0.20444	0.49361	0.56208
O247	0.19538	0.62875	0.55837
O248	0.00079	0.44793	0.78949
O249	0.98644	0.6334	0.78177
O250	0.14093	0.55707	0.22924
O251	0.21735	0.56145	0.39157
O252	0.31065	0.5672	0.53271
O253	0.40196	0.56584	0.38749
O254	0.40163	0.55805	0.19256
O255	0.27191	0.53375	0.21928
O256	0.14267	0.32572	0.25272
O257	0.19944	0.34148	0.42673
O258	0.31674	0.35176	0.51725
O259	0.42203	0.33186	0.40177
O260	0.39896	0.33103	0.20584
O261	0.27445	0.34574	0.26285
O262	0.19071	0.4449	0.30209
O263	0.41427	0.44661	0.3019
O264	0.07498	0.62067	0.08435
O265	0.09204	0.48953	0.07088
O266	0.11735	0.35906	0.0636
O267	0.31424	0.62395	0.08737
O268	0.33389	0.49211	0.05715
O269	0.3066	0.36012	0.06875
O270	0.51358	0.53469	0.28561
O271	0.51789	0.36366	0.27418

O272	0.44337	0.74625	0.64188
O273	0.19866	0.74311	0.65632
O274	0.27468	0.7472	0.05358
O275	0.11247	0.74591	0.05509
O276	0.06922	0.24678	0.13684
O277	0.30753	0.24117	0.1509
O278	0.23732	0.24813	0.55892
O279	0.39786	0.24684	0.54938
O280	0.56301	0.24909	0.35046
O281	0.80118	0.2405	0.3311
O282	0.73036	0.24304	0.95473
O283	0.88992	0.24463	0.94081
O284	0.93924	0.74628	0.86191
O285	0.69572	0.7505	0.86148
O286	0.77074	0.74452	0.43679
O287	0.6084	0.74581	0.45014
O288	0.96008	0.26463	0.44475
O289	0.90216	0.17103	0.5466
O290	0.86019	0.29331	0.55892
O291	0.96832	0.25624	0.63303
O292	0.09868	0.22697	0.59817
O293	0.05888	0.32847	0.66711
GA29	0.9206	0.39783	0.6177
H295	0.93842	0.28761	0.386
H296	0.83422	0.31936	0.49968
H297	0.86444	0.15613	0.50241
H298	0.96764	0.53411	0.61128
H299	0.99646	0.3325	0.65231
H300	0.10097	0.55446	0.54078
H301	0.09847	0.56425	0.40985
H302	0.98906	0.60419	0.41068
H303	0.01845	0.63379	0.52777
H304	0.90558	0.57688	0.54243
H305	0.98275	0.40809	0.38442
H306	0.097	0.44645	0.41255
H307	0.89092	0.47614	0.44271
H308	0.07032	0.44489	0.53712
AL30	0.81777	0.32478	0.31103
AL31	0.80381	0.47403	0.70146
P311	0.92243	0.24629	0.54459
C312	0.95149	0.54739	0.53448
C313	0.07045	0.54574	0.47437
C314	0.00714	0.58814	0.48456
C315	0.99176	0.45035	0.43452

C316	0.9403	0.48613	0.47105
C317	0.06059	0.46857	0.46394
C318	0.07184	0.27363	0.63148
<b>C<sub>6</sub>H<sub>10</sub>+COOH</b>			
SI2	0.42629	0.0528	0.64309
SI3	0.30592	0.02311	0.78524
SI4	0.28183	0.05669	0.00829
SI5	0.12202	0.06042	0.01078
SI6	0.07088	0.02407	0.79792
SI7	0.17985	0.05137	0.6488
SI8	0.42278	0.82279	0.67059
SI9	0.30599	0.86511	0.80904
SI10	0.26947	0.82655	0.02958
SI11	0.11508	0.82329	0.01786
SI12	0.06698	0.86603	0.80265
SI13	0.18377	0.82232	0.67362
SI14	0.07719	0.94009	0.15018
SI15	0.19791	0.96911	0.29464
SI16	0.2193	0.93114	0.51385
SI17	0.37851	0.92896	0.51424
SI18	0.43133	0.96579	0.3049
SI19	0.322	0.94253	0.15494
SI20	0.08296	0.16961	0.1639
SI21	0.19907	0.12559	0.30831
SI22	0.23555	0.17024	0.5242
SI23	0.38977	0.17033	0.50967
SI24	0.43705	0.12324	0.29943
SI25	0.31968	0.16176	0.16843
SI26	0.58101	0.55548	0.34338
SI27	0.68795	0.53169	0.18258
SI28	0.72006	0.55336	0.96679
SI29	0.87763	0.55989	0.98013
SI30	0.93174	0.52572	0.18946
SI31	0.8094	0.55219	0.31667
SI32	0.57902	0.32666	0.32446
SI33	0.69573	0.37383	0.1843
SI34	0.73205	0.32386	0.97079
SI35	0.88654	0.32206	0.97953
SI36	0.93981	0.36738	0.18899
SI37	0.92819	0.43879	0.84779
SI38	0.77824	0.43417	0.47778
SI39	0.61987	0.42998	0.48541
SI40	0.56597	0.46744	0.70023

SI41	0.6794	0.43035	0.82822
SI42	0.91912	0.67079	0.82531
SI43	0.80471	0.63605	0.68376
SI44	0.76664	0.66484	0.46505
SI45	0.61196	0.66839	0.4851
SI46	0.56736	0.62471	0.7031
SI47	0.68756	0.67399	0.8182
SI48	0.57671	0.93907	0.36176
SI49	0.69424	0.96435	0.21636
SI50	0.7211	0.93466	0.99549
SI51	0.88077	0.93042	0.99442
SI52	0.9326	0.96715	0.20358
SI53	0.8207	0.94179	0.35315
SI54	0.57918	0.17064	0.33219
SI55	0.69597	0.11931	0.19743
SI56	0.73442	0.16423	0.97891
SI57	0.88835	0.16819	0.98219
SI58	0.9386	0.1247	0.1942
SI59	0.8189	0.16242	0.32404
SI60	0.92544	0.04921	0.85373
SI61	0.80245	0.02068	0.70992
SI62	0.7809	0.06125	0.49148
SI63	0.62122	0.06741	0.48938
SI64	0.57164	0.02577	0.70042
SI65	0.67979	0.04977	0.85289
SI66	0.92188	0.82379	0.8373
SI67	0.80269	0.86312	0.69234
SI68	0.76879	0.82129	0.47528
SI69	0.61466	0.82213	0.49446
SI70	0.5668	0.86841	0.70365
SI71	0.68227	0.82751	0.83553
SI72	0.42421	0.44252	0.64384
SI73	0.30921	0.47004	0.79848
SI74	0.29117	0.42969	0.01174
SI75	0.1329	0.43216	0.01363
SI76	0.07716	0.469	0.80397
SI77	0.19033	0.44389	0.66149
SI78	0.4286	0.66788	0.66443
SI79	0.30524	0.62584	0.79949
SI80	0.27115	0.67099	0.01313
SI81	0.1164	0.67017	0.01351
SI82	0.06557	0.62651	0.80355
SI83	0.1822	0.66393	0.6669
SI84	0.08015	0.5524	0.15129

SI85	0.20429	0.52496	0.28681
SI86	0.23115	0.56254	0.51355
SI87	0.38889	0.5662	0.50782
SI88	0.43262	0.5263	0.29424
SI89	0.32871	0.55217	0.14037
SI90	0.08724	0.32435	0.1646
SI91	0.20029	0.36565	0.31156
SI92	0.23707	0.3274	0.53107
SI93	0.3919	0.3245	0.51431
SI94	0.43636	0.36896	0.29638
SI95	0.31932	0.31993	0.17281
O96	0.3616	0.05906	0.71547
O97	0.30399	0.06131	0.8922
O98	0.2016	0.04653	0.01991
O99	0.09971	0.06392	0.89469
O100	0.10558	0.05363	0.69754
O101	0.23259	0.02896	0.73472
O102	0.36202	0.82148	0.75072
O103	0.30722	0.84325	0.92535
O104	0.19182	0.85047	0.02091
O105	0.08777	0.82698	0.90423
O106	0.10642	0.83257	0.70848
O107	0.23232	0.85067	0.76195
O108	0.32472	0.94424	0.79884
O109	0.08757	0.94471	0.81156
O110	0.43538	0.12168	0.57917
O111	0.4194	0.99035	0.56544
O112	0.39895	0.85868	0.56741
O113	0.19653	0.12602	0.60749
O114	0.18047	0.99624	0.55902
O115	0.19687	0.86227	0.5696
O116	0.99114	0.03614	0.78576
O117	0.98687	0.85917	0.78581
O118	0.14252	0.93658	0.22113
O119	0.20016	0.92457	0.39639
O120	0.29913	0.94277	0.52848
O121	0.39772	0.92408	0.39675
O122	0.39709	0.94371	0.20014
O123	0.27064	0.96767	0.24129
O124	0.14484	0.16493	0.24091
O125	0.19937	0.16142	0.41663
O126	0.31262	0.1443	0.51606
O127	0.41457	0.16901	0.39421
O128	0.39701	0.14788	0.20006

O129	0.27241	0.13107	0.25654
O130	0.17868	0.04678	0.31968
O131	0.41969	0.04548	0.32531
O132	0.06927	0.86935	0.09069
O133	0.08252	0.00061	0.06862
O134	0.10213	0.1322	0.05987
O135	0.30495	0.86628	0.12085
O136	0.31864	0.99228	0.05874
O137	0.30412	0.12612	0.062
O138	0.5103	0.94919	0.29447
O139	0.51667	0.13204	0.2791
O140	0.63797	0.56964	0.25975
O141	0.68059	0.56425	0.07208
O142	0.79933	0.54002	0.98584
O143	0.90848	0.56806	0.09161
O144	0.88763	0.55046	0.28458
O145	0.76485	0.54507	0.21673
O146	0.64317	0.33074	0.25168
O147	0.69243	0.34389	0.0717
O148	0.8099	0.34922	0.9762
O149	0.91511	0.32449	0.09272
O150	0.90541	0.33431	0.2882
O151	0.76998	0.36723	0.22901
O152	0.67106	0.45195	0.1831
O153	0.91895	0.44564	0.17272
O154	0.5684	0.62382	0.40711
O155	0.60346	0.496	0.41908
O156	0.5934	0.36238	0.43136
O157	0.79681	0.6234	0.37142
O158	0.78935	0.49011	0.39133
O159	0.80878	0.36086	0.43403
O160	0.01053	0.54051	0.21157
O161	0.02053	0.36353	0.20179
O162	0.8712	0.43484	0.76306
O163	0.82017	0.44669	0.57822
O164	0.70008	0.42439	0.49849
O165	0.58476	0.43381	0.59344
O166	0.60128	0.42954	0.79298
O167	0.72623	0.44449	0.73419
O168	0.86559	0.6782	0.73535
O169	0.81074	0.64751	0.56323
O170	0.68925	0.64262	0.48311
O171	0.58235	0.66066	0.59674
O172	0.6096	0.66096	0.79101

O173	0.73287	0.66852	0.71744
O174	0.81094	0.55914	0.71493
O175	0.58788	0.54613	0.69721
O176	0.93362	0.36747	0.9073
O177	0.91899	0.49966	0.92641
O178	0.88844	0.62981	0.91987
O179	0.69483	0.35682	0.8761
O180	0.68817	0.4878	0.9144
O181	0.71238	0.62134	0.90188
O182	0.48583	0.4606	0.71725
O183	0.48844	0.63395	0.7297
O184	0.64035	0.92774	0.28845
O185	0.69832	0.92491	0.11072
O186	0.80133	0.9453	0.98514
O187	0.90207	0.92412	0.11095
O188	0.8955	0.947	0.30717
O189	0.7678	0.96263	0.2669
O190	0.64437	0.16492	0.26086
O191	0.69827	0.14745	0.08435
O192	0.81212	0.13947	0.98394
O193	0.91822	0.16675	0.09479
O194	0.89634	0.15175	0.2897
O195	0.77006	0.12203	0.24797
O196	0.67101	0.0417	0.19836
O197	0.92164	0.04598	0.17682
O198	0.56723	0.87256	0.43075
O199	0.58613	0.0041	0.434
O200	0.59442	0.13731	0.44131
O201	0.8079	0.86595	0.39243
O202	0.81413	0.99346	0.44692
O203	0.81429	0.12766	0.43729
O204	0.01149	0.95125	0.21918
O205	0.01775	0.13529	0.21595
O206	0.86055	0.04987	0.78164
O207	0.79946	0.06679	0.60915
O208	0.70141	0.06175	0.47155
O209	0.60449	0.0675	0.6078
O210	0.60524	0.04858	0.8055
O211	0.73116	0.02436	0.76675
O212	0.86023	0.82941	0.75998
O213	0.8051	0.82775	0.58336
O214	0.69188	0.84776	0.48526
O215	0.59134	0.82214	0.61057
O216	0.60501	0.84273	0.80397

O217	0.72983	0.85182	0.74331
O218	0.81724	0.94317	0.67979
O219	0.58523	0.94636	0.67996
O220	0.93314	0.12214	0.90761
O221	0.92039	0.99183	0.94004
O222	0.9015	0.86022	0.94157
O223	0.69683	0.12577	0.88805
O224	0.68369	1.00032	0.94949
O225	0.69966	0.86742	0.93705
O226	0.49247	0.04149	0.71076
O227	0.4865	0.86167	0.71947
O228	0.35663	0.44249	0.71007
O229	0.31675	0.42272	0.89682
O230	0.21216	0.44917	0.01688
O231	0.10795	0.42799	0.89828
O232	0.11269	0.44968	0.69804
O233	0.23256	0.46487	0.75998
O234	0.35913	0.65922	0.72479
O235	0.30338	0.66957	0.90171
O236	0.19391	0.64485	0.01006
O237	0.08619	0.67037	0.90094
O238	0.10554	0.65337	0.70515
O239	0.23154	0.62839	0.74806
O240	0.32519	0.54836	0.82513
O241	0.08488	0.54873	0.82586
O242	0.4348	0.36914	0.59315
O243	0.42005	0.49746	0.55385
O244	0.42486	0.6317	0.55563
O245	0.20579	0.36794	0.62535
O246	0.20717	0.49359	0.56848
O247	0.19231	0.62785	0.55877
O248	-0.00086	0.44896	0.78908
O249	0.98596	0.63325	0.7828
O250	0.14082	0.56029	0.23156
O251	0.21756	0.55945	0.39458
O252	0.31022	0.57085	0.53471
O253	0.40123	0.56668	0.38869
O254	0.40085	0.55887	0.19404
O255	0.2711	0.53492	0.22137
O256	0.14126	0.32514	0.25471
O257	0.1982	0.34529	0.42815
O258	0.31473	0.35014	0.51589
O259	0.42128	0.33192	0.40206
O260	0.39641	0.33167	0.20616

O261	0.27239	0.34692	0.2636
O262	0.18721	0.44573	0.299
O263	0.41291	0.4471	0.30319
O264	0.07378	0.62114	0.08627
O265	0.09281	0.49012	0.07459
O266	0.11832	0.35961	0.06509
O267	0.31371	0.6231	0.08644
O268	0.33345	0.49064	0.06125
O269	0.30361	0.35911	0.06903
O270	0.51268	0.5347	0.28714
O271	0.51553	0.3633	0.27099
O272	0.44366	0.74648	0.64402
O273	0.19862	0.74323	0.6545
O274	0.27443	0.74717	0.05533
O275	0.11147	0.74619	0.05699
O276	0.06802	0.24751	0.13684
O277	0.30526	0.24104	0.15363
O278	0.23353	0.24813	0.55782
O279	0.39681	0.24673	0.55004
O280	0.56102	0.24887	0.34843
O281	0.80118	0.24013	0.33278
O282	0.73084	0.24329	0.95585
O283	0.89113	0.24474	0.94035
O284	0.93847	0.74598	0.86314
O285	0.69415	0.74932	0.86292
O286	0.77118	0.74411	0.43756
O287	0.60731	0.74653	0.45078
O288	0.97147	0.26035	0.42464
O289	0.92205	0.16698	0.53447
O290	0.8767	0.28802	0.54792
O291	-0.0108	0.25025	0.61482
O292	0.08656	0.28911	0.54226
O293	0.07598	0.27934	0.70951
GA29	0.93348	0.39883	0.61753
H295	0.94753	0.28947	0.37347
H296	0.8341	0.33053	0.48597
H297	0.88002	0.15109	0.50045
H298	0.97149	0.53187	0.6154
H299	0.04108	0.2644	0.75582
H300	0.11015	0.54016	0.53074
H301	0.09669	0.54915	0.40105
H302	0.00028	0.60951	0.42306
H303	0.03604	0.62622	0.54164
H304	0.91548	0.58608	0.55292

H305	0.96822	0.41345	0.38191
H306	0.08717	0.4315	0.41873
H307	0.8862	0.49272	0.44712
H308	0.05876	0.43768	0.54174
AL30	0.81903	0.32332	0.3104
AL31	0.80357	0.47366	0.70144
P311	0.93572	0.24359	0.52492
C312	0.95691	0.55109	0.54056
C313	0.0731	0.53532	0.4717
C314	0.01722	0.58593	0.49298
C315	0.98274	0.45265	0.43438
C316	0.93715	0.49532	0.4719
C317	0.05314	0.46021	0.46653
C318	0.05466	0.2746	0.61505
<b>T<sub>SCO+OH</sub></b>			
SI2	0.42631	0.0533	0.64205
SI3	0.3062	0.02344	0.78486
SI4	0.28135	0.05681	0.00748
SI5	0.12133	0.05986	0.00919
SI6	0.06995	0.02486	0.79581
SI7	0.1802	0.05225	0.64868
SI8	0.4234	0.82285	0.66944
SI9	0.3065	0.86525	0.80823
SI10	0.26932	0.82662	0.02796
SI11	0.11481	0.82359	0.01711
SI12	0.0658	0.86674	0.80193
SI13	0.1835	0.82279	0.6737
SI14	0.07792	0.93995	0.15012
SI15	0.19838	0.96964	0.29485
SI16	0.21924	0.93188	0.51394
SI17	0.37845	0.92913	0.51367
SI18	0.43084	0.96514	0.3033
SI19	0.32128	0.94257	0.15415
SI20	0.08206	0.16883	0.16331
SI21	0.1986	0.1261	0.30811
SI22	0.23512	0.17106	0.52349
SI23	0.39	0.17122	0.50822
SI24	0.43739	0.12296	0.29821
SI25	0.31944	0.1621	0.16812
SI26	0.57832	0.55268	0.34849
SI27	0.69192	0.52668	0.19016
SI28	0.71529	0.561	0.97969
SI29	0.874	0.56065	0.97803

SI30	0.93413	0.52465	0.18775
SI31	0.81604	0.55137	0.32015
SI32	0.57675	0.32653	0.33272
SI33	0.6999	0.37092	0.1977
SI34	0.73068	0.31972	0.98669
SI35	0.885	0.32264	0.9824
SI36	0.94063	0.36585	0.19372
SI37	0.92793	0.43813	0.84269
SI38	0.77402	0.43446	0.47183
SI39	0.61746	0.42893	0.4836
SI40	0.57613	0.46735	0.70073
SI41	0.68078	0.4325	0.85288
SI42	0.91965	0.67068	0.82568
SI43	0.80469	0.63059	0.68852
SI44	0.76737	0.66193	0.46751
SI45	0.61267	0.66807	0.48216
SI46	0.56799	0.62485	0.69989
SI47	0.68504	0.67501	0.82064
SI48	0.57537	0.93835	0.36026
SI49	0.69324	0.96493	0.21472
SI50	0.72074	0.93589	0.99491
SI51	0.88033	0.93161	0.99105
SI52	0.93371	0.96619	0.19987
SI53	0.82072	0.9388	0.34778
SI54	0.58042	0.17031	0.32849
SI55	0.69543	0.12024	0.19208
SI56	0.73481	0.16318	0.97352
SI57	0.88862	0.16866	0.98075
SI58	0.93781	0.12369	0.19246
SI59	0.818	0.16154	0.32301
SI60	0.92477	0.05135	0.84968
SI61	0.80339	0.0203	0.70767
SI62	0.78006	0.05602	0.48658
SI63	0.62137	0.06477	0.48522
SI64	0.57202	0.02644	0.69605
SI65	0.6807	0.04862	0.84907
SI66	0.92089	0.82354	0.83414
SI67	0.80478	0.86381	0.6889
SI68	0.76966	0.82023	0.47235
SI69	0.61571	0.82171	0.49257
SI70	0.56739	0.86947	0.70014
SI71	0.68378	0.83056	0.83078
SI72	0.43007	0.4433	0.64063
SI73	0.31115	0.47074	0.79223

SI74	0.29222	0.42933	0.00801
SI75	0.13475	0.43116	0.01165
SI76	0.08132	0.47184	0.80537
SI77	0.18825	0.44615	0.6519
SI78	0.42811	0.66772	0.6607
SI79	0.30491	0.62642	0.79678
SI80	0.27134	0.67117	0.01063
SI81	0.11711	0.6711	0.00925
SI82	0.06708	0.62825	0.80116
SI83	0.18241	0.66441	0.66317
SI84	0.08111	0.55246	0.14373
SI85	0.20489	0.52575	0.28076
SI86	0.22959	0.56327	0.50635
SI87	0.38835	0.56601	0.50428
SI88	0.43345	0.52663	0.2899
SI89	0.32981	0.55152	0.13564
SI90	0.08729	0.32373	0.16176
SI91	0.20202	0.36698	0.30525
SI92	0.2374	0.32815	0.52707
SI93	0.39206	0.32549	0.51191
SI94	0.4361	0.36877	0.2928
SI95	0.32103	0.32051	0.16684
O96	0.36189	0.05938	0.71506
O97	0.30456	0.06165	0.89183
O98	0.20109	0.04669	0.01739
O99	0.0984	0.06392	0.89355
O100	0.1059	0.05448	0.69656
O101	0.2328	0.02948	0.7346
O102	0.36259	0.82181	0.74963
O103	0.30814	0.84351	0.92467
O104	0.19174	0.85024	0.01709
O105	0.08523	0.82888	0.90504
O106	0.10632	0.83202	0.70973
O107	0.23272	0.85042	0.76167
O108	0.32484	0.94448	0.79803
O109	0.08656	0.94535	0.80877
O110	0.43477	0.12244	0.57843
O111	0.41914	0.99079	0.56458
O112	0.39938	0.85876	0.56632
O113	0.19753	0.12707	0.60818
O114	0.18119	0.99773	0.55809
O115	0.19578	0.86354	0.57019
O116	0.99048	0.0371	0.78223
O117	0.98586	0.85969	0.78369

O118	0.1435	0.93738	0.22051
O119	0.2004	0.92492	0.39641
O120	0.29911	0.94265	0.52903
O121	0.39685	0.9244	0.39588
O122	0.39648	0.94318	0.19861
O123	0.27109	0.96853	0.2415
O124	0.14395	0.16463	0.24057
O125	0.19842	0.16217	0.41644
O126	0.31242	0.14661	0.5145
O127	0.41498	0.16874	0.39308
O128	0.39677	0.14794	0.19944
O129	0.27203	0.13253	0.25689
O130	0.17912	0.04721	0.32032
O131	0.42024	0.04505	0.32331
O132	0.07026	0.86834	0.09311
O133	0.08281	0.99916	0.06645
O134	0.10137	0.13109	0.05974
O135	0.30323	0.86644	0.12046
O136	0.31777	0.9922	0.0579
O137	0.30327	0.12605	0.06222
O138	0.50924	0.94654	0.29179
O139	0.51692	0.13179	0.27791
O140	0.64385	0.55481	0.27823
O141	0.68048	0.57055	0.08906
O142	0.79512	0.54889	0.99357
O143	0.9118	0.56177	0.08514
O144	0.89341	0.55465	0.28296
O145	0.76916	0.53842	0.22368
O146	0.64499	0.33713	0.2717
O147	0.70118	0.32323	0.09911
O148	0.8077	0.34826	0.98286
O149	0.91647	0.32587	0.09385
O150	0.90779	0.33214	0.29257
O151	0.77242	0.37198	0.24846
O152	0.67704	0.44753	0.16916
O153	0.92015	0.44455	0.18001
O154	0.56867	0.62501	0.40289
O155	0.58383	0.49552	0.43484
O156	0.58147	0.36118	0.44294
O157	0.79944	0.62253	0.37318
O158	0.80633	0.49016	0.39862
O159	0.81177	0.36047	0.44466
O160	0.01313	0.54014	0.20727
O161	0.02195	0.3631	0.20302

O162	0.88485	0.43001	0.73897
O163	0.79301	0.44791	0.58413
O164	0.69536	0.42642	0.44989
O165	0.60856	0.43142	0.60308
O166	0.60778	0.43344	0.79882
O167	0.74231	0.43529	0.77788
O168	0.8654	0.67532	0.73628
O169	0.80846	0.64186	0.56756
O170	0.68931	0.64044	0.48102
O171	0.58243	0.66099	0.59356
O172	0.60739	0.66337	0.78894
O173	0.7324	0.66061	0.72426
O174	0.81428	0.55425	0.72185
O175	0.59254	0.54735	0.69542
O176	0.92905	0.36876	0.90628
O177	0.90343	0.49899	0.91191
O178	0.88971	0.63112	0.922
O179	0.68237	0.36248	0.91502
O180	0.68099	0.49634	0.92905
O181	0.7044	0.62857	0.91503
O182	0.49584	0.45687	0.70694
O183	0.488	0.6307	0.72232
O184	0.64	0.92897	0.28855
O185	0.69506	0.92535	0.10878
O186	0.80097	0.94811	0.9903
O187	0.90652	0.92323	0.105
O188	0.89522	0.94372	0.30104
O189	0.7675	0.96195	0.2631
O190	0.6431	0.16738	0.25209
O191	0.69711	0.14495	0.0772
O192	0.81262	0.13937	0.98182
O193	0.91854	0.16637	0.09329
O194	0.89478	0.14915	0.28748
O195	0.7693	0.12473	0.24227
O196	0.67062	0.04254	0.19797
O197	0.92189	0.04487	0.1734
O198	0.56762	0.87163	0.42923
O199	0.58061	0.00383	0.43263
O200	0.5999	0.13575	0.43501
O201	0.80703	0.86237	0.38465
O202	0.81626	0.98942	0.4432
O203	0.80912	0.12445	0.43354
O204	0.01257	0.95182	0.21933
O205	0.01686	0.13499	0.21569

O206	0.85999	0.05438	0.77732
O207	0.79689	0.0631	0.60451
O208	0.70046	0.05103	0.46672
O209	0.6047	0.0686	0.60371
O210	0.60631	0.04788	0.80113
O211	0.73209	0.02017	0.76497
O212	0.86017	0.82523	0.75488
O213	0.80731	0.8313	0.57826
O214	0.6929	0.84703	0.48275
O215	0.59235	0.82175	0.60879
O216	0.6064	0.84692	0.80133
O217	0.73093	0.85457	0.73789
O218	0.82351	0.94318	0.68239
O219	0.58428	0.94716	0.67268
O220	0.93373	0.12328	0.90583
O221	0.91851	0.99274	0.9342
O222	0.89755	0.86119	0.93584
O223	0.69928	0.12487	0.8807
O224	0.68305	0.00109	0.94792
O225	0.70264	0.86894	0.9331
O226	0.49302	0.04261	0.70858
O227	0.48732	0.86166	0.71766
O228	0.36546	0.44335	0.71329
O229	0.3121	0.42323	0.89079
O230	0.2136	0.44773	0.02385
O231	0.11697	0.42871	0.89316
O232	0.11244	0.45402	0.69563
O233	0.23742	0.46605	0.74271
O234	0.35918	0.65956	0.72271
O235	0.30295	0.67024	0.89883
O236	0.19423	0.64469	0.008
O237	0.08918	0.67445	0.89534
O238	0.10537	0.65251	0.69964
O239	0.2313	0.62874	0.74491
O240	0.32467	0.54888	0.82234
O241	0.0885	0.5514	0.82798
O242	0.43747	0.37071	0.58621
O243	0.42288	0.50029	0.55421
O244	0.42023	0.63413	0.55047
O245	0.19908	0.3691	0.61551
O246	0.19961	0.49469	0.55585
O247	0.19402	0.62935	0.55459
O248	0.00304	0.45196	0.80075
O249	0.987	0.6332	0.78382

O250	0.14282	0.56067	0.22198
O251	0.21552	0.56323	0.38727
O252	0.30896	0.56508	0.52898
O253	0.40172	0.56581	0.38537
O254	0.40157	0.55904	0.18975
O255	0.27286	0.53298	0.21733
O256	0.14383	0.32548	0.24855
O257	0.20178	0.34374	0.42093
O258	0.31495	0.35171	0.52081
O259	0.4165	0.33188	0.39709
O260	0.39801	0.33189	0.2006
O261	0.27407	0.35158	0.25486
O262	0.18696	0.44701	0.29777
O263	0.41428	0.44734	0.29884
O264	0.07307	0.62068	0.078
O265	0.09226	0.48964	0.06746
O266	0.11612	0.35877	0.06023
O267	0.31397	0.62258	0.08274
O268	0.33546	0.4904	0.05559
O269	0.30768	0.35767	0.0607
O270	0.51328	0.53707	0.28064
O271	0.51552	0.36152	0.27144
O272	0.4445	0.74639	0.64359
O273	0.19839	0.74385	0.65269
O274	0.27459	0.74715	0.05359
O275	0.11197	0.74621	0.05545
O276	0.06788	0.24683	0.13562
O277	0.30536	0.24149	0.15261
O278	0.23119	0.24943	0.55642
O279	0.3973	0.24787	0.54786
O280	0.56098	0.24766	0.35016
O281	0.80145	0.23933	0.33603
O282	0.73028	0.24232	0.94962
O283	0.89045	0.24585	0.94179
O284	0.93897	0.74624	0.86164
O285	0.69453	0.75208	0.85554
O286	0.77262	0.74156	0.4427
O287	0.60915	0.74624	0.44833
O288	0.94242	0.22802	0.45403
O289	0.84966	0.20629	0.58117
O290	0.89876	0.32083	0.56873
O291	0.96966	0.22305	0.63896
O292	0.06534	0.31429	0.5125
O293	0.04222	0.30981	0.68853

GA29	0.96486	0.38515	0.63423
H295	0.93819	0.26323	0.40262
H296	0.8438	0.34345	0.50075
H297	0.83575	0.17461	0.52734
H298	0.97958	0.54529	0.63298
H299	0.00981	0.27433	0.71462
H300	0.09261	0.54626	0.5359
H301	0.0943	0.57412	0.41085
H302	0.97304	0.59732	0.41726
H303	0.01414	0.63687	0.51916
H304	0.90824	0.57544	0.57142
H305	0.96848	0.40223	0.41689
H306	0.06192	0.46774	0.35093
H307	0.89063	0.46182	0.52476
H308	0.08664	0.43961	0.46778
AL30	0.82269	0.32246	0.32109
AL31	0.80516	0.4684	0.70744
P311	0.91745	0.24405	0.56455
C312	0.95562	0.54918	0.55887
C313	0.06384	0.54757	0.46623
C314	0.00063	0.58786	0.48698
C315	0.98363	0.44953	0.45207
C316	0.94131	0.48101	0.51611
C317	0.05139	0.47489	0.43087
C318	0.0655	0.29072	0.5937

### C<sub>6</sub>H<sub>10</sub>Ga-OH+CO

SI2	0.42648	0.05478	0.64204
SI3	0.30643	0.02426	0.7847
SI4	0.28146	0.05779	0.00726
SI5	0.12128	0.06031	0.00911
SI6	0.07016	0.02572	0.79544
SI7	0.18053	0.05335	0.64853
SI8	0.4239	0.82353	0.66978
SI9	0.30687	0.86617	0.80831
SI10	0.26912	0.82736	0.02776
SI11	0.11438	0.82426	0.01832
SI12	0.06565	0.86751	0.80266
SI13	0.18369	0.8238	0.67411
SI14	0.07846	0.9407	0.15082
SI15	0.19896	0.97075	0.29544
SI16	0.21953	0.93308	0.51443

SI17	0.37876	0.93032	0.5141
SI18	0.43054	0.96569	0.30325
SI19	0.32114	0.94342	0.15377
SI20	0.08092	0.16905	0.16434
SI21	0.1984	0.12715	0.30863
SI22	0.23547	0.17193	0.524
SI23	0.38935	0.17218	0.5087
SI24	0.43752	0.12369	0.299
SI25	0.31962	0.16295	0.16809
SI26	0.57693	0.55148	0.34958
SI27	0.69121	0.52425	0.19228
SI28	0.71354	0.56476	0.98378
SI29	0.8725	0.56237	0.97724
SI30	0.9349	0.52528	0.18508
SI31	0.81714	0.55125	0.32059
SI32	0.57816	0.32663	0.33576
SI33	0.70144	0.36998	0.19984
SI34	0.73259	0.31974	0.98923
SI35	0.88702	0.32322	0.98226
SI36	0.9412	0.36675	0.19361
SI37	0.92849	0.4402	0.84565
SI38	0.77527	0.43588	0.47095
SI39	0.61957	0.43091	0.48402
SI40	0.57999	0.46773	0.70083
SI41	0.68364	0.43322	0.85691
SI42	0.92118	0.67102	0.82338
SI43	0.80449	0.62969	0.68942
SI44	0.7674	0.66221	0.46713
SI45	0.61231	0.66828	0.4799
SI46	0.56778	0.62537	0.69826
SI47	0.68325	0.67616	0.82181
SI48	0.57493	0.93862	0.35984
SI49	0.69223	0.96559	0.21342
SI50	0.72123	0.93679	0.99476
SI51	0.88063	0.93199	0.98959
SI52	0.93439	0.96689	0.19808
SI53	0.82049	0.93962	0.34477
SI54	0.58119	0.17086	0.32827
SI55	0.69535	0.12054	0.19137
SI56	0.73522	0.16396	0.97231
SI57	0.88929	0.16956	0.98028
SI58	0.93624	0.12447	0.1932
SI59	0.81614	0.16265	0.32353
SI60	0.9251	0.05248	0.84851

SI61	0.80437	0.02126	0.70692
SI62	0.78002	0.05653	0.48481
SI63	0.62172	0.06431	0.48442
SI64	0.57214	0.02703	0.69497
SI65	0.68133	0.0493	0.8479
SI66	0.92064	0.82397	0.83231
SI67	0.80568	0.86491	0.68724
SI68	0.7697	0.82096	0.47084
SI69	0.61538	0.82186	0.49202
SI70	0.56782	0.87019	0.69953
SI71	0.68487	0.83223	0.82912
SI72	0.43195	0.44376	0.64111
SI73	0.31114	0.47053	0.79056
SI74	0.29127	0.42932	0.00743
SI75	0.13353	0.43082	0.00971
SI76	0.08148	0.47552	0.80547
SI77	0.1861	0.44715	0.64868
SI78	0.42735	0.66823	0.65947
SI79	0.30452	0.62665	0.79651
SI80	0.27117	0.67176	0.01056
SI81	0.11698	0.67224	0.00837
SI82	0.06884	0.63057	0.80031
SI83	0.18311	0.66599	0.66172
SI84	0.08111	0.55271	0.14137
SI85	0.20444	0.52623	0.28005
SI86	0.22836	0.564	0.50437
SI87	0.38751	0.56622	0.50418
SI88	0.43282	0.52632	0.28941
SI89	0.32918	0.5518	0.13513
SI90	0.08679	0.32424	0.15951
SI91	0.20316	0.36743	0.30283
SI92	0.23553	0.32881	0.52602
SI93	0.38942	0.32683	0.51175
SI94	0.43612	0.36872	0.29387
SI95	0.32271	0.32125	0.1661
O96	0.36216	0.06035	0.71525
O97	0.30456	0.06253	0.89161
O98	0.20119	0.04829	0.01751
O99	0.0984	0.06462	0.89352
O100	0.10626	0.05494	0.69621
O101	0.23313	0.03008	0.73418
O102	0.36288	0.82261	0.74963
O103	0.30827	0.84446	0.92479
O104	0.19144	0.85059	0.0166

O105	0.08372	0.83043	0.90701
O106	0.10666	0.83171	0.71174
O107	0.23308	0.85131	0.76188
O108	0.32529	0.94534	0.79797
O109	0.08661	0.94608	0.80837
O110	0.43478	0.12454	0.57982
O111	0.41909	0.99274	0.56368
O112	0.40075	0.86027	0.56689
O113	0.19766	0.12822	0.60856
O114	0.18177	0.99948	0.55704
O115	0.19477	0.8654	0.57111
O116	0.99078	0.03806	0.78118
O117	0.98575	0.86069	0.78331
O118	0.14397	0.93861	0.22127
O119	0.20152	0.92574	0.39664
O120	0.2994	0.94286	0.53085
O121	0.39631	0.92527	0.39601
O122	0.39628	0.94382	0.19842
O123	0.27135	0.96998	0.24123
O124	0.14238	0.16501	0.24258
O125	0.19839	0.16368	0.41675
O126	0.31227	0.14586	0.51391
O127	0.41517	0.16943	0.39396
O128	0.3967	0.1485	0.20029
O129	0.27131	0.13393	0.25615
O130	0.17965	0.04818	0.32177
O131	0.42051	0.04566	0.32342
O132	0.07054	0.86838	0.096
O133	0.08367	0.99853	0.06516
O134	0.1003	0.1307	0.06144
O135	0.30268	0.86728	0.1205
O136	0.31761	0.99287	0.05734
O137	0.3039	0.12682	0.06214
O138	0.50876	0.94639	0.29142
O139	0.51702	0.13277	0.27878
O140	0.64347	0.55025	0.28187
O141	0.67834	0.57007	0.09342
O142	0.79379	0.55934	-0.00004
O143	0.91442	0.56079	0.08061
O144	0.89334	0.55634	0.27873
O145	0.76822	0.53574	0.22747
O146	0.64517	0.33654	0.27179
O147	0.70618	0.32043	0.10341
O148	0.80951	0.3483	0.98243

O149	0.91844	0.32615	0.09356
O150	0.90753	0.33503	0.29201
O151	0.77266	0.37453	0.25379
O152	0.67732	0.44556	0.16675
O153	0.92109	0.44542	0.17788
O154	0.56847	0.62505	0.40067
O155	0.5801	0.49529	0.43808
O156	0.58627	0.36112	0.4459
O157	0.80004	0.62242	0.37343
O158	0.81331	0.49093	0.4025
O159	0.80984	0.36001	0.44566
O160	0.01364	0.54097	0.20669
O161	0.02269	0.36396	0.20463
O162	0.88725	0.42888	0.73828
O163	0.79328	0.44627	0.5851
O164	0.6967	0.43419	0.44534
O165	0.61566	0.43332	0.60423
O166	0.61178	0.43461	0.79955
O167	0.74674	0.43234	0.78408
O168	0.86597	0.67424	0.73511
O169	0.80675	0.6413	0.56849
O170	0.68911	0.64116	0.4783
O171	0.58238	0.66027	0.59121
O172	0.60615	0.66623	0.78609
O173	0.73254	0.65765	0.7292
O174	0.81511	0.553	0.72109
O175	0.59386	0.54829	0.69729
O176	0.93119	0.37072	0.90767
O177	0.89154	0.49729	0.90931
O178	0.89286	0.63079	0.9198
O179	0.6827	0.36495	0.92311
O180	0.68486	0.49886	0.92922
O181	0.69741	0.63197	0.92071
O182	0.50016	0.45448	0.70306
O183	0.48752	0.62991	0.71888
O184	0.63966	0.92944	0.28826
O185	0.69333	0.92587	0.10744
O186	0.80147	0.94919	0.99408
O187	0.91016	0.92365	0.10171
O188	0.89484	0.94269	0.29733
O189	0.76689	0.96254	0.26052
O190	0.64271	0.16849	0.24974
O191	0.69838	0.14524	0.07644
O192	0.81317	0.14069	0.97911

O193	0.9173	0.16732	0.09406
O194	0.89338	0.14951	0.28885
O195	0.76868	0.12287	0.24348
O196	0.66916	0.04311	0.19678
O197	0.921	0.04557	0.173
O198	0.56734	0.87208	0.42925
O199	0.57961	0.00421	0.43209
O200	0.60229	0.13555	0.43345
O201	0.80594	0.86349	0.38261
O202	0.81801	0.99168	0.43878
O203	0.80564	0.12732	0.43519
O204	0.0133	0.95415	0.21984
O205	0.01532	0.13612	0.21726
O206	0.86052	0.05687	0.77573
O207	0.79754	0.06276	0.60274
O208	0.70043	0.04811	0.46696
O209	0.60464	0.06934	0.6027
O210	0.60697	0.04793	0.79988
O211	0.73302	0.0209	0.76411
O212	0.86061	0.82456	0.75177
O213	0.80781	0.83356	0.57592
O214	0.69267	0.84659	0.48174
O215	0.59258	0.82189	0.60857
O216	0.60745	0.84902	0.80081
O217	0.73162	0.8562	0.73574
O218	0.82555	0.94408	0.68349
O219	0.5839	0.94778	0.67049
O220	0.93475	0.12337	0.90708
O221	0.91789	0.99268	0.93082
O222	0.89545	0.86131	0.93335
O223	0.69922	0.1257	0.87973
O224	0.68401	0.00188	0.94679
O225	0.70487	0.86995	0.93149
O226	0.49326	0.04353	0.70828
O227	0.48802	0.8616	0.71865
O228	0.36979	0.44379	0.71828
O229	0.30905	0.42347	0.88958
O230	0.21244	0.44528	0.02657
O231	0.11756	0.4306	0.89076
O232	0.11177	0.45946	0.695
O233	0.23962	0.4649	0.73491
O234	0.3592	0.65983	0.72317
O235	0.30289	0.67014	0.89888
O236	0.19399	0.64551	0.00749

O237	0.08944	0.67778	0.89432
O238	0.10593	0.65516	0.69802
O239	0.23128	0.62981	0.74375
O240	0.323	0.54883	0.82155
O241	0.09265	0.55488	0.82916
O242	0.43636	0.37181	0.58421
O243	0.4233	0.50243	0.55749
O244	0.41746	0.63578	0.5488
O245	0.19419	0.37023	0.61037
O246	0.19641	0.49586	0.55211
O247	0.19422	0.63061	0.55327
O248	0.00135	0.46346	0.80706
O249	0.98874	0.63425	0.78118
O250	0.14296	0.56042	0.21923
O251	0.21306	0.56542	0.38557
O252	0.30782	0.5632	0.52667
O253	0.40172	0.56523	0.38548
O254	0.40109	0.55864	0.18909
O255	0.2729	0.53281	0.21772
O256	0.14608	0.32687	0.24226
O257	0.20069	0.34129	0.41755
O258	0.31275	0.35471	0.52099
O259	0.41374	0.33184	0.39672
O260	0.39992	0.33169	0.19994
O261	0.27588	0.35346	0.25379
O262	0.18715	0.44751	0.29987
O263	0.41367	0.44712	0.2984
O264	0.07283	0.62079	0.07538
O265	0.09131	0.48952	0.06575
O266	0.11229	0.35838	0.05552
O267	0.31335	0.62335	0.08362
O268	0.33379	0.49146	0.05368
O269	0.30991	0.35826	0.05974
O270	0.51265	0.53663	0.27996
O271	0.51608	0.36241	0.27749
O272	0.44448	0.74689	0.64364
O273	0.19977	0.74528	0.65122
O274	0.2747	0.74784	0.05305
O275	0.11176	0.74679	0.0565
O276	0.06699	0.24703	0.13647
O277	0.30588	0.24243	0.15259
O278	0.23372	0.25025	0.55669
O279	0.39432	0.24918	0.5479
O280	0.56174	0.2479	0.35312

O281	0.79667	0.24014	0.32798
O282	0.73042	0.24322	0.9483
O283	0.8923	0.24668	0.94097
O284	0.93927	0.74675	0.8596
O285	0.69512	0.75358	0.85255
O286	0.77367	0.7419	0.44292
O287	0.60827	0.74657	0.44711
O288	0.91193	0.22995	0.45835
O289	0.83938	0.20694	0.6011
O290	0.88747	0.32125	0.58349
O291	0.96664	0.22577	0.63522
O292	0.04813	0.26983	0.4195
O293	0.02239	0.34715	0.68752
GA29	0.94674	0.38565	0.64108
H295	0.95407	0.24137	0.42575
H296	0.83786	0.34243	0.50518
H297	0.82468	0.17575	0.54755
H298	0.98469	0.53935	0.64171
H299	0.01404	0.29821	0.68045
H300	0.08985	0.54841	0.52969
H301	0.08185	0.57343	0.40389
H302	0.959	0.58498	0.42604
H303	0.0016	0.63086	0.52005
H304	0.90689	0.56109	0.59087
H305	0.97289	0.3914	0.43115
H306	0.0509	0.46498	0.35103
H307	0.89228	0.45103	0.53306
H308	0.09189	0.44103	0.45903
AL30	0.82369	0.32205	0.32193
AL31	0.80517	0.46751	0.70837
P311	0.90683	0.24345	0.57575
C312	0.95541	0.53901	0.57212
C313	0.05703	0.54573	0.46428
C314	0.99149	0.57995	0.49192
C315	0.98697	0.43917	0.46636
C316	0.94446	0.46845	0.534
C317	0.04914	0.47163	0.43294
C318	0.08303	0.25826	0.48537
<b>TS<sub>CO+H2O</sub></b>			
SI2	0.42651	0.05487	0.64181
SI3	0.3061	0.02439	0.78354
SI4	0.28162	0.05778	0.00673
SI5	0.12149	0.06004	0.00807

SI6	0.07049	0.02613	0.79396
SI7	0.18045	0.05299	0.64635
SI8	0.42371	0.82366	0.66843
SI9	0.30684	0.86631	0.80718
SI10	0.26954	0.8275	0.0268
SI11	0.11486	0.82424	0.01679
SI12	0.06546	0.86761	0.80114
SI13	0.18366	0.82376	0.67317
SI14	0.07869	0.94051	0.1494
SI15	0.19947	0.97067	0.29431
SI16	0.21957	0.93255	0.51281
SI17	0.37886	0.9306	0.51294
SI18	0.43144	0.96593	0.30206
SI19	0.32171	0.94345	0.1527
SI20	0.08085	0.16832	0.16323
SI21	0.19929	0.12703	0.30697
SI22	0.23606	0.17181	0.52199
SI23	0.39001	0.17211	0.50762
SI24	0.4389	0.12417	0.2981
SI25	0.32073	0.16296	0.16696
SI26	0.57806	0.55075	0.34995
SI27	0.6924	0.5241	0.1916
SI28	0.71348	0.56525	0.9834
SI29	0.873	0.56226	0.97865
SI30	0.93516	0.52569	0.18642
SI31	0.81699	0.55153	0.32122
SI32	0.57916	0.32736	0.33629
SI33	0.70304	0.36989	0.20001
SI34	0.73315	0.32006	0.98977
SI35	0.88735	0.32261	0.98571
SI36	0.94167	0.36717	0.19604
SI37	0.92758	0.43814	0.8483
SI38	0.7761	0.43642	0.47509
SI39	0.61927	0.43113	0.48749
SI40	0.57747	0.46741	0.70432
SI41	0.68071	0.43343	0.85836
SI42	0.92154	0.67026	0.8229
SI43	0.80439	0.62899	0.69095
SI44	0.76818	0.66163	0.46881
SI45	0.61268	0.6679	0.47941
SI46	0.56752	0.62512	0.69813
SI47	0.68314	0.6767	0.82126
SI48	0.57546	0.93885	0.35937
SI49	0.69336	0.9667	0.2135

SI50	0.7214	0.93728	0.99439
SI51	0.88106	0.93136	0.98882
SI52	0.93453	0.96629	0.19819
SI53	0.82111	0.93883	0.34469
SI54	0.58246	0.1715	0.32831
SI55	0.6968	0.12214	0.19118
SI56	0.7354	0.1646	0.97161
SI57	0.88913	0.16899	0.98286
SI58	0.93622	0.12395	0.1957
SI59	0.8173	0.16304	0.32579
SI60	0.92554	0.05292	0.8494
SI61	0.8053	0.0217	0.70844
SI62	0.77995	0.05527	0.48489
SI63	0.62178	0.06396	0.48438
SI64	0.57207	0.02712	0.69482
SI65	0.68151	0.04996	0.84766
SI66	0.92093	0.82304	0.83227
SI67	0.80616	0.86548	0.68905
SI68	0.77036	0.82113	0.47215
SI69	0.61564	0.82161	0.49179
SI70	0.56754	0.87032	0.69883
SI71	0.68448	0.83275	0.82916
SI72	0.43093	0.44347	0.64116
SI73	0.31073	0.47059	0.79068
SI74	0.29104	0.42994	0.00754
SI75	0.1331	0.43054	0.01005
SI76	0.07957	0.47349	0.8055
SI77	0.18584	0.44648	0.65064
SI78	0.42712	0.66842	0.65893
SI79	0.30525	0.62674	0.79715
SI80	0.27163	0.6717	0.01124
SI81	0.11744	0.67169	0.00733
SI82	0.06865	0.62895	0.7994
SI83	0.18365	0.66561	0.66245
SI84	0.08113	0.55257	0.14157
SI85	0.20485	0.5256	0.27959
SI86	0.22852	0.56276	0.50518
SI87	0.38782	0.5655	0.50364
SI88	0.43377	0.5259	0.28931
SI89	0.32976	0.55217	0.13611
SI90	0.08712	0.32343	0.16027
SI91	0.20357	0.36624	0.30284
SI92	0.23614	0.3287	0.52608
SI93	0.39	0.32661	0.51123

SI94	0.43693	0.36857	0.29359
SI95	0.32327	0.32112	0.16611
O96	0.36207	0.06081	0.71483
O97	0.30337	0.06253	0.89049
O98	0.20143	0.04894	0.01933
O99	0.10052	0.06405	0.89169
O100	0.10626	0.05521	0.69426
O101	0.23311	0.02975	0.73194
O102	0.36263	0.82269	0.74818
O103	0.30849	0.84435	0.92358
O104	0.19188	0.85077	0.01565
O105	0.08433	0.83091	0.90551
O106	0.10659	0.83181	0.71025
O107	0.23296	0.85142	0.76093
O108	0.32521	0.9455	0.79702
O109	0.08603	0.94625	0.80578
O110	0.43507	0.12443	0.57914
O111	0.4189	0.99279	0.56357
O112	0.40062	0.86039	0.56551
O113	0.19794	0.12763	0.60564
O114	0.18131	0.99865	0.55547
O115	0.19532	0.8647	0.56969
O116	0.99121	0.03956	0.78145
O117	0.98562	0.86005	0.78229
O118	0.14433	0.93939	0.21968
O119	0.20151	0.92505	0.39502
O120	0.29938	0.94297	0.52893
O121	0.39689	0.92594	0.39499
O122	0.39685	0.94426	0.19733
O123	0.27188	0.96976	0.24023
O124	0.14326	0.16381	0.23977
O125	0.199	0.16458	0.41447
O126	0.31284	0.14579	0.51169
O127	0.41642	0.16972	0.39322
O128	0.3978	0.14899	0.19963
O129	0.27233	0.13395	0.25493
O130	0.18108	0.04811	0.32194
O131	0.42232	0.04601	0.32214
O132	0.07116	0.86789	0.09525
O133	0.08369	0.99788	0.06297
O134	0.09905	0.1302	0.05966
O135	0.30339	0.86726	0.11945
O136	0.31789	0.99262	0.05594
O137	0.30532	0.12657	0.06114

O138	0.50945	0.94583	0.29027
O139	0.51833	0.13371	0.27808
O140	0.6446	0.54819	0.28237
O141	0.67875	0.57055	0.09354
O142	0.79383	0.55949	0.99844
O143	0.91335	0.56288	0.08378
O144	0.89395	0.55517	0.28163
O145	0.76934	0.53688	0.22629
O146	0.64627	0.33799	0.27277
O147	0.70731	0.31952	0.10436
O148	0.81006	0.34868	0.98269
O149	0.91686	0.32493	0.09841
O150	0.909	0.33795	0.29675
O151	0.77422	0.37422	0.25385
O152	0.6797	0.44538	0.16499
O153	0.92278	0.44579	0.17625
O154	0.56967	0.62504	0.3987
O155	0.58083	0.49592	0.4403
O156	0.58639	0.36185	0.44642
O157	0.80047	0.6231	0.37355
O158	0.81079	0.4913	0.40245
O159	0.80924	0.36042	0.44822
O160	0.01406	0.54177	0.2082
O161	0.02334	0.36337	0.20547
O162	0.88218	0.42648	0.74619
O163	0.79617	0.44791	0.58796
O164	0.69694	0.43454	0.45286
O165	0.61216	0.43235	0.60751
O166	0.60749	0.43435	0.80447
O167	0.74071	0.43268	0.78038
O168	0.86611	0.67397	0.73501
O169	0.80697	0.63811	0.56944
O170	0.68962	0.64144	0.47884
O171	0.58192	0.6586	0.59002
O172	0.60613	0.66686	0.78479
O173	0.73256	0.65875	0.72855
O174	0.81381	0.5532	0.72756
O175	0.5927	0.54775	0.69975
O176	0.93311	0.36969	0.91282
O177	0.89385	0.49617	0.91464
O178	0.89398	0.62996	0.91966
O179	0.68242	0.36565	0.92563
O180	0.68389	0.49952	0.92958
O181	0.6971	0.63235	0.9201

O182	0.4974	0.45514	0.70652
O183	0.48722	0.63031	0.71846
O184	0.64058	0.93084	0.28835
O185	0.69402	0.92707	0.10746
O186	0.80183	0.94836	0.99224
O187	0.90996	0.92376	0.10139
O188	0.89561	0.94107	0.29751
O189	0.76807	0.96267	0.26022
O190	0.64402	0.16969	0.24995
O191	0.69856	0.14647	0.07603
O192	0.81302	0.14021	0.97861
O193	0.91547	0.16693	0.09756
O194	0.89481	0.14844	0.29315
O195	0.7703	0.12563	0.24239
O196	0.67119	0.04449	0.19743
O197	0.92084	0.04511	0.17496
O198	0.56828	0.872	0.42819
O199	0.57881	0.00444	0.4319
O200	0.60355	0.1354	0.43294
O201	0.80585	0.86273	0.38221
O202	0.81856	0.99088	0.43857
O203	0.80419	0.12647	0.43565
O204	0.01364	0.9537	0.21866
O205	0.01569	0.13549	0.21723
O206	0.86092	0.05866	0.77674
O207	0.7982	0.06088	0.60254
O208	0.70026	0.04609	0.46814
O209	0.60419	0.06961	0.60247
O210	0.60712	0.04781	0.79963
O211	0.73343	0.02182	0.76414
O212	0.86022	0.82323	0.75276
O213	0.80847	0.83645	0.5764
O214	0.69304	0.84587	0.48239
O215	0.59224	0.82186	0.60808
O216	0.60712	0.8493	0.80015
O217	0.73172	0.85689	0.73638
O218	0.82742	0.94428	0.68891
O219	0.58366	0.94791	0.66977
O220	0.93548	0.12251	0.91122
O221	0.9185	0.99155	0.92923
O222	0.89657	0.86037	0.93379
O223	0.69879	0.12652	0.87934
O224	0.68467	0.00273	0.94672
O225	0.70355	0.87049	0.93187

O226	0.49313	0.04354	0.70836
O227	0.48769	0.86171	0.71766
O228	0.36706	0.44302	0.71521
O229	0.30978	0.42375	0.88998
O230	0.21208	0.44608	0.02504
O231	0.11578	0.42917	0.89161
O232	0.1112	0.45712	0.69592
O233	0.23825	0.46576	0.73751
O234	0.35913	0.66053	0.72324
O235	0.30436	0.6693	0.90029
O236	0.19456	0.64518	0.00713
O237	0.09005	0.67607	0.89312
O238	0.10639	0.65297	0.69706
O239	0.23166	0.6303	0.74538
O240	0.32401	0.54878	0.82064
O241	0.09104	0.55292	0.82844
O242	0.43652	0.3716	0.58429
O243	0.42389	0.50207	0.55706
O244	0.41626	0.63546	0.54875
O245	0.1958	0.36988	0.6119
O246	0.19463	0.49586	0.55406
O247	0.19564	0.63007	0.55399
O248	-0.00001	0.46002	0.80585
O249	0.98884	0.63368	0.77939
O250	0.14362	0.56003	0.21878
O251	0.21079	0.56342	0.38689
O252	0.30796	0.56048	0.52523
O253	0.40245	0.56507	0.38509
O254	0.40213	0.5583	0.18883
O255	0.2742	0.53306	0.22014
O256	0.14641	0.32515	0.24343
O257	0.20015	0.34234	0.41862
O258	0.31324	0.35453	0.51953
O259	0.41464	0.33162	0.39643
O260	0.40049	0.33169	0.19963
O261	0.27655	0.35205	0.25521
O262	0.1873	0.44651	0.2975
O263	0.41396	0.44685	0.29826
O264	0.07346	0.62062	0.07534
O265	0.0908	0.48913	0.06631
O266	0.11359	0.35807	0.05725
O267	0.31332	0.62403	0.08613
O268	0.33315	0.49235	0.05383
O269	0.30948	0.35923	0.06091

O270	0.51366	0.53552	0.28047
O271	0.51685	0.36242	0.27721
O272	0.44413	0.74699	0.64204
O273	0.19928	0.74496	0.65115
O274	0.27477	0.74803	0.05255
O275	0.11219	0.74658	0.05414
O276	0.06718	0.24645	0.13598
O277	0.30672	0.2424	0.15088
O278	0.23422	0.25	0.55575
O279	0.39455	0.249	0.54747
O280	0.56311	0.2485	0.35373
O281	0.80003	0.24092	0.33213
O282	0.73134	0.24387	0.9473
O283	0.8927	0.24615	0.9442
O284	0.9401	0.74592	0.85919
O285	0.69476	0.75409	0.85254
O286	0.77544	0.74164	0.44768
O287	0.60818	0.74628	0.44729
O288	0.9114	0.22482	0.47285
O289	0.83836	0.19859	0.61412
O290	0.87545	0.31643	0.5926
O291	0.96232	0.23035	0.65205
O292	0.0486	0.25825	0.41827
O293	0.01608	0.35755	0.64892
GA29	0.93018	0.39253	0.62754
H295	0.95453	0.23589	0.44319
H296	0.83344	0.33895	0.51018
H297	0.82294	0.17161	0.55655
H298	0.97826	0.53229	0.63701
H299	1.01201	0.30792	0.65441
H300	0.08942	0.56012	0.5342
H301	0.08212	0.58152	0.4092
H302	0.95792	0.58547	0.42411
H303	0.99136	0.63025	0.52706
H304	0.90097	0.55034	0.58126
H305	1.00477	0.393	0.42179
H306	0.10397	0.46204	0.40836
H307	0.90689	0.45815	0.46633
H308	0.03786	0.40224	0.53858
AL30	0.82511	0.32342	0.32508
AL31	0.80312	0.4679	0.71237
P311	0.90229	0.24133	0.5893
C312	0.95145	0.53198	0.56503
C313	0.05614	0.55327	0.4685

C314	0.98673	0.58004	0.49352
C315	0.01028	0.43524	0.47502
C316	0.94648	0.46073	0.52248
C317	0.05962	0.48146	0.44631
C318	0.0837	0.25276	0.48557

### C<sub>6</sub>H<sub>9</sub>Ga-H<sub>2</sub>O+CO

SI2	0.42674	0.05479	0.64182
SI3	0.30613	0.02452	0.78294
SI4	0.28194	0.05779	0.00652
SI5	0.12171	0.06003	0.00743
SI6	0.07085	0.02652	0.79318
SI7	0.18062	0.05289	0.64514
SI8	0.42356	0.82371	0.66761
SI9	0.30696	0.86663	0.80673
SI10	0.26991	0.8277	0.02621
SI11	0.11542	0.82425	0.01564
SI12	0.06561	0.86765	0.79989
SI13	0.18417	0.82411	0.67277
SI14	0.07926	0.9403	0.14819
SI15	0.20002	0.97057	0.29362
SI16	0.21984	0.93243	0.51181
SI17	0.37915	0.93076	0.51209
SI18	0.43217	0.96602	0.3012
SI19	0.32219	0.94326	0.1522
SI20	0.08098	0.16812	0.16253
SI21	0.20023	0.12689	0.30558
SI22	0.23684	0.17153	0.52041
SI23	0.3909	0.17203	0.50727
SI24	0.44001	0.12427	0.29774
SI25	0.32204	0.16293	0.16602
SI26	0.57817	0.5514	0.34871
SI27	0.69196	0.52444	0.18965
SI28	0.7138	0.56466	0.98135
SI29	0.87293	0.56115	0.97731
SI30	0.93581	0.5257	0.18646
SI31	0.81663	0.55289	0.31868
SI32	0.57949	0.32764	0.336
SI33	0.70216	0.36993	0.19759
SI34	0.73295	0.31972	0.98848
SI35	0.88742	0.32267	0.98588
SI36	0.94285	0.36695	0.197
SI37	0.92692	0.43759	0.84627
SI38	0.77638	0.43799	0.47333

SI39	0.6185	0.43207	0.48768
SI40	0.57561	0.46737	0.70509
SI41	0.68134	0.43282	0.85501
SI42	0.92237	0.66907	0.82185
SI43	0.80487	0.62902	0.68945
SI44	0.76812	0.66194	0.46806
SI45	0.61268	0.66805	0.4789
SI46	0.56709	0.62524	0.69767
SI47	0.68366	0.67676	0.81974
SI48	0.57594	0.93899	0.35917
SI49	0.69425	0.96714	0.21428
SI50	0.72173	0.93691	0.99445
SI51	0.88173	0.93049	0.98834
SI52	0.93505	0.96632	0.19823
SI53	0.82205	0.93877	0.3451
SI54	0.58337	0.17185	0.32883
SI55	0.6973	0.12276	0.19153
SI56	0.73549	0.16422	0.9717
SI57	0.889	0.16879	0.9847
SI58	0.93647	0.1241	0.19734
SI59	0.81774	0.16289	0.32734
SI60	0.92591	0.05306	0.85035
SI61	0.80607	0.02147	0.70957
SI62	0.78041	0.05467	0.48592
SI63	0.62221	0.06378	0.48469
SI64	0.57216	0.02691	0.69496
SI65	0.68183	0.04971	0.84766
SI66	0.92164	0.822	0.83246
SI67	0.80644	0.86532	0.69075
SI68	0.77059	0.82153	0.47322
SI69	0.6159	0.82183	0.49188
SI70	0.56742	0.87018	0.69874
SI71	0.68413	0.83257	0.82988
SI72	0.4299	0.44332	0.64218
SI73	0.30936	0.4701	0.79123
SI74	0.29117	0.43099	0.00834
SI75	0.13327	0.43117	0.01195
SI76	0.07932	0.47243	0.80598
SI77	0.18501	0.4448	0.65268
SI78	0.42677	0.66854	0.65857
SI79	0.30525	0.62673	0.79718
SI80	0.27238	0.67182	0.01097
SI81	0.11825	0.67112	0.00645
SI82	0.06963	0.62837	0.79686

SI83	0.18458	0.66627	0.6621
SI84	0.08163	0.55313	0.14327
SI85	0.20508	0.52507	0.28054
SI86	0.22843	0.56201	0.5072
SI87	0.38788	0.56484	0.50413
SI88	0.43406	0.52616	0.2892
SI89	0.32981	0.55308	0.13735
SI90	0.08822	0.32291	0.16129
SI91	0.20391	0.36534	0.30339
SI92	0.23697	0.32846	0.52578
SI93	0.39097	0.32656	0.51115
SI94	0.43746	0.36873	0.2931
SI95	0.32343	0.32085	0.16675
O96	0.36223	0.06114	0.71463
O97	0.30285	0.06247	0.88994
O98	0.20169	0.05038	0.02064
O99	0.10188	0.06399	0.89056
O100	0.10643	0.05578	0.6933
O101	0.23328	0.02992	0.73082
O102	0.36244	0.82289	0.74728
O103	0.30897	0.84475	0.92312
O104	0.19231	0.85128	0.01506
O105	0.08492	0.83138	0.90437
O106	0.10688	0.83228	0.70889
O107	0.23285	0.85236	0.761
O108	0.3256	0.94578	0.79634
O109	0.08543	0.94652	0.80422
O110	0.43566	0.12428	0.57908
O111	0.41909	0.99277	0.56351
O112	0.40058	0.86046	0.56462
O113	0.19817	0.12735	0.60357
O114	0.18118	0.99826	0.55477
O115	0.19618	0.86465	0.56906
O116	0.99161	0.04101	0.78185
O117	0.98578	0.85933	0.78141
O118	0.14499	0.93988	0.21827
O119	0.20149	0.92476	0.39414
O120	0.29965	0.94346	0.52727
O121	0.39769	0.92621	0.39429
O122	0.39747	0.94457	0.19642
O123	0.2726	0.96948	0.24006
O124	0.14413	0.16272	0.23746
O125	0.19982	0.16493	0.41281
O126	0.31367	0.14571	0.5108

O127	0.4176	0.16964	0.39306
O128	0.39906	0.14931	0.19938
O129	0.27333	0.134	0.25375
O130	0.18221	0.04805	0.32184
O131	0.42336	0.04611	0.32139
O132	0.07162	0.86749	0.09467
O133	0.08421	0.99716	0.06097
O134	0.09741	0.12967	0.05856
O135	0.30401	0.86704	0.11911
O136	0.31768	0.99215	0.05516
O137	0.30726	0.1261	0.0604
O138	0.5102	0.94581	0.28946
O139	0.51953	0.13388	0.2782
O140	0.64454	0.54869	0.28074
O141	0.6779	0.5699	0.0907
O142	0.79393	0.55954	-0.0014
O143	0.91434	0.5599	0.0811
O144	0.89306	0.55705	0.27855
O145	0.76881	0.53754	0.22407
O146	0.64687	0.33824	0.27293
O147	0.70465	0.31958	0.10184
O148	0.80994	0.34829	0.98408
O149	0.91819	0.32636	0.09743
O150	0.90917	0.3352	0.29567
O151	0.77439	0.37332	0.24861
O152	0.67914	0.44557	0.1638
O153	0.92338	0.44555	0.1804
O154	0.57002	0.62579	0.39713
O155	0.5809	0.49682	0.43941
O156	0.58668	0.36258	0.44569
O157	0.79945	0.62413	0.37153
O158	0.81023	0.49241	0.39982
O159	0.80783	0.36147	0.44385
O160	0.01394	0.54345	0.20794
O161	0.02422	0.36257	0.20567
O162	0.8829	0.4258	0.74245
O163	0.80057	0.44716	0.58506
O164	0.69681	0.43625	0.45614
O165	0.60916	0.43257	0.60723
O166	0.60735	0.43397	0.80379
O167	0.7404	0.43174	0.7751
O168	0.86719	0.67305	0.73359
O169	0.80729	0.63775	0.56796
O170	0.68962	0.64166	0.47893

O171	0.58135	0.65791	0.58898
O172	0.60669	0.66708	0.78314
O173	0.73345	0.66002	0.727
O174	0.8127	0.55306	0.72634
O175	0.59134	0.54758	0.70042
O176	0.93206	0.36896	0.91022
O177	0.89147	0.4951	0.91123
O178	0.89427	0.62877	0.9183
O179	0.68353	0.36487	0.92174
O180	0.68574	0.49858	0.92662
O181	0.69762	0.63155	0.91761
O182	0.49549	0.45492	0.71007
O183	0.48701	0.63111	0.71881
O184	0.64141	0.93112	0.28877
O185	0.69504	0.92789	0.10805
O186	0.80229	0.94666	0.99028
O187	0.90992	0.92415	0.10144
O188	0.89649	0.94063	0.29769
O189	0.76901	0.96305	0.26086
O190	0.64498	0.17066	0.25045
O191	0.69842	0.14646	0.0761
O192	0.81301	0.13969	0.97959
O193	0.91465	0.16728	0.09979
O194	0.89533	0.14832	0.29543
O195	0.77107	0.12738	0.24204
O196	0.67218	0.04509	0.19916
O197	0.92102	0.04531	0.17637
O198	0.56865	0.87225	0.42813
O199	0.57904	0.00471	0.43154
O200	0.60493	0.13543	0.43306
O201	0.80632	0.86298	0.38326
O202	0.81974	0.99113	0.43872
O203	0.80347	0.12645	0.43693
O204	0.01428	0.9539	0.21753
O205	0.01591	0.13599	0.21788
O206	0.86125	0.05938	0.77769
O207	0.79931	0.06028	0.60326
O208	0.70071	0.04514	0.4697
O209	0.60411	0.06958	0.6026
O210	0.60743	0.04742	0.79975
O211	0.73384	0.0219	0.76409
O212	0.8601	0.82245	0.75424
O213	0.80843	0.83703	0.57765
O214	0.69327	0.84636	0.48292

O215	0.59227	0.8218	0.60803
O216	0.60689	0.84899	0.80006
O217	0.73191	0.85736	0.73804
O218	0.82846	0.94401	0.6915
O219	0.58383	0.94775	0.66982
O220	0.93565	0.12206	0.91383
O221	0.91897	0.99071	0.92839
O222	0.89835	0.85927	0.93471
O223	0.69892	0.12633	0.87931
O224	0.68552	0.00269	0.94683
O225	0.70211	0.8701	0.93325
O226	0.49325	0.04333	0.70867
O227	0.48752	0.86176	0.71703
O228	0.36417	0.44266	0.71282
O229	0.31128	0.42386	0.89126
O230	0.21218	0.4482	0.02278
O231	0.11357	0.42885	0.89424
O232	0.10873	0.447	0.6979
O233	0.23514	0.46408	0.74304
O234	0.35881	0.66055	0.72277
O235	0.30607	0.6689	0.90068
O236	0.19549	0.6451	0.0056
O237	0.09029	0.67391	0.89251
O238	0.10701	0.65475	0.69592
O239	0.2313	0.63113	0.747
O240	0.3233	0.54842	0.81934
O241	0.09375	0.5518	0.82086
O242	0.43679	0.37151	0.58525
O243	0.42495	0.502	0.55794
O244	0.41606	0.63513	0.54875
O245	0.19723	0.36863	0.61331
O246	0.19447	0.49694	0.56087
O247	0.19857	0.63119	0.55426
O248	-0.00063	0.46102	0.80548
O249	0.98957	0.63204	0.77885
O250	0.14444	0.56026	0.2195
O251	0.21112	0.56072	0.38912
O252	0.30829	0.55843	0.52577
O253	0.40323	0.56465	0.38575
O254	0.40247	0.5591	0.18925
O255	0.27476	0.53455	0.22191
O256	0.14694	0.32311	0.24517
O257	0.20007	0.34293	0.41978
O258	0.31404	0.35393	0.5189

O259	0.41612	0.33201	0.39665
O260	0.40081	0.3318	0.19942
O261	0.27726	0.34882	0.25823
O262	0.18947	0.44527	0.29267
O263	0.41465	0.44698	0.29751
O264	0.07469	0.6207	0.07567
O265	0.09068	0.48923	0.06825
O266	0.11596	0.35828	0.05952
O267	0.31374	0.62496	0.08721
O268	0.33318	0.49327	0.0549
O269	0.30799	0.36043	0.06331
O270	0.51392	0.53576	0.27943
O271	0.51737	0.36219	0.27607
O272	0.44391	0.74707	0.6412
O273	0.20067	0.74559	0.65154
O274	0.27491	0.7483	0.05163
O275	0.11287	0.74644	0.05174
O276	0.06799	0.24624	0.13486
O277	0.30813	0.24215	0.14845
O278	0.2343	0.24957	0.55489
O279	0.39557	0.24886	0.5471
O280	0.56392	0.24876	0.35463
O281	0.80216	0.24098	0.33786
O282	0.73187	0.24337	0.94673
O283	0.89264	0.24584	0.94546
O284	0.94094	0.74474	0.85836
O285	0.69483	0.75393	0.85278
O286	0.77545	0.74212	0.44869
O287	0.60854	0.74655	0.44736
O288	0.91904	0.21264	0.48419
O289	0.83492	0.19926	0.6152
O290	0.88148	0.31573	0.58253
O291	0.9537	0.22905	0.66983
O292	0.05433	0.25058	0.41525
O293	0.00207	0.34037	0.68946
GA29	0.93278	0.3947	0.624
H295	0.94595	0.24108	0.44058
H296	0.83293	0.34019	0.50291
H297	0.81799	0.17456	0.55601
H298	0.97034	0.53423	0.6337
H299	-0.01238	0.28712	0.6849
H300	0.08458	0.56716	0.54882
H301	0.08291	0.59272	0.42324
H302	0.9607	0.58588	0.41873

H303	0.98305	0.63237	0.52666
H304	0.8958	0.54646	0.56635
H305	1.01903	0.39236	0.43075
H306	0.10665	0.47211	0.40481
H307	0.90975	0.45072	0.46504
H308	0.04826	0.34982	0.67059
AL30	0.82469	0.32361	0.32141
AL31	0.80369	0.4679	0.70982
P311	0.90028	0.23937	0.59252
C312	0.94834	0.53183	0.55826
C313	0.05751	0.56023	0.47782
C314	0.98518	0.58223	0.49203
C315	1.01442	0.4429	0.46221
C316	0.95176	0.45997	0.51614
C317	0.06255	0.48824	0.44562
C318	0.07996	0.25735	0.49103
<b>C<sub>6</sub>H<sub>8</sub>+Ga(H)+CO<sub>2</sub></b>			
SI2	0.42696	0.05451	0.64388
SI3	0.3054	0.02237	0.78274
SI4	0.28327	0.05226	0.00883
SI5	0.12334	0.05756	0.01019
SI6	0.0718	0.02497	0.79602
SI7	0.17943	0.05364	0.64623
SI8	0.42169	0.82187	0.67165
SI9	0.3046	0.86402	0.80804
SI10	0.26971	0.82589	0.02932
SI11	0.11506	0.82247	0.01777
SI12	0.0658	0.86668	0.80153
SI13	0.182	0.82176	0.67367
SI14	0.07798	0.93845	0.15033
SI15	0.19953	0.96858	0.29469
SI16	0.21897	0.93221	0.51441
SI17	0.37838	0.9309	0.51554
SI18	0.43288	0.96497	0.30636
SI19	0.32366	0.93908	0.15596
SI20	0.08317	0.16692	0.16295
SI21	0.20194	0.12564	0.3052
SI22	0.23666	0.17132	0.52096
SI23	0.3903	0.1714	0.5103
SI24	0.43984	0.12308	0.30123
SI25	0.32418	0.15938	0.16533
SI26	0.5773	0.55999	0.33533
SI27	0.68507	0.53006	0.1775

SI28	0.7127	0.55074	0.96109
SI29	0.87054	0.55854	0.96668
SI30	0.92958	0.52579	0.17714
SI31	0.80789	0.55843	0.30365
SI32	0.58127	0.32704	0.32378
SI33	0.69384	0.37152	0.17776
SI34	0.72742	0.32083	0.96735
SI35	0.8816	0.3195	0.98091
SI36	0.93595	0.36715	0.1887
SI37	0.92327	0.43209	0.83868
SI38	0.77503	0.44321	0.46687
SI39	0.6173	0.43823	0.48128
SI40	0.5645	0.46795	0.69765
SI41	0.67918	0.42513	0.82148
SI42	0.91755	0.66925	0.81634
SI43	0.80447	0.63087	0.67824
SI44	0.76492	0.66403	0.46026
SI45	0.60992	0.66997	0.47595
SI46	0.56439	0.62459	0.69429
SI47	0.68401	0.67245	0.81006
SI48	0.57889	0.93961	0.36511
SI49	0.69689	0.96274	0.22205
SI50	0.72269	0.92962	0.99909
SI51	0.88254	0.92679	0.99751
SI52	0.93309	0.96686	0.20714
SI53	0.8237	0.94207	0.36038
SI54	0.58174	0.17173	0.34018
SI55	0.69952	0.11838	0.20837
SI56	0.73345	0.16133	0.98639
SI57	0.88739	0.16621	0.98782
SI58	0.93873	0.12446	0.19932
SI59	0.82259	0.16402	0.33396
SI60	0.92665	0.04766	0.85909
SI61	0.80359	0.02119	0.71513
SI62	0.78512	0.06436	0.49697
SI63	0.62496	0.06806	0.49309
SI64	0.57221	0.02363	0.70261
SI65	0.67937	0.04612	0.85758
SI66	0.92221	0.82241	0.84098
SI67	0.80186	0.86461	0.69958
SI68	0.77018	0.82152	0.48341
SI69	0.61602	0.82354	0.50001
SI70	0.5666	0.86585	0.70863
SI71	0.68219	0.82607	0.84001

SI72	0.42265	0.44381	0.6429
SI73	0.30556	0.47005	0.79562
SI74	0.28729	0.42811	0.01017
SI75	0.12943	0.42875	0.00898
SI76	0.07398	0.46487	0.80001
SI77	0.18594	0.44374	0.65644
SI78	0.42468	0.66712	0.65636
SI79	0.30181	0.62551	0.79326
SI80	0.27045	0.67077	0.00517
SI81	0.11621	0.66827	0.00422
SI82	0.06431	0.62331	0.79516
SI83	0.17997	0.66331	0.65987
SI84	0.07704	0.55031	0.14092
SI85	0.20177	0.52461	0.27879
SI86	0.22581	0.56178	0.50636
SI87	0.38549	0.56472	0.50101
SI88	0.43201	0.52642	0.28616
SI89	0.32646	0.55331	0.13512
SI90	0.08409	0.32209	0.16095
SI91	0.19995	0.36337	0.30463
SI92	0.23787	0.32897	0.52401
SI93	0.39191	0.32628	0.51056
SI94	0.43744	0.36821	0.29176
SI95	0.31983	0.31665	0.16759
O96	0.36253	0.05947	0.71704
O97	0.30324	0.05686	0.8921
O98	0.20298	0.04542	0.02431
O99	0.10407	0.06147	0.89309
O100	0.10534	0.05616	0.69571
O101	0.23271	0.03161	0.73154
O102	0.36074	0.81931	0.7515
O103	0.30692	0.8459	0.92581
O104	0.19188	0.84953	0.02253
O105	0.08693	0.83063	0.90524
O106	0.10454	0.83082	0.70865
O107	0.23058	0.84733	0.76386
O108	0.32261	0.94277	0.79083
O109	0.08742	0.94508	0.8039
O110	0.43594	0.12463	0.58263
O111	0.41897	0.99363	0.56372
O112	0.39923	0.8618	0.57135
O113	0.19621	0.12812	0.6039
O114	0.17989	0.99795	0.55713
O115	0.1962	0.8641	0.57207

O116	0.99197	0.0377	0.78914
O117	0.98551	0.85922	0.78686
O118	0.14342	0.93754	0.2212
O119	0.20042	0.92427	0.39683
O120	0.2988	0.94403	0.5291
O121	0.39786	0.92437	0.39824
O122	0.39875	0.94204	0.2016
O123	0.2723	0.96518	0.24165
O124	0.14671	0.16314	0.23725
O125	0.20201	0.16309	0.41237
O126	0.31348	0.14435	0.51661
O127	0.41539	0.16855	0.3952
O128	0.40113	0.14724	0.2005
O129	0.27529	0.13196	0.2538
O130	0.18277	0.04682	0.31953
O131	0.42266	0.04503	0.32514
O132	0.07026	0.86574	0.09584
O133	0.08367	0.9961	0.06421
O134	0.10071	0.1284	0.05936
O135	0.30628	0.86252	0.12284
O136	0.31917	0.98669	0.05746
O137	0.30997	0.12023	0.0616
O138	0.51191	0.94792	0.29838
O139	0.51965	0.13365	0.28495
O140	0.63772	0.56907	0.25651
O141	0.67123	0.55761	0.06536
O142	0.792	0.54622	0.98551
O143	0.91062	0.56116	0.0715
O144	0.88462	0.55805	0.26584
O145	0.76198	0.5484	0.20538
O146	0.64362	0.32709	0.24726
O147	0.68496	0.34637	0.06312
O148	0.80501	0.34642	0.97431
O149	0.90906	0.32334	0.0944
O150	0.90188	0.33781	0.29055
O151	0.76972	0.36121	0.21354
O152	0.67101	0.45	0.18676
O153	0.91631	0.44537	0.16911
O154	0.5662	0.63159	0.39113
O155	0.59219	0.50299	0.41893
O156	0.59947	0.36878	0.4245
O157	0.79409	0.62901	0.35998
O158	0.79143	0.49651	0.38003
O159	0.7934	0.36656	0.42282

O160	0.00752	0.54174	0.20159
O161	0.01676	0.3606	0.19659
O162	0.87215	0.42011	0.74235
O163	0.82108	0.45104	0.56601
O164	0.69742	0.44515	0.49654
O165	0.58145	0.43607	0.58893
O166	0.60129	0.42666	0.78569
O167	0.7279	0.43863	0.72885
O168	0.86519	0.67646	0.72418
O169	0.80704	0.63756	0.55643
O170	0.68681	0.64293	0.47431
O171	0.5775	0.65498	0.58396
O172	0.60628	0.66767	0.77569
O173	0.73242	0.6621	0.71344
O174	0.81344	0.55474	0.71512
O175	0.58759	0.5465	0.70004
O176	0.92741	0.36564	0.90767
O177	0.89901	0.49629	0.90088
O178	0.88356	0.62874	0.90869
O179	0.69278	0.35074	0.86788
O180	0.689	0.48196	0.90811
O181	0.69901	0.61692	0.8947
O182	0.48445	0.46171	0.71627
O183	0.48503	0.63187	0.7192
O184	0.64166	0.92517	0.29112
O185	0.702	0.92439	0.11567
O186	0.80283	0.93949	0.98385
O187	0.90144	0.924	0.11518
O188	0.89798	0.94543	0.31183
O189	0.76977	0.95963	0.27411
O190	0.6475	0.16433	0.27059
O191	0.70157	0.14693	0.09546
O192	0.81128	0.13703	0.98754
O193	0.91619	0.16684	0.10116
O194	0.8993	0.15302	0.29633
O195	0.77303	0.12105	0.26086
O196	0.67446	0.04067	0.20704
O197	0.92037	0.04583	0.1829
O198	0.5688	0.87601	0.43985
O199	0.59075	0.00653	0.43227
O200	0.59592	0.13855	0.44973
O201	0.8115	0.86723	0.40449
O202	0.81809	0.99698	0.45013
O203	0.81966	0.13207	0.44878

O204	0.01246	0.95176	0.21877
O205	0.01862	0.13315	0.21749
O206	0.86122	0.04934	0.78831
O207	0.80198	0.06796	0.61534
O208	0.70541	0.06493	0.47591
O209	0.60778	0.06416	0.61123
O210	0.60517	0.04509	0.80879
O211	0.7319	0.0253	0.77045
O212	0.85745	0.83104	0.77059
O213	0.8045	0.82601	0.59314
O214	0.69341	0.84872	0.49132
O215	0.59307	0.81962	0.6163
O216	0.60469	0.84208	0.81022
O217	0.72855	0.85674	0.75058
O218	0.8182	0.9439	0.68292
O219	0.58317	0.94381	0.68258
O220	0.93372	0.11884	0.91762
O221	0.92239	0.98724	0.94103
O222	0.90612	0.85552	0.9496
O223	0.69365	0.12093	0.89981
O224	0.68393	0.99323	0.94976
O225	0.69964	0.86032	0.94645
O226	0.49341	0.04179	0.71029
O227	0.48644	0.857	0.72365
O228	0.35512	0.44287	0.70937
O229	0.31177	0.42301	0.89448
O230	0.20829	0.44687	0.01696
O231	0.10722	0.42457	0.89278
O232	0.10864	0.44376	0.6945
O233	0.22982	0.46452	0.75338
O234	0.35574	0.65707	0.71728
O235	0.30013	0.67243	0.89221
O236	0.19379	0.64307	0.00425
O237	0.08783	0.66829	0.89038
O238	0.10314	0.64914	0.69489
O239	0.22842	0.62664	0.74111
O240	0.32087	0.54844	0.82327
O241	0.08185	0.54513	0.81865
O242	0.43354	0.37078	0.59098
O243	0.41848	0.49911	0.55353
O244	0.41761	0.63293	0.5466
O245	0.20431	0.36889	0.61712
O246	0.19674	0.49695	0.56608
O247	0.19323	0.63079	0.55008

O248	0.99597	0.44447	0.78981
O249	0.98457	0.63092	0.77692
O250	0.13745	0.55574	0.2215
O251	0.20622	0.5568	0.38957
O252	0.30583	0.56375	0.52159
O253	0.40138	0.56427	0.38306
O254	0.39876	0.55927	0.18769
O255	0.26916	0.54414	0.21954
O256	0.13752	0.32581	0.25198
O257	0.19639	0.34632	0.42291
O258	0.31484	0.35306	0.50831
O259	0.42252	0.33321	0.3991
O260	0.3962	0.33103	0.20283
O261	0.27058	0.33719	0.25956
O262	0.19379	0.44362	0.28548
O263	0.4152	0.44668	0.29503
O264	0.07288	0.61861	0.07472
O265	0.08676	0.48663	0.06594
O266	0.11498	0.35647	0.06085
O267	0.31535	0.62174	0.0731
O268	0.32876	0.48822	0.06265
O269	0.30163	0.35737	0.06606
O270	0.51125	0.53856	0.27426
O271	0.51673	0.36073	0.26855
O272	0.44026	0.74591	0.63892
O273	0.19567	0.7429	0.65128
O274	0.27412	0.74592	0.05063
O275	0.11101	0.74384	0.04916
O276	0.06729	0.24449	0.13552
O277	0.31057	0.2379	0.14266
O278	0.23597	0.24991	0.55246
O279	0.39571	0.24875	0.54734
O280	0.56439	0.25038	0.3568
O281	0.80237	0.24139	0.33899
O282	0.72696	0.23987	0.95996
O283	0.88802	0.24212	0.94356
O284	0.93818	0.74336	0.85699
O285	0.69591	0.74671	0.85622
O286	0.77226	0.74451	0.44514
O287	0.60781	0.74962	0.4511
O288	0.95134	0.2624	0.44472
O289	0.90422	0.19904	0.58987
O290	0.86296	0.32147	0.55382
O291	0.96932	0.30604	0.62864

O292	0.09239	0.24759	0.57204
O293	0.10041	0.2684	0.74461
GA29	0.91935	0.3958	0.61541
H295	0.93785	0.29451	0.38992
H296	0.8203	0.34069	0.48122
H297	0.87777	0.17206	0.54123
H298	0.09035	0.5779	0.51587
H299	0.06586	0.57916	0.38971
H300	0.97678	0.62391	0.53015
H301	0.96892	0.45363	0.60115
H302	0.88306	0.55081	0.4899
H303	0.01404	0.3975	0.37162
H304	0.11027	0.46503	0.4257
H305	0.90176	0.44672	0.38253
H306	0.06382	0.4603	0.53672
AL30	0.81521	0.32399	0.30625
AL30	0.80295	0.47051	0.69247
P309	0.92376	0.27094	0.55346
C310	0.93346	0.53571	0.46947
C311	0.05456	0.55624	0.46309
C312	0.98515	0.57571	0.49307
C313	0.00548	0.4455	0.40874
C314	0.94402	0.47247	0.4163
C315	0.0625	0.47971	0.45906
C316	0.09588	0.25824	0.65841
<b>TS<sub>COOH</sub></b>			
SI2	0.42593	0.05394	0.64458
SI3	0.30525	0.02301	0.78556
SI4	0.28151	0.0547	0.00963
SI5	0.12138	0.05864	0.01085
SI6	0.07042	0.02517	0.79683
SI7	0.17967	0.05245	0.64867
SI8	0.42214	0.82263	0.67144
SI9	0.30565	0.86511	0.81021
SI10	0.26973	0.82608	0.03028
SI11	0.11527	0.82272	0.0193
SI12	0.06561	0.86675	0.80374
SI13	0.18293	0.82238	0.67658
SI14	0.07797	0.93896	0.15151
SI15	0.1988	0.96935	0.2973
SI16	0.21878	0.93125	0.51591
SI17	0.37814	0.93026	0.51535
SI18	0.43158	0.96509	0.30508

SI19	0.32159	0.94081	0.15624
SI20	0.08212	0.16739	0.16544
SI21	0.20043	0.12608	0.3093
SI22	0.23553	0.17191	0.52427
SI23	0.38981	0.17134	0.511
SI24	0.43913	0.12338	0.30147
SI25	0.32187	0.16044	0.16888
SI26	0.58135	0.55769	0.33621
SI27	0.6876	0.53035	0.17901
SI28	0.71666	0.55128	0.96119
SI29	0.87456	0.55786	0.97142
SI30	0.93134	0.5257	0.1827
SI31	0.81022	0.55461	0.31016
SI32	0.58166	0.32654	0.3251
SI33	0.69437	0.3727	0.18043
SI34	0.72987	0.32187	0.96827
SI35	0.88415	0.32027	0.97853
SI36	0.93809	0.36698	0.18854
SI37	0.92828	0.43418	0.83999
SI38	0.77957	0.43668	0.47121
SI39	0.62222	0.43524	0.48209
SI40	0.56625	0.4685	0.69684
SI41	0.67994	0.42624	0.82238
SI42	0.91889	0.66936	0.8199
SI43	0.80484	0.63317	0.67945
SI44	0.76527	0.66382	0.46136
SI45	0.61056	0.66827	0.47948
SI46	0.56612	0.62502	0.69879
SI47	0.68623	0.6739	0.81331
SI48	0.57547	0.93815	0.36333
SI49	0.69389	0.96381	0.22009
SI50	0.72064	0.93283	0.99829
SI51	0.88053	0.92811	0.99416
SI52	0.93321	0.96613	0.20323
SI53	0.82182	0.9408	0.35396
SI54	0.58169	0.17137	0.33594
SI55	0.69518	0.11864	0.19803
SI56	0.73295	0.16181	0.98045
SI57	0.88699	0.16648	0.9872
SI58	0.93795	0.12355	0.19795
SI59	0.81759	0.16136	0.32421
SI60	0.92464	0.04876	0.85417
SI61	0.80265	0.02033	0.71013
SI62	0.77968	0.05866	0.49104

SI63	0.62101	0.06464	0.48986
SI64	0.5713	0.02436	0.7011
SI65	0.68012	0.04724	0.8532
SI66	0.92114	0.82231	0.8378
SI67	0.80263	0.86374	0.69413
SI68	0.76828	0.82103	0.4774
SI69	0.61433	0.82199	0.49677
SI70	0.56657	0.8668	0.70594
SI71	0.68278	0.82749	0.83732
SI72	0.42382	0.44365	0.64316
SI73	0.30892	0.47056	0.79853
SI74	0.28937	0.42897	0.01295
SI75	0.1317	0.42929	0.01145
SI76	0.07782	0.46848	0.80395
SI77	0.18973	0.4466	0.65842
SI78	0.42675	0.66767	0.66039
SI79	0.30457	0.62568	0.79762
SI80	0.27137	0.67082	0.0098
SI81	0.11705	0.66943	0.00726
SI82	0.06579	0.62514	0.80028
SI83	0.18216	0.66354	0.6652
SI84	0.07872	0.55066	0.1425
SI85	0.20277	0.52528	0.28201
SI86	0.22798	0.56417	0.50719
SI87	0.38789	0.56626	0.50219
SI88	0.43471	0.52591	0.28904
SI89	0.32847	0.55297	0.13963
SI90	0.08591	0.32261	0.16322
SI91	0.20044	0.36451	0.30926
SI92	0.23764	0.3291	0.52912
SI93	0.39184	0.32569	0.51302
SI94	0.4374	0.36838	0.29513
SI95	0.32009	0.31808	0.17154
O96	0.36151	0.05964	0.71757
O97	0.30292	0.05993	0.8934
O98	0.20118	0.04733	0.02302
O99	0.10075	0.06292	0.89436
O100	0.10541	0.0549	0.69704
O101	0.23217	0.02919	0.73472
O102	0.36104	0.82099	0.75102
O103	0.30813	0.84424	0.92701
O104	0.19207	0.84984	0.02098
O105	0.08582	0.83006	0.90742
O106	0.10547	0.83157	0.71133

O107	0.2314	0.85019	0.76541
O108	0.3244	0.94402	0.79757
O109	0.08602	0.94538	0.80832
O110	0.43503	0.12369	0.58272
O111	0.41837	0.99262	0.56509
O112	0.39986	0.86064	0.56934
O113	0.19834	0.12643	0.6074
O114	0.17995	0.9967	0.5595
O115	0.1963	0.86271	0.57291
O116	0.99072	0.03792	0.7864
O117	0.98557	0.85885	0.78678
O118	0.14308	0.93869	0.22281
O119	0.20014	0.92385	0.39822
O120	0.29867	0.94275	0.53041
O121	0.39691	0.92489	0.39765
O122	0.3969	0.9436	0.20035
O123	0.27129	0.96684	0.24329
O124	0.1455	0.16269	0.23967
O125	0.20001	0.16413	0.41591
O126	0.31271	0.14568	0.51557
O127	0.4161	0.16866	0.39636
O128	0.39915	0.14773	0.20196
O129	0.27383	0.13209	0.25767
O130	0.18169	0.04716	0.32421
O131	0.42299	0.04514	0.32536
O132	0.0709	0.86619	0.09738
O133	0.08291	0.99659	0.06536
O134	0.09864	0.12901	0.06142
O135	0.30464	0.86411	0.12379
O136	0.31665	0.98868	0.05813
O137	0.30702	0.12258	0.06421
O138	0.50984	0.94544	0.29363
O139	0.51872	0.13388	0.28253
O140	0.63937	0.57168	0.25454
O141	0.6775	0.55936	0.06699
O142	0.79593	0.54149	0.98206
O143	0.9093	0.56359	0.0803
O144	0.88765	0.555	0.27535
O145	0.76482	0.54376	0.21156
O146	0.64296	0.32761	0.24675
O147	0.68922	0.34632	0.06612
O148	0.80752	0.34754	0.97354
O149	0.91278	0.32525	0.09134
O150	0.90324	0.33522	0.28811

O151	0.76925	0.36491	0.22212
O152	0.66982	0.45088	0.1861
O153	0.91806	0.44545	0.17231
O154	0.56728	0.62669	0.39749
O155	0.60388	0.49968	0.41428
O156	0.60207	0.36584	0.4272
O157	0.79463	0.62549	0.3641
O158	0.7946	0.49287	0.38799
O159	0.80184	0.36104	0.42913
O160	0.0097	0.5416	0.20482
O161	0.01888	0.36173	0.19915
O162	0.87607	0.42783	0.74517
O163	0.82603	0.44461	0.5718
O164	0.70244	0.43668	0.50268
O165	0.58363	0.43808	0.58736
O166	0.60262	0.42621	0.78423
O167	0.72956	0.43842	0.73029
O168	0.86627	0.67595	0.72817
O169	0.80898	0.64184	0.55824
O170	0.68768	0.64187	0.47822
O171	0.57932	0.6567	0.58919
O172	0.60814	0.66632	0.78204
O173	0.73323	0.66515	0.71466
O174	0.81192	0.55606	0.71194
O175	0.5894	0.54689	0.7014
O176	0.92997	0.36471	0.90299
O177	0.90916	0.49636	0.91104
O178	0.8864	0.62801	0.91264
O179	0.69356	0.35268	0.87095
O180	0.68813	0.48484	0.90678
O181	0.70559	0.61914	0.89725
O182	0.48631	0.46244	0.71462
O183	0.48689	0.63271	0.72418
O184	0.64053	0.92683	0.29277
O185	0.69749	0.92507	0.11374
O186	0.80091	0.94288	0.98785
O187	0.90364	0.92326	0.10994
O188	0.896	0.94414	0.30584
O189	0.76787	0.96194	0.26926
O190	0.64585	0.16624	0.26238
O191	0.69415	0.14396	0.0834
O192	0.81061	0.13797	0.99005
O193	0.91692	0.16703	0.10001
O194	0.89548	0.1484	0.29463

O195	0.77064	0.1225	0.24357
O196	0.66998	0.04119	0.20435
O197	0.92142	0.04499	0.17738
O198	0.5664	0.87292	0.43512
O199	0.58108	0.00476	0.43337
O200	0.59881	0.13667	0.4434
O201	0.80796	0.86552	0.39506
O202	0.81823	0.99382	0.44647
O203	0.80672	0.12797	0.4371
O204	0.01218	0.95138	0.21971
O205	0.01708	0.13441	0.22005
O206	0.85999	0.05161	0.78131
O207	0.79685	0.06568	0.60894
O208	0.70032	0.05178	0.47087
O209	0.60487	0.06552	0.60847
O210	0.60548	0.04651	0.80604
O211	0.73144	0.02106	0.76758
O212	0.85901	0.82804	0.7615
O213	0.8037	0.82714	0.58603
O214	0.69145	0.84766	0.48689
O215	0.59175	0.82023	0.61327
O216	0.60533	0.8423	0.80644
O217	0.72979	0.85542	0.74666
O218	0.82002	0.94312	0.68033
O219	0.58365	0.94475	0.68044
O220	0.93167	0.11918	0.91473
O221	0.91912	0.98812	0.93546
O222	0.90054	0.8568	0.94346
O223	0.69797	0.1233	0.88733
O224	0.68351	0.99794	0.95006
O225	0.69902	0.86459	0.94181
O226	0.49239	0.04136	0.71131
O227	0.48648	0.85905	0.72261
O228	0.35792	0.44198	0.71277
O229	0.31376	0.42334	0.89734
O230	0.21039	0.44796	0.02082
O231	0.11081	0.42539	0.89447
O232	0.11318	0.45319	0.69738
O233	0.23352	0.46717	0.7555
O234	0.35754	0.65824	0.72088
O235	0.30321	0.67117	0.89806
O236	0.19448	0.64371	0.00603
O237	0.0883	0.67217	0.8937
O238	0.1053	0.64878	0.69957

O239	0.23083	0.6269	0.74626
O240	0.32536	0.54877	0.82584
O241	0.08342	0.54799	0.83013
O242	0.43482	0.37068	0.59138
O243	0.4174	0.49879	0.55403
O244	0.42112	0.63282	0.55096
O245	0.20636	0.3708	0.62222
O246	0.2025	0.49739	0.56547
O247	0.19461	0.63153	0.55489
O248	1.00055	0.44653	0.78979
O249	0.98624	0.63216	0.77936
O250	0.14023	0.55706	0.22101
O251	0.2059	0.56039	0.3911
O252	0.30803	0.56887	0.51853
O253	0.40613	0.56625	0.38503
O254	0.40158	0.55898	0.19034
O255	0.27217	0.54046	0.22487
O256	0.1396	0.32582	0.25391
O257	0.19667	0.34596	0.42699
O258	0.31494	0.3524	0.5124
O259	0.42157	0.3322	0.401
O260	0.39707	0.33124	0.20517
O261	0.27199	0.34163	0.26329
O262	0.19163	0.44486	0.29274
O263	0.41492	0.44687	0.29934
O264	0.07338	0.61876	0.07592
O265	0.08815	0.48669	0.06804
O266	0.11685	0.35682	0.06277
O267	0.31467	0.62245	0.08127
O268	0.33117	0.48945	0.06407
O269	0.30321	0.35819	0.06892
O270	0.51462	0.5343	0.27819
O271	0.51695	0.36195	0.27322
O272	0.44193	0.7464	0.64198
O273	0.19747	0.74321	0.65782
O274	0.27428	0.74639	0.05396
O275	0.11204	0.74455	0.0537
O276	0.06763	0.24532	0.13805
O277	0.30805	0.23935	0.1492
O278	0.23515	0.25015	0.55738
O279	0.39637	0.24826	0.54985
O280	0.56441	0.24966	0.35608
O281	0.8011	0.23946	0.33286
O282	0.72827	0.24108	0.95861

O283	0.88843	0.2424	0.94307
O284	0.93792	0.74399	0.85974
O285	0.69646	0.7486	0.85875
O286	0.77073	0.74374	0.44022
O287	0.60692	0.74721	0.45029
O288	0.95552	0.2557	0.43853
O289	0.88965	0.18403	0.56493
O290	0.87212	0.31153	0.558
O291	0.97793	0.25868	0.62587
O292	0.08967	0.23153	0.57164
O293	0.06081	0.34259	0.59437
GA29	0.91884	0.40115	0.60766
H295	0.93802	0.2866	0.38537
H296	0.83005	0.33365	0.48697
H297	0.85603	0.16675	0.51571
H298	0.09156	0.57935	0.52163
H299	0.06149	0.581	0.39832
H300	0.97691	0.6213	0.54613
H301	-0.00057	0.37703	0.60864
H302	0.88409	0.54633	0.51007
H303	0.01617	0.39887	0.37682
H304	0.11183	0.46818	0.42786
H305	0.90351	0.44389	0.39698
H306	0.06939	0.46028	0.54154
AL30	0.81695	0.3225	0.307
AL30	0.80458	0.47121	0.69682
P309	0.92395	0.25281	0.54618
C310	0.93439	0.53179	0.48845
C311	0.05432	0.55678	0.47203
C312	0.98568	0.57339	0.50846
C313	0.0076	0.44556	0.41747
C314	0.94537	0.46964	0.43189
C315	0.06487	0.48076	0.46514
C316	0.05766	0.28047	0.58981

### C<sub>6</sub>H<sub>8</sub>+COOH

SI2	0.42617	0.05373	0.64377
SI3	0.30487	0.02213	0.78312
SI4	0.28215	0.05209	0.00877
SI5	0.12231	0.05794	0.01093
SI6	0.07109	0.02453	0.79724
SI7	0.17872	0.0529	0.64642
SI8	0.42171	0.82195	0.67087
SI9	0.30497	0.86394	0.80855

SI10	0.27006	0.82509	0.02958
SI11	0.11542	0.82193	0.01793
SI12	0.06576	0.86632	0.8026
SI13	0.18216	0.82228	0.67419
SI14	0.07753	0.93825	0.15026
SI15	0.19904	0.96844	0.29424
SI16	0.21858	0.93197	0.51406
SI17	0.37781	0.93018	0.51512
SI18	0.43204	0.96448	0.30575
SI19	0.32301	0.93896	0.15542
SI20	0.08298	0.16767	0.16353
SI21	0.20119	0.12545	0.30577
SI22	0.23419	0.17229	0.52228
SI23	0.38945	0.17141	0.51007
SI24	0.43864	0.12245	0.30076
SI25	0.32301	0.15917	0.16586
SI26	0.5803	0.55834	0.33599
SI27	0.68749	0.53103	0.17746
SI28	0.71576	0.55076	0.9592
SI29	0.87373	0.55888	0.97267
SI30	0.92843	0.52735	0.18233
SI31	0.80815	0.55459	0.31059
SI32	0.57842	0.32684	0.32316
SI33	0.69569	0.37294	0.18414
SI34	0.72861	0.32153	0.96978
SI35	0.8827	0.32074	0.97945
SI36	0.93624	0.36848	0.18704
SI37	0.9255	0.43611	0.84607
SI38	0.77709	0.43849	0.4738
SI39	0.61803	0.43443	0.48065
SI40	0.56433	0.4679	0.69782
SI41	0.67702	0.42567	0.82388
SI42	0.91792	0.66931	0.81943
SI43	0.80305	0.63273	0.68173
SI44	0.76491	0.66293	0.46368
SI45	0.60993	0.6687	0.47921
SI46	0.56448	0.62458	0.69788
SI47	0.6847	0.67398	0.81235
SI48	0.57745	0.93878	0.36491
SI49	0.69572	0.96302	0.22159
SI50	0.72179	0.93182	0.99889
SI51	0.88156	0.92791	0.9971
SI52	0.93299	0.96625	0.20652
SI53	0.82269	0.9406	0.35862

SI54	0.58077	0.17108	0.33735
SI55	0.69737	0.11856	0.20334
SI56	0.73333	0.16196	0.98329
SI57	0.88739	0.16687	0.98713
SI58	0.93892	0.12391	0.19833
SI59	0.82064	0.16277	0.32903
SI60	0.92565	0.04817	0.85777
SI61	0.80289	0.02052	0.71342
SI62	0.78237	0.06122	0.49498
SI63	0.6227	0.06707	0.4919
SI64	0.5715	0.02437	0.70209
SI65	0.67938	0.04711	0.85581
SI66	0.92164	0.82243	0.84064
SI67	0.8018	0.86367	0.69792
SI68	0.76975	0.82033	0.4815
SI69	0.61558	0.82242	0.49909
SI70	0.56637	0.86675	0.70732
SI71	0.68157	0.82695	0.8396
SI72	0.42192	0.44376	0.64175
SI73	0.30641	0.47124	0.79653
SI74	0.28766	0.42847	0.01096
SI75	0.13045	0.42935	0.01002
SI76	0.07541	0.46653	0.80177
SI77	0.18743	0.44611	0.65783
SI78	0.42549	0.66735	0.65751
SI79	0.30236	0.62617	0.79323
SI80	0.27127	0.6703	0.00574
SI81	0.1171	0.66832	0.00514
SI82	0.0652	0.62431	0.79686
SI83	0.18035	0.66367	0.66055
SI84	0.07687	0.55054	0.1413
SI85	0.20237	0.52617	0.2781
SI86	0.22631	0.56361	0.50599
SI87	0.38603	0.56557	0.50064
SI88	0.43337	0.52609	0.28722
SI89	0.32815	0.55329	0.13595
SI90	0.08472	0.32311	0.16071
SI91	0.19951	0.36502	0.30523
SI92	0.23617	0.32992	0.52529
SI93	0.39191	0.32542	0.50959
SI94	0.43622	0.36802	0.29041
SI95	0.31808	0.31648	0.16719
O96	0.36176	0.05914	0.71691
O97	0.30185	0.05741	0.89197

O98	0.20183	0.04508	0.02437
O99	0.10261	0.06243	0.89386
O100	0.10481	0.05498	0.69662
O101	0.23226	0.03051	0.73116
O102	0.36095	0.81962	0.75113
O103	0.30732	0.84464	0.92592
O104	0.19226	0.84882	0.02235
O105	0.08742	0.82911	0.90513
O106	0.10469	0.83203	0.70864
O107	0.23082	0.84832	0.76392
O108	0.32294	0.94287	0.79306
O109	0.08678	0.9449	0.80789
O110	0.43449	0.12319	0.58101
O111	0.41876	0.99214	0.56468
O112	0.39823	0.8606	0.56992
O113	0.19445	0.12776	0.60461
O114	0.17913	0.99751	0.55692
O115	0.19622	0.86371	0.57167
O116	0.99135	0.03757	0.78876
O117	0.98556	0.85884	0.7875
O118	0.14317	0.93709	0.22063
O119	0.20001	0.92423	0.39646
O120	0.29834	0.94411	0.52886
O121	0.39698	0.92399	0.39768
O122	0.39812	0.94211	0.20063
O123	0.27182	0.96525	0.24125
O124	0.14662	0.16367	0.23742
O125	0.20026	0.16217	0.4134
O126	0.31169	0.14758	0.51852
O127	0.41357	0.16775	0.39452
O128	0.40014	0.14692	0.19995
O129	0.27481	0.1318	0.25531
O130	0.18168	0.04662	0.31861
O131	0.42157	0.04443	0.32493
O132	0.07027	0.86601	0.09447
O133	0.0823	0.99691	0.06539
O134	0.10029	0.12919	0.05969
O135	0.30611	0.86225	0.12301
O136	0.31806	0.9863	0.05661
O137	0.30842	0.11988	0.06236
O138	0.51087	0.94681	0.29723
O139	0.51847	0.13222	0.28408
O140	0.63832	0.57055	0.2538
O141	0.67791	0.56096	0.06588

O142	0.79543	0.53902	0.9763
O143	0.90339	0.56828	0.08444
O144	0.88601	0.55489	0.27726
O145	0.7643	0.54609	0.20995
O146	0.64361	0.33	0.25258
O147	0.69095	0.34318	0.07159
O148	0.80623	0.34755	0.97062
O149	0.90756	0.32435	0.09451
O150	0.90509	0.33758	0.29011
O151	0.76996	0.36552	0.22843
O152	0.67135	0.45117	0.18328
O153	0.91621	0.44684	0.16914
O154	0.5673	0.62852	0.39497
O155	0.6011	0.50121	0.41647
O156	0.58978	0.36747	0.42686
O157	0.7934	0.62549	0.36524
O158	0.7907	0.49191	0.38494
O159	0.80692	0.36336	0.43499
O160	0.00722	0.54287	0.202
O161	0.01719	0.36269	0.19211
O162	0.8701	0.43224	0.75967
O163	0.81842	0.45428	0.57312
O164	0.69838	0.429	0.49173
O165	0.58316	0.43806	0.58877
O166	0.59934	0.42558	0.78628
O167	0.72619	0.43764	0.73177
O168	0.86554	0.67619	0.72753
O169	0.80801	0.63875	0.55992
O170	0.68691	0.64222	0.47945
O171	0.57733	0.65563	0.58771
O172	0.60666	0.66648	0.7803
O173	0.73221	0.66839	0.71378
O174	0.80712	0.55716	0.72076
O175	0.587	0.54645	0.70266
O176	0.93087	0.36592	0.90862
O177	0.91634	0.49839	0.92222
O178	0.88512	0.62853	0.91225
O179	0.68943	0.35253	0.87535
O180	0.68456	0.48441	0.9084
O181	0.70456	0.61833	0.89454
O182	0.48404	0.4618	0.71412
O183	0.48503	0.63248	0.7224
O184	0.64101	0.9259	0.29189
O185	0.70035	0.92485	0.11504

O186	0.802	0.94187	0.98536
O187	0.90141	0.92364	0.11433
O188	0.89709	0.94539	0.31081
O189	0.76897	0.96001	0.2728
O190	0.64608	0.16474	0.2664
O191	0.69825	0.14551	0.08959
O192	0.81127	0.13787	0.98829
O193	0.91717	0.16648	0.09995
O194	0.898	0.15089	0.29507
O195	0.77179	0.12246	0.25267
O196	0.67294	0.04077	0.20615
O197	0.92159	0.04522	0.18093
O198	0.56817	0.87436	0.43819
O199	0.58671	0.00556	0.43348
O200	0.59623	0.138	0.4466
O201	0.81048	0.86525	0.40057
O202	0.81678	0.99402	0.45036
O203	0.81506	0.12857	0.44249
O204	0.01214	0.95045	0.21944
O205	0.01847	0.13387	0.21824
O206	0.86058	0.0496	0.78604
O207	0.80008	0.06687	0.61294
O208	0.70289	0.06046	0.47405
O209	0.60608	0.06547	0.61033
O210	0.60492	0.04593	0.80793
O211	0.73128	0.02369	0.76922
O212	0.85787	0.82995	0.76798
O213	0.80465	0.82619	0.59065
O214	0.69298	0.84749	0.48961
O215	0.59292	0.82014	0.61558
O216	0.60423	0.84325	0.80915
O217	0.72858	0.85488	0.74885
O218	0.81807	0.94317	0.6825
O219	0.5831	0.94473	0.68129
O220	0.933	0.11998	0.91483
O221	0.92127	0.98865	0.94101
O222	0.90403	0.85689	0.9477
O223	0.69552	0.12263	0.89358
O224	0.68369	0.99632	0.95073
O225	0.69921	0.86331	0.94423
O226	0.4926	0.042	0.71069
O227	0.48611	0.85834	0.72183
O228	0.3548	0.44315	0.70938
O229	0.3127	0.42419	0.89545

O230	0.20899	0.44902	0.01704
O231	0.10807	0.42481	0.89376
O232	0.10985	0.44676	0.69536
O233	0.23019	0.46743	0.75576
O234	0.35578	0.65824	0.71694
O235	0.29966	0.67316	0.89208
O236	0.19454	0.64267	0.00653
O237	0.08987	0.66996	0.89068
O238	0.1035	0.64901	0.69539
O239	0.229	0.62637	0.7408
O240	0.32278	0.54953	0.82375
O241	0.08313	0.5465	0.82241
O242	0.43268	0.37088	0.5897
O243	0.41702	0.49874	0.55214
O244	0.41933	0.63263	0.548
O245	0.20818	0.37193	0.62004
O246	0.19776	0.49916	0.56699
O247	0.19328	0.63246	0.54976
O248	0.99759	0.44539	0.78946
O249	0.98543	0.63192	0.77919
O250	0.13746	0.55695	0.22158
O251	0.20619	0.5579	0.38936
O252	0.30628	0.56663	0.5201
O253	0.4025	0.56525	0.38286
O254	0.40068	0.55931	0.18828
O255	0.27	0.54635	0.21979
O256	0.13639	0.32756	0.25382
O257	0.1964	0.35025	0.42389
O258	0.31424	0.3493	0.50754
O259	0.4219	0.33264	0.3977
O260	0.3943	0.33156	0.20167
O261	0.26922	0.33696	0.25951
O262	0.1946	0.44509	0.28324
O263	0.41465	0.4467	0.29576
O264	0.07275	0.61806	0.07327
O265	0.08693	0.48598	0.06812
O266	0.11755	0.35628	0.06084
O267	0.31734	0.62072	0.07117
O268	0.33003	0.4868	0.06619
O269	0.29967	0.35666	0.06514
O270	0.51313	0.53564	0.27832
O271	0.51495	0.35941	0.26388
O272	0.44124	0.74606	0.63947
O273	0.19584	0.74329	0.65353

O274	0.2749	0.74528	0.05209
O275	0.11153	0.74361	0.05114
O276	0.06741	0.24537	0.13613
O277	0.30898	0.23756	0.14304
O278	0.22862	0.25082	0.55279
O279	0.39796	0.24827	0.54743
O280	0.56259	0.24942	0.35327
O281	0.80375	0.24066	0.33799
O282	0.72819	0.24067	0.95871
O283	0.88928	0.24287	0.94323
O284	0.93796	0.74378	0.8597
O285	0.69392	0.74801	0.86086
O286	0.772	0.7431	0.44445
O287	0.60715	0.74804	0.45185
O288	0.96895	0.26006	0.42795
O289	0.91617	0.17585	0.5492
O290	0.88113	0.30127	0.55416
O291	0.99211	0.25417	0.61775
O292	0.07477	0.31947	0.54669
O293	0.08024	0.28567	0.70744
GA29	0.94601	0.4192	0.60598
H295	0.94777	0.29206	0.37822
H296	0.83496	0.33726	0.4889
H297	0.87616	0.1586	0.51149
H298	0.09102	0.58284	0.51748
H299	0.0622	0.58624	0.39358
H300	0.97588	0.62316	0.54193
H301	0.05133	0.26037	0.75308
H302	0.88382	0.54751	0.50089
H303	0.0186	0.40371	0.36553
H304	0.11304	0.47324	0.42015
H305	0.90454	0.44705	0.38688
H306	0.06999	0.46292	0.5323
AL30	0.81901	0.32409	0.31284
AL30	0.8021	0.47152	0.70008
P309	0.93495	0.2507	0.53192
C310	0.93449	0.53472	0.47863
C311	0.05447	0.56083	0.46628
C312	0.98535	0.57625	0.50192
C313	0.00906	0.45013	0.40629
C314	0.94652	0.47377	0.41956
C315	0.06557	0.48503	0.45647
C316	0.05193	0.28957	0.61709

**TS<sub>CO+OH</sub>**

SI2	0.42637	0.05374	0.64305
SI3	0.3048	0.02308	0.78319
SI4	0.2813	0.05448	0.00772
SI5	0.12113	0.0582	0.00962
SI6	0.07018	0.02473	0.79543
SI7	0.17878	0.05353	0.64604
SI8	0.42161	0.82263	0.6693
SI9	0.30463	0.86466	0.80777
SI10	0.26928	0.82573	0.02819
SI11	0.11471	0.82183	0.01562
SI12	0.06495	0.86654	0.80072
SI13	0.18192	0.82326	0.67292
SI14	0.07779	0.93743	0.14891
SI15	0.19838	0.96835	0.29309
SI16	0.21854	0.93301	0.51304
SI17	0.37776	0.93062	0.51352
SI18	0.4314	0.96463	0.30347
SI19	0.32184	0.94057	0.15367
SI20	0.08103	0.16731	0.16324
SI21	0.19971	0.12497	0.30441
SI22	0.23428	0.17126	0.52046
SI23	0.38938	0.17116	0.50929
SI24	0.43904	0.12278	0.30002
SI25	0.32221	0.15984	0.1666
SI26	0.58038	0.55553	0.34077
SI27	0.69023	0.52869	0.18342
SI28	0.71585	0.5526	0.9669
SI29	0.87437	0.55936	0.9741
SI30	0.93104	0.52621	0.18251
SI31	0.81214	0.55248	0.31508
SI32	0.58117	0.32594	0.32794
SI33	0.69806	0.37093	0.18677
SI34	0.73066	0.31993	0.97309
SI35	0.88483	0.31942	0.98224
SI36	0.93781	0.36865	0.18933
SI37	0.92682	0.43461	0.84563
SI38	0.77734	0.43599	0.47609
SI39	0.61807	0.43285	0.48728
SI40	0.5647	0.46673	0.70297
SI41	0.67777	0.42743	0.83242
SI42	0.91977	0.66893	0.82072
SI43	0.80441	0.63257	0.68399

SI44	0.76614	0.66211	0.46398
SI45	0.61132	0.66736	0.47975
SI46	0.56507	0.62412	0.69852
SI47	0.68465	0.67338	0.81585
SI48	0.57538	0.93784	0.36336
SI49	0.6947	0.96381	0.22049
SI50	0.72007	0.93224	0.99908
SI51	0.88011	0.92757	0.9934
SI52	0.93346	0.96477	0.20299
SI53	0.82269	0.93902	0.3537
SI54	0.58204	0.1706	0.33494
SI55	0.69819	0.11933	0.20067
SI56	0.73438	0.16095	0.98013
SI57	0.88794	0.16574	0.98724
SI58	0.93739	0.1226	0.1998
SI59	0.81999	0.16225	0.33188
SI60	0.92459	0.04872	0.85397
SI61	0.80252	0.01854	0.7124
SI62	0.77999	0.05686	0.49046
SI63	0.62182	0.06369	0.48865
SI64	0.57208	0.02421	0.69961
SI65	0.67957	0.04614	0.85477
SI66	0.92135	0.82137	0.83753
SI67	0.80269	0.86184	0.69586
SI68	0.7689	0.81989	0.47806
SI69	0.61496	0.82131	0.49628
SI70	0.56642	0.86667	0.70462
SI71	0.68166	0.82698	0.83796
SI72	0.42318	0.44366	0.64399
SI73	0.30634	0.4715	0.79661
SI74	0.29075	0.42843	0.01125
SI75	0.13278	0.42888	0.01209
SI76	0.07648	0.46687	0.80434
SI77	0.18972	0.44497	0.65586
SI78	0.42545	0.66762	0.65761
SI79	0.30185	0.62701	0.79403
SI80	0.27156	0.67096	0.00738
SI81	0.11784	0.668	0.00412
SI82	0.06701	0.62493	0.79344
SI83	0.18111	0.6652	0.65854
SI84	0.07875	0.55127	0.14134
SI85	0.20347	0.52628	0.27716
SI86	0.22769	0.56306	0.50574
SI87	0.38744	0.56429	0.50188

SI88	0.43463	0.52573	0.28738
SI89	0.32983	0.55357	0.13548
SI90	0.08473	0.32256	0.16085
SI91	0.20042	0.36562	0.30281
SI92	0.23764	0.3291	0.5219
SI93	0.39241	0.32563	0.51122
SI94	0.43874	0.36803	0.29281
SI95	0.32124	0.31732	0.16905
O96	0.36214	0.05907	0.71658
O97	0.30169	0.05978	0.89108
O98	0.20107	0.04765	0.02297
O99	0.1015	0.062	0.89267
O100	0.10484	0.05485	0.6953
O101	0.23238	0.03088	0.73056
O102	0.36052	0.821	0.74898
O103	0.30723	0.84365	0.92451
O104	0.1915	0.84893	0.01887
O105	0.086	0.82895	0.90336
O106	0.10438	0.8313	0.70772
O107	0.2305	0.84919	0.76278
O108	0.32239	0.9438	0.79514
O109	0.08638	0.94491	0.80552
O110	0.43436	0.12366	0.5811
O111	0.41847	0.99263	0.5633
O112	0.39879	0.8609	0.5677
O113	0.19515	0.12857	0.60507
O114	0.17996	0.99921	0.55505
O115	0.19516	0.86528	0.57098
O116	0.99059	0.03719	0.78576
O117	0.98479	0.85927	0.78536
O118	0.14352	0.93561	0.21923
O119	0.20006	0.92453	0.3956
O120	0.29835	0.94405	0.52851
O121	0.39606	0.92468	0.3958
O122	0.39699	0.94311	0.19839
O123	0.2713	0.96654	0.24047
O124	0.14542	0.1635	0.23621
O125	0.1992	0.1613	0.41258
O126	0.31173	0.14665	0.5157
O127	0.41452	0.16811	0.39432
O128	0.39933	0.14744	0.20029
O129	0.27363	0.13127	0.25473
O130	0.17976	0.04628	0.31703
O131	0.42215	0.04466	0.32354

O132	0.06998	0.86511	0.09339
O133	0.08318	0.99575	0.06381
O134	0.09757	0.12854	0.05946
O135	0.30451	0.86396	0.12115
O136	0.31683	0.9884	0.05547
O137	0.30771	0.12225	0.06167
O138	0.50962	0.94481	0.29349
O139	0.51865	0.13272	0.28261
O140	0.64204	0.56531	0.26433
O141	0.67973	0.56329	0.07471
O142	0.79583	0.54195	0.98135
O143	0.90679	0.56779	0.08435
O144	0.88979	0.55139	0.28012
O145	0.76736	0.54252	0.21547
O146	0.64567	0.32957	0.2568
O147	0.69276	0.33809	0.0761
O148	0.80811	0.34655	0.97539
O149	0.91251	0.32302	0.0956
O150	0.9049	0.34316	0.29173
O151	0.77192	0.36555	0.23113
O152	0.67312	0.44914	0.18107
O153	0.91989	0.44678	0.16292
O154	0.56741	0.62636	0.39793
O155	0.59438	0.49776	0.42351
O156	0.59486	0.36395	0.43343
O157	0.79747	0.62422	0.36779
O158	0.79464	0.49183	0.39248
O159	0.80251	0.36093	0.43757
O160	0.00986	0.54246	0.20315
O161	0.01946	0.36361	0.19686
O162	0.87427	0.42834	0.7528
O163	0.81991	0.44808	0.5778
O164	0.69853	0.43535	0.49853
O165	0.5838	0.43354	0.59618
O166	0.60024	0.42769	0.79409
O167	0.7275	0.44046	0.74096
O168	0.86715	0.6756	0.72925
O169	0.80787	0.64021	0.56266
O170	0.68814	0.6403	0.47817
O171	0.57982	0.65568	0.58939
O172	0.60694	0.66478	0.78252
O173	0.73326	0.66586	0.71887
O174	0.81101	0.55635	0.72039
O175	0.58623	0.54559	0.70224

O176	0.93121	0.36608	0.91002
O177	0.9123	0.49826	0.91671
O178	0.88698	0.62903	0.91426
O179	0.69082	0.35402	0.88141
O180	0.68472	0.48554	0.91786
O181	0.70334	0.61923	0.9008
O182	0.48421	0.4597	0.71927
O183	0.48543	0.63275	0.72141
O184	0.64059	0.92773	0.29303
O185	0.69724	0.92437	0.11457
O186	0.80041	0.94231	0.98787
O187	0.90384	0.92271	0.10889
O188	0.89692	0.94131	0.30535
O189	0.76878	0.95981	0.2689
O190	0.64583	0.16626	0.26109
O191	0.69867	0.14463	0.08598
O192	0.81192	0.13635	0.98594
O193	0.91573	0.1652	0.1014
O194	0.89702	0.14663	0.29843
O195	0.77199	0.12345	0.2508
O196	0.67274	0.04165	0.2049
O197	0.92177	0.04376	0.17925
O198	0.56692	0.87207	0.43432
O199	0.57987	0.00422	0.43408
O200	0.59965	0.13577	0.44219
O201	0.80876	0.86382	0.39532
O202	0.81955	0.99276	0.4452
O203	0.80672	0.12782	0.44331
O204	0.01268	0.94983	0.2182
O205	0.01709	0.13393	0.21962
O206	0.86018	0.05218	0.78074
O207	0.79449	0.061	0.60941
O208	0.70059	0.04915	0.46809
O209	0.60652	0.06531	0.60772
O210	0.6055	0.04555	0.80535
O211	0.73183	0.01906	0.77118
O212	0.85854	0.82438	0.76229
O213	0.80419	0.82721	0.58652
O214	0.69208	0.84685	0.4866
O215	0.59199	0.81969	0.61271
O216	0.60455	0.84301	0.80603
O217	0.72947	0.85291	0.74693
O218	0.82133	0.94108	0.68617
O219	0.58322	0.94451	0.67826

O220	0.93351	0.11841	0.91566
O221	0.91859	0.9874	0.93422
O222	0.90031	0.85613	0.94276
O223	0.69671	0.12197	0.88977
O224	0.68182	0.99695	0.95181
O225	0.69852	0.86424	0.94199
O226	0.49311	0.04178	0.70891
O227	0.48615	0.85855	0.72035
O228	0.35414	0.44499	0.70791
O229	0.31293	0.42367	0.89425
O230	0.21166	0.4465	0.02086
O231	0.11223	0.42693	0.89422
O232	0.10985	0.43989	0.69522
O233	0.22956	0.4659	0.75534
O234	0.35625	0.65785	0.71843
O235	0.29978	0.67327	0.89348
O236	0.19521	0.64223	0.00796
O237	0.09256	0.6684	0.88861
O238	0.10375	0.65172	0.69206
O239	0.22876	0.62805	0.74055
O240	0.32032	0.54976	0.82463
O241	0.08841	0.54654	0.81213
O242	0.43245	0.37024	0.59303
O243	0.42091	0.49896	0.55451
O244	0.41818	0.6328	0.54819
O245	0.20606	0.37032	0.61636
O246	0.19624	0.49926	0.56722
O247	0.19501	0.63198	0.54905
O248	0.99954	0.44595	0.79191
O249	0.98685	0.63006	0.78084
O250	0.14005	0.55983	0.22032
O251	0.20897	0.55757	0.38883
O252	0.30745	0.56206	0.52259
O253	0.40326	0.56376	0.38397
O254	0.40189	0.55968	0.18893
O255	0.27186	0.543	0.21881
O256	0.13978	0.32537	0.25037
O257	0.1964	0.34996	0.42202
O258	0.31487	0.35127	0.50773
O259	0.42324	0.33368	0.40046
O260	0.39777	0.32947	0.20477
O261	0.27232	0.342	0.25943
O262	0.19173	0.44564	0.28314
O263	0.41552	0.44634	0.29458

O264	0.07279	0.61784	0.07149
O265	0.09012	0.48667	0.06853
O266	0.1169	0.35589	0.05999
O267	0.31777	0.62222	0.07412
O268	0.33273	0.48892	0.06181
O269	0.30608	0.35748	0.06565
O270	0.51428	0.53566	0.27779
O271	0.51798	0.361	0.27047
O272	0.44048	0.74628	0.63897
O273	0.19702	0.74454	0.65007
O274	0.27432	0.7461	0.05284
O275	0.11151	0.74338	0.04879
O276	0.06623	0.24527	0.13605
O277	0.30804	0.2388	0.14715
O278	0.23014	0.25049	0.54956
O279	0.39605	0.24818	0.54757
O280	0.56318	0.24851	0.35494
O281	0.80432	0.24037	0.3368
O282	0.7298	0.23975	0.95512
O283	0.89002	0.24203	0.94504
O284	0.94082	0.74349	0.85907
O285	0.69337	0.74816	0.86146
O286	0.77142	0.74217	0.44304
O287	0.60782	0.7463	0.45061
O288	0.92614	0.2144	0.498
O289	0.8383	0.19822	0.62452
O290	0.86752	0.31648	0.57299
O291	0.94919	0.25449	0.68158
O292	0.04698	0.26477	0.50453
O293	0.02649	0.36202	0.61563
GA29	0.9219	0.39805	0.61244
H295	0.97198	0.2284	0.48188
H296	0.83075	0.33348	0.50141
H297	0.8235	0.17284	0.56496
H298	0.08704	0.60221	0.48391
H299	0.04067	0.5937	0.37306
H300	0.97297	0.6325	0.54125
H301	0.05989	0.39741	0.65839
H302	0.88657	0.54593	0.53928
H303	0.01383	0.40937	0.37513
H304	0.10665	0.48857	0.39705
H305	0.90235	0.44389	0.4239
H306	0.07968	0.48266	0.5212
AL30	0.82151	0.32405	0.31641

AL30	0.80274	0.47123	0.7028
P309	0.8996	0.24516	0.601
C310	0.93451	0.53661	0.50386
C311	0.04639	0.57344	0.44953
C312	0.98222	0.58423	0.5049
C313	0.00614	0.45596	0.41657
C314	0.94474	0.47378	0.44867
C315	0.06396	0.49855	0.44556
C316	0.0595	0.30823	0.56261

### C<sub>6</sub>H<sub>8</sub>+Ga(OH)+CO

SI2	0.42518	0.05473	0.64538
SI3	0.30359	0.02331	0.78452
SI4	0.28236	0.05544	0.01013
SI5	0.12207	0.05908	0.01075
SI6	0.07096	0.02577	0.79605
SI7	0.17827	0.05367	0.64673
SI8	0.42199	0.82251	0.66948
SI9	0.30466	0.86446	0.80776
SI10	0.26997	0.82549	0.02834
SI11	0.11524	0.82298	0.01682
SI12	0.06609	0.86739	0.80059
SI13	0.1824	0.8215	0.673
SI14	0.07804	0.93833	0.14997
SI15	0.19869	0.96842	0.29474
SI16	0.2186	0.93231	0.51466
SI17	0.378	0.93168	0.51456
SI18	0.43196	0.96527	0.30407
SI19	0.32218	0.93998	0.15505
SI20	0.08122	0.16768	0.16358
SI21	0.20068	0.12528	0.30425
SI22	0.235	0.1714	0.52035
SI23	0.3895	0.17187	0.51142
SI24	0.44039	0.12374	0.30187
SI25	0.32347	0.16129	0.16795
SI26	0.57742	0.55435	0.34394
SI27	0.6918	0.52539	0.18967
SI28	0.71164	0.55863	0.97794
SI29	0.87122	0.56136	0.97184
SI30	0.93461	0.52712	0.18042
SI31	0.81768	0.55369	0.31457
SI32	0.58025	0.32638	0.33446
SI33	0.69956	0.36847	0.19208
SI34	0.72917	0.31783	0.98074

SI35	0.88345	0.32108	0.98682
SI36	0.94032	0.36908	0.19425
SI37	0.92672	0.43529	0.84592
SI38	0.7766	0.43971	0.46827
SI39	0.61821	0.43574	0.48305
SI40	0.57427	0.46926	0.7006
SI41	0.68026	0.43009	0.847
SI42	0.91946	0.6705	0.81874
SI43	0.80454	0.62846	0.68661
SI44	0.76645	0.66085	0.46571
SI45	0.61128	0.66872	0.47596
SI46	0.56501	0.62642	0.69434
SI47	0.68176	0.67311	0.81708
SI48	0.57636	0.93888	0.36285
SI49	0.69663	0.96563	0.22175
SI50	0.72157	0.93166	0.9987
SI51	0.88143	0.92796	0.99565
SI52	0.93313	0.96592	0.20545
SI53	0.82356	0.93928	0.35837
SI54	0.58407	0.17098	0.33662
SI55	0.69839	0.12165	0.19774
SI56	0.73406	0.16098	0.97834
SI57	0.88731	0.16708	0.99085
SI58	0.93796	0.12338	0.20217
SI59	0.81973	0.16243	0.32991
SI60	0.92557	0.04994	0.85856
SI61	0.80419	0.01997	0.71374
SI62	0.78142	0.05708	0.49313
SI63	0.62235	0.06349	0.49219
SI64	0.56986	0.02405	0.70131
SI65	0.67985	0.04568	0.8529
SI66	0.9226	0.8233	0.83837
SI67	0.8033	0.86463	0.69649
SI68	0.77024	0.81942	0.47966
SI69	0.61621	0.82208	0.4953
SI70	0.56697	0.8665	0.70418
SI71	0.6827	0.82814	0.83769
SI72	0.42821	0.44412	0.63795
SI73	0.30796	0.46977	0.78801
SI74	0.29012	0.42656	0.00459
SI75	0.13214	0.42765	0.0048
SI76	0.07831	0.47038	0.79976
SI77	0.1847	0.4461	0.64602
SI78	0.42455	0.66747	0.65401

SI79	0.30264	0.62538	0.79226
SI80	0.27129	0.67003	0.00551
SI81	0.11697	0.67031	0.9993
SI82	0.06589	0.62676	0.79329
SI83	0.181	0.66325	0.65765
SI84	0.08096	0.55137	0.13254
SI85	0.20343	0.52568	0.27389
SI86	0.22664	0.5631	0.49853
SI87	0.38674	0.56547	0.49699
SI88	0.43496	0.52562	0.28315
SI89	0.32904	0.55007	0.1319
SI90	0.08533	0.32298	0.15671
SI91	0.20222	0.36675	0.29805
SI92	0.23506	0.32858	0.52134
SI93	0.38968	0.32649	0.5093
SI94	0.43759	0.36718	0.29087
SI95	0.32281	0.31944	0.1632
O96	0.36036	0.05978	0.71752
O97	0.30179	0.05914	0.89305
O98	0.20199	0.0504	0.0264
O99	0.10338	0.06193	0.89331
O100	0.10393	0.05685	0.69529
O101	0.23082	0.03213	0.73334
O102	0.36123	0.82134	0.74962
O103	0.30758	0.84468	0.92488
O104	0.19224	0.84943	0.02088
O105	0.08674	0.83172	0.90468
O106	0.10506	0.83101	0.7084
O107	0.23089	0.84706	0.76328
O108	0.32096	0.94385	0.79388
O109	0.08709	0.94596	0.80302
O110	0.4342	0.12538	0.58557
O111	0.41786	0.99448	0.56393
O112	0.39971	0.86226	0.56889
O113	0.19509	0.12767	0.60304
O114	0.17918	0.9975	0.55837
O115	0.19629	0.86387	0.57146
O116	0.99109	0.03903	0.78936
O117	0.98584	0.86052	0.78505
O118	0.14315	0.93649	0.22126
O119	0.19963	0.92472	0.39728
O120	0.29839	0.94426	0.52909
O121	0.39695	0.92581	0.39704
O122	0.39741	0.94289	0.19956

O123	0.27156	0.96509	0.24229
O124	0.14603	0.16324	0.23562
O125	0.19987	0.16223	0.41194
O126	0.31222	0.14575	0.51523
O127	0.41675	0.16783	0.39762
O128	0.40062	0.14998	0.20299
O129	0.27454	0.13098	0.25442
O130	0.18092	0.04662	0.31822
O131	0.42296	0.04542	0.3227
O132	0.07027	0.86598	0.0948
O133	0.0843	0.99632	0.06449
O134	0.09644	0.12909	0.05921
O135	0.30567	0.86337	0.12141
O136	0.31667	0.9888	0.05804
O137	0.31067	0.12309	0.06266
O138	0.51032	0.94584	0.29381
O139	0.52032	0.13316	0.28529
O140	0.64532	0.55387	0.27914
O141	0.67715	0.56726	0.08748
O142	0.79225	0.55612	0.99127
O143	0.91236	0.56162	0.07554
O144	0.8937	0.5602	0.27311
O145	0.76929	0.53906	0.21991
O146	0.64719	0.33336	0.26905
O147	0.69421	0.3256	0.08896
O148	0.80615	0.34682	0.98156
O149	0.91389	0.32605	0.09801
O150	0.90792	0.33996	0.29485
O151	0.77414	0.36587	0.23446
O152	0.67681	0.44617	0.17208
O153	0.92073	0.44729	0.17345
O154	0.56788	0.62851	0.39272
O155	0.57909	0.49946	0.43446
O156	0.58883	0.36544	0.44057
O157	0.79845	0.62371	0.36935
O158	0.81189	0.49099	0.39181
O159	0.80174	0.36158	0.43669
O160	0.01361	0.54255	0.19844
O161	0.02185	0.36412	0.20004
O162	0.88088	0.4195	0.74283
O163	0.80325	0.44732	0.57903
O164	0.69667	0.44316	0.45423
O165	0.60766	0.43509	0.60237
O166	0.60559	0.43476	0.79883

O167	0.738	0.43682	0.76556
O168	0.86413	0.67659	0.73053
O169	0.80547	0.63664	0.56545
O170	0.68778	0.64083	0.47625
O171	0.5786	0.65799	0.58492
O172	0.60479	0.66973	0.77813
O173	0.73179	0.65552	0.72507
O174	0.81807	0.55271	0.72245
O175	0.59084	0.54934	0.69896
O176	0.92875	0.3671	0.91118
O177	0.89394	0.4966	0.90481
O178	0.88948	0.63004	0.9137
O179	0.6845	0.35665	0.89919
O180	0.6858	0.48853	0.93171
O181	0.69151	0.62264	0.9102
O182	0.49412	0.45798	0.70416
O183	0.48496	0.63141	0.7159
O184	0.64126	0.92917	0.29162
O185	0.70114	0.92662	0.11553
O186	0.80174	0.94094	0.98425
O187	0.90194	0.92357	0.11256
O188	0.89754	0.9435	0.30927
O189	0.76938	0.96226	0.27494
O190	0.64685	0.16819	0.2603
O191	0.69556	0.1453	0.08224
O192	0.81162	0.1368	0.98898
O193	0.91556	0.16639	0.10452
O194	0.89808	0.14792	0.30131
O195	0.77375	0.12842	0.24197
O196	0.67482	0.0435	0.20587
O197	0.92101	0.04485	0.18144
O198	0.56839	0.87318	0.43385
O199	0.58157	0.00495	0.43399
O200	0.60471	0.13554	0.44215
O201	0.81044	0.86304	0.39648
O202	0.81994	0.99057	0.4536
O203	0.80411	0.12472	0.43638
O204	0.01244	0.95116	0.21829
O205	0.01774	0.13382	0.22108
O206	0.86042	0.05245	0.7857
O207	0.80126	0.06788	0.61245
O208	0.70158	0.04626	0.48269
O209	0.60182	0.06681	0.60926
O210	0.60518	0.04487	0.80611

O211	0.73154	0.02093	0.76617
O212	0.85889	0.82917	0.76524
O213	0.80461	0.82812	0.58875
O214	0.6936	0.84701	0.48635
O215	0.59341	0.82028	0.61189
O216	0.60564	0.84364	0.80563
O217	0.73041	0.85833	0.7492
O218	0.82224	0.94385	0.68166
O219	0.58235	0.9448	0.67812
O220	0.93313	0.12068	0.91789
O221	0.92008	0.98916	0.93938
O222	0.90416	0.85735	0.9453
O223	0.69826	0.12126	0.88713
O224	0.68386	0.99592	0.94895
O225	0.69824	0.86297	0.94453
O226	0.49094	0.04093	0.71318
O227	0.48708	0.85729	0.72085
O228	0.36394	0.443	0.71111
O229	0.30826	0.42226	0.88663
O230	0.21105	0.44169	0.02303
O231	0.11663	0.42743	0.88564
O232	0.1091	0.45414	0.6899
O233	0.23506	0.46507	0.73621
O234	0.35586	0.65781	0.71585
O235	0.30316	0.66993	0.89376
O236	0.19414	0.64418	-0.00003
O237	0.08981	0.67484	0.88496
O238	0.10379	0.64964	0.69097
O239	0.22885	0.62788	0.74107
O240	0.3215	0.54785	0.81899
O241	0.08516	0.55002	0.82379
O242	0.43578	0.37188	0.58258
O243	0.4206	0.5014	0.55219
O244	0.41637	0.63461	0.5435
O245	0.19573	0.36963	0.60797
O246	0.1962	0.4961	0.5515
O247	0.19414	0.63018	0.54828
O248	0.99968	0.45022	0.80052
O249	0.98596	0.63298	0.77578
O250	0.14466	0.5598	0.20699
O251	0.20788	0.56389	0.38085
O252	0.30668	0.56274	0.51486
O253	0.4044	0.56477	0.37937
O254	0.40198	0.55675	0.18287

O255	0.27437	0.53381	0.21803
O256	0.14479	0.32529	0.23929
O257	0.20089	0.34287	0.41348
O258	0.31271	0.35322	0.51624
O259	0.41525	0.33133	0.39472
O260	0.39976	0.33089	0.19778
O261	0.27495	0.35145	0.24941
O262	0.18653	0.44662	0.29038
O263	0.41742	0.44619	0.29424
O264	0.07247	0.61841	0.06448
O265	0.0895	0.48658	0.05944
O266	0.11087	0.35527	0.05123
O267	0.31306	0.62068	0.07761
O268	0.33194	0.48838	0.05272
O269	0.30979	0.35533	0.05586
O270	0.51462	0.53755	0.27206
O271	0.51733	0.35843	0.27349
O272	0.44023	0.74636	0.63775
O273	0.19633	0.74294	0.64915
O274	0.27499	0.74554	0.05019
O275	0.11142	0.74447	0.04897
O276	0.06523	0.2453	0.13663
O277	0.30735	0.24011	0.15047
O278	0.23154	0.24983	0.55153
O279	0.39449	0.24933	0.5478
O280	0.56507	0.24828	0.36043
O281	0.80578	0.24058	0.34212
O282	0.73045	0.23935	0.94977
O283	0.88876	0.24362	0.94977
O284	0.94005	0.74499	0.85755
O285	0.69644	0.74903	0.85475
O286	0.77354	0.74127	0.44744
O287	0.60909	0.7478	0.44737
O288	0.91517	0.18529	0.56065
O289	0.81675	0.19425	0.67049
O290	0.85775	0.3021	0.58023
O291	0.92145	0.26203	0.71979
O292	0.02304	0.23975	0.4369
O293	0.00576	0.35763	0.60558
GA29	0.92441	0.35253	0.66205
H295	0.94943	0.20496	0.517
H296	0.819	0.33425	0.49599
H297	0.8114	0.14722	0.64336
H298	0.07271	0.62382	0.45609

H299	0.0073	0.60875	0.37099
H300	0.97175	0.6376	0.56282
H301	0.01096	0.40027	0.56917
H302	0.90459	0.53821	0.59946
H303	0.01204	0.41884	0.38369
H304	0.0843	0.51561	0.35141
H305	0.91281	0.43606	0.48761
H306	0.09518	0.50607	0.48073
AL30	0.82422	0.32325	0.31695
AL30	0.80492	0.46809	0.70326
P309	0.87795	0.2348	0.63371
C310	0.94325	0.53607	0.54252
C311	0.03109	0.58945	0.43987
C312	0.98043	0.59078	0.52238
C313	0.00534	0.46522	0.42619
C314	0.95152	0.47448	0.4849
C315	0.05809	0.51833	0.42275
C316	0.07213	0.26072	0.46837

### TS<sub>CO+H2O</sub>

SI2	0.42496	0.05433	0.64524
SI3	0.3034	0.02259	0.78485
SI4	0.28218	0.05518	0.01021
SI5	0.12209	0.05846	0.01063
SI6	0.07085	0.02506	0.79625
SI7	0.17811	0.05261	0.64675
SI8	0.42172	0.82206	0.66871
SI9	0.30433	0.86373	0.80732
SI10	0.26935	0.82475	0.02794
SI11	0.11457	0.82256	0.01582
SI12	0.06564	0.86692	0.79976
SI13	0.1819	0.82128	0.67215
SI14	0.07748	0.93779	0.14953
SI15	0.19831	0.96769	0.2935
SI16	0.21849	0.93176	0.51382
SI17	0.37784	0.93119	0.51428
SI18	0.43195	0.96499	0.30388
SI19	0.3223	0.93956	0.15447
SI20	0.08098	0.16722	0.16272
SI21	0.19982	0.1246	0.30378
SI22	0.23397	0.17044	0.51993
SI23	0.38886	0.17148	0.51048
SI24	0.4399	0.12337	0.30102
SI25	0.32258	0.16121	0.16822

SI26	0.57641	0.55367	0.34511
SI27	0.69246	0.52478	0.19175
SI28	0.71214	0.55991	0.97921
SI29	0.87201	0.56059	0.9721
SI30	0.9323	0.52604	0.18212
SI31	0.81741	0.55074	0.32219
SI32	0.57839	0.32621	0.336
SI33	0.69946	0.36984	0.19692
SI34	0.72783	0.31771	0.98783
SI35	0.88221	0.3217	0.98851
SI36	0.93927	0.36843	0.19437
SI37	0.92689	0.43487	0.84336
SI38	0.77175	0.4369	0.47374
SI39	0.61595	0.43384	0.4821
SI40	0.57575	0.46796	0.70064
SI41	0.67851	0.43142	0.85571
SI42	0.91725	0.67133	0.82176
SI43	0.80238	0.62904	0.68829
SI44	0.76734	0.66165	0.46641
SI45	0.61204	0.66823	0.47808
SI46	0.56536	0.6254	0.69672
SI47	0.6812	0.67399	0.81926
SI48	0.57699	0.93846	0.36246
SI49	0.69682	0.96543	0.22187
SI50	0.7221	0.93289	0.99794
SI51	0.8818	0.92932	0.99637
SI52	0.93284	0.96578	0.20625
SI53	0.82371	0.94117	0.36015
SI54	0.58352	0.17047	0.33482
SI55	0.69829	0.12107	0.1977
SI56	0.73361	0.16151	0.97767
SI57	0.88725	0.16798	0.98892
SI58	0.93769	0.12333	0.20095
SI59	0.81982	0.16385	0.32882
SI60	0.92557	0.05032	0.85864
SI61	0.80415	0.02136	0.71179
SI62	0.78291	0.06093	0.49439
SI63	0.62345	0.06401	0.49116
SI64	0.57008	0.02471	0.70016
SI65	0.68015	0.04645	0.85173
SI66	0.92189	0.82448	0.83869
SI67	0.80247	0.86602	0.69605
SI68	0.77037	0.81969	0.48049
SI69	0.61605	0.82177	0.49567

SI70	0.56637	0.86731	0.70364
SI71	0.68199	0.82994	0.83697
SI72	0.42828	0.44294	0.63984
SI73	0.30771	0.46959	0.78769
SI74	0.28724	0.42615	0.00574
SI75	0.13035	0.4279	0.00579
SI76	0.07816	0.46973	0.80003
SI77	0.18439	0.4465	0.64231
SI78	0.42405	0.66697	0.65438
SI79	0.30211	0.62508	0.79282
SI80	0.26973	0.66936	0.0064
SI81	0.11543	0.66977	0.00046
SI82	0.06342	0.62662	0.79411
SI83	0.17983	0.66284	0.65878
SI84	0.07818	0.55086	0.13337
SI85	0.20148	0.52545	0.27377
SI86	0.22411	0.5628	0.49718
SI87	0.38437	0.56438	0.49855
SI88	0.43365	0.52532	0.28444
SI89	0.32751	0.54915	0.13215
SI90	0.08386	0.32265	0.15503
SI91	0.20146	0.36642	0.29675
SI92	0.23373	0.32758	0.51948
SI93	0.38856	0.326	0.50831
SI94	0.4367	0.36678	0.29014
SI95	0.32187	0.31948	0.16261
O96	0.36018	0.05886	0.71765
O97	0.30128	0.05907	0.89297
O98	0.20191	0.04913	0.02683
O99	0.10385	0.06133	0.89307
O100	0.10381	0.05594	0.69523
O101	0.23071	0.03078	0.73311
O102	0.36082	0.82086	0.74869
O103	0.3069	0.84277	0.92401
O104	0.19167	0.8488	0.02028
O105	0.08657	0.83046	0.90326
O106	0.10453	0.83096	0.70703
O107	0.23058	0.84689	0.76209
O108	0.32079	0.94321	0.79539
O109	0.08721	0.94529	0.80347
O110	0.43304	0.12492	0.58492
O111	0.41782	0.99366	0.56438
O112	0.39911	0.86138	0.5679
O113	0.19513	0.12685	0.6038

O114	0.17895	0.99682	0.55785
O115	0.19619	0.86305	0.57018
O116	0.99114	0.03831	0.78979
O117	0.98548	0.86032	0.78392
O118	0.14292	0.93513	0.22034
O119	0.19957	0.9244	0.39643
O120	0.2982	0.94396	0.52864
O121	0.39685	0.92558	0.39682
O122	0.39739	0.94197	0.19957
O123	0.27126	0.96459	0.24124
O124	0.14568	0.16338	0.23523
O125	0.19834	0.16075	0.41212
O126	0.31138	0.14592	0.51378
O127	0.41652	0.16749	0.39697
O128	0.39982	0.14999	0.20258
O129	0.27396	0.13073	0.25498
O130	0.17997	0.04588	0.31621
O131	0.42204	0.04514	0.32185
O132	0.06948	0.86589	0.09311
O133	0.08381	0.99628	0.06484
O134	0.09698	0.1289	0.05846
O135	0.30548	0.86313	0.12013
O136	0.31743	0.98896	0.05794
O137	0.30949	0.12334	0.0627
O138	0.51044	0.94622	0.29447
O139	0.51973	0.13241	0.28372
O140	0.64395	0.55255	0.27955
O141	0.68275	0.57036	0.09184
O142	0.79271	0.54867	0.98351
O143	0.90717	0.56364	0.08144
O144	0.89409	0.55349	0.28139
O145	0.76941	0.5348	0.22781
O146	0.64662	0.33684	0.27524
O147	0.69669	0.32129	0.09932
O148	0.80461	0.3465	0.98634
O149	0.91238	0.32332	0.10102
O150	0.90729	0.34376	0.29815
O151	0.77333	0.37177	0.24214
O152	0.67592	0.44636	0.1682
O153	0.92096	0.44629	0.16852
O154	0.56805	0.6273	0.39623
O155	0.57653	0.49765	0.43406
O156	0.58306	0.36384	0.444
O157	0.80026	0.62311	0.37173

O158	0.81045	0.49127	0.40463
O159	0.80106	0.36029	0.44241
O160	0.01153	0.54218	0.20125
O161	0.02096	0.36311	0.2016
O162	0.88239	0.4251	0.74052
O163	0.78934	0.44442	0.5879
O164	0.69323	0.43887	0.44608
O165	0.61004	0.43537	0.602
O166	0.6068	0.43211	0.79762
O167	0.74183	0.43681	0.78459
O168	0.86134	0.67701	0.73466
O169	0.80597	0.63904	0.5673
O170	0.68874	0.64108	0.47604
O171	0.58103	0.6578	0.58832
O172	0.60347	0.66746	0.78382
O173	0.72918	0.65625	0.72477
O174	0.81494	0.55308	0.72226
O175	0.59093	0.54827	0.70098
O176	0.92621	0.37045	0.91676
O177	0.90421	0.5005	0.90527
O178	0.88831	0.63173	0.91835
O179	0.67999	0.36026	0.91488
O180	0.67608	0.49418	0.93409
O181	0.69581	0.62673	0.9148
O182	0.49566	0.45596	0.70232
O183	0.48477	0.63031	0.71456
O184	0.64114	0.9278	0.29
O185	0.7022	0.92752	0.11149
O186	0.80224	0.94206	0.98298
O187	0.90113	0.92362	0.11364
O188	0.89763	0.94374	0.31035
O189	0.7692	0.96223	0.27604
O190	0.6462	0.16823	0.25842
O191	0.69619	0.14357	0.0817
O192	0.81145	0.13801	0.98699
O193	0.91595	0.16553	0.10237
O194	0.89802	0.14892	0.29952
O195	0.77321	0.12742	0.24365
O196	0.67408	0.04315	0.20717
O197	0.92098	0.04465	0.18191
O198	0.56845	0.87275	0.43346
O199	0.58388	0.00437	0.43344
O200	0.60386	0.13541	0.44057
O201	0.8108	0.86532	0.40025

O202	0.82109	0.99451	0.45266
O203	0.80605	0.12889	0.43803
O204	0.01219	0.95043	0.21839
O205	0.01761	0.13345	0.22016
O206	0.86035	0.05094	0.78657
O207	0.8017	0.07091	0.61336
O208	0.70305	0.04949	0.48156
O209	0.60222	0.06723	0.60805
O210	0.60534	0.04514	0.80508
O211	0.73157	0.02157	0.76504
O212	0.85766	0.83165	0.76697
O213	0.80401	0.82666	0.5904
O214	0.69344	0.84652	0.48669
O215	0.59306	0.82044	0.61223
O216	0.60473	0.84571	0.8059
O217	0.72934	0.86026	0.74829
O218	0.82106	0.94494	0.67778
O219	0.58146	0.94539	0.67622
O220	0.93301	0.12222	0.91486
O221	0.92106	0.99116	0.94249
O222	0.90536	0.85912	0.94572
O223	0.69804	0.12226	0.8857
O224	0.68427	0.9971	0.94835
O225	0.69841	0.86425	0.94386
O226	0.49115	0.04187	0.71243
O227	0.48643	0.85748	0.71989
O228	0.3666	0.44045	0.71802
O229	0.30119	0.4227	0.88649
O230	0.20879	0.44096	0.03046
O231	0.11982	0.42943	0.88548
O232	0.1103	0.45534	0.69026
O233	0.23806	0.46714	0.72646
O234	0.35585	0.65806	0.71797
O235	0.3013	0.66926	0.89455
O236	0.19255	0.64327	0.00174
O237	0.08851	0.67378	0.88603
O238	0.10259	0.6487	0.69205
O239	0.22844	0.6273	0.74088
O240	0.32132	0.54752	0.81912
O241	0.08122	0.54947	0.82386
O242	0.43416	0.37155	0.58175
O243	0.41768	0.50118	0.55622
O244	0.41327	0.63403	0.54425
O245	0.19401	0.3695	0.60523

O246	0.19034	0.4953	0.54481
O247	0.19215	0.62937	0.5491
O248	1.00201	0.44308	0.79832
O249	0.98375	0.63438	0.7765
O250	0.14159	0.55822	0.2085
O251	0.20428	0.56529	0.37975
O252	0.30386	0.56043	0.51442
O253	0.40232	0.56332	0.38114
O254	0.39991	0.55606	0.18435
O255	0.27219	0.53271	0.21772
O256	0.14542	0.32633	0.23398
O257	0.19865	0.34058	0.41158
O258	0.31119	0.35237	0.51457
O259	0.41387	0.33072	0.39368
O260	0.39884	0.3311	0.19648
O261	0.2747	0.35308	0.24892
O262	0.18448	0.44661	0.29491
O263	0.4167	0.44577	0.29476
O264	0.07051	0.61838	0.06623
O265	0.08653	0.4865	0.05939
O266	0.10682	0.35519	0.0483
O267	0.31161	0.61977	0.07806
O268	0.3304	0.48756	0.05265
O269	0.30833	0.35455	0.05468
O270	0.51293	0.5389	0.2733
O271	0.51626	0.35787	0.27253
O272	0.44012	0.74574	0.63755
O273	0.19533	0.74234	0.64935
O274	0.27388	0.74484	0.05105
O275	0.11051	0.7442	0.04914
O276	0.0647	0.24481	0.13581
O277	0.30603	0.24016	0.15184
O278	0.22882	0.24912	0.55077
O279	0.39334	0.24898	0.54712
O280	0.56391	0.2476	0.35837
O281	0.80499	0.24204	0.3351
O282	0.72808	0.24018	0.95127
O283	0.88861	0.24472	0.94921
O284	0.9385	0.74608	0.85866
O285	0.6949	0.75077	0.85317
O286	0.77423	0.74191	0.44559
O287	0.60865	0.74717	0.4488
O288	0.92721	0.18543	0.60347
O289	0.82113	0.21492	0.68179

O290	0.87668	0.30128	0.55879
O291	0.92228	0.28967	0.72476
O292	0.03404	0.21348	0.45555
O293	0.02627	0.34612	0.60763
GA29	0.93705	0.37363	0.62942
H295	0.96548	0.19559	0.56058
H296	0.8257	0.33373	0.49848
H297	0.81314	0.16979	0.65354
H298	0.08584	0.57536	0.50055
H299	0.03486	0.58134	0.3956
H300	0.97242	0.61632	0.56208
H301	0.0474	0.32423	0.66442
H302	0.89261	0.53043	0.59961
H303	0.00673	0.38525	0.42079
H304	0.09239	0.46907	0.39427
H305	0.89861	0.43241	0.47156
H306	0.04958	0.42797	0.5201
AL30	0.82344	0.32553	0.32041
AL30	0.80372	0.46703	0.71001
P309	0.88756	0.24895	0.6441
C310	0.93573	0.51716	0.55436
C311	0.03984	0.55429	0.4682
C312	0.9799	0.56559	0.53318
C313	0.00203	0.43328	0.46008
C314	0.94078	0.44648	0.51927
C315	0.04836	0.48342	0.43766
C316	0.04748	0.26383	0.41922

### **C<sub>6</sub>H<sub>7</sub>Ga+H<sub>2</sub>O+CO**

SI2	0.42473	0.05389	0.64538
SI3	0.30311	0.02206	0.78481
SI4	0.28216	0.05422	0.01038
SI5	0.12211	0.05743	0.01066
SI6	0.07082	0.02439	0.79665
SI7	0.17769	0.05183	0.64664
SI8	0.42121	0.82173	0.66959
SI9	0.30374	0.86329	0.80771
SI10	0.26886	0.82388	0.02825
SI11	0.11408	0.8212	0.01523
SI12	0.06546	0.86636	0.79951
SI13	0.18162	0.82098	0.6721
SI14	0.07722	0.93645	0.1489
SI15	0.19787	0.96661	0.29293
SI16	0.21829	0.93117	0.51355

SI17	0.3776	0.93074	0.51454
SI18	0.43186	0.96415	0.30427
SI19	0.32216	0.93861	0.15466
SI20	0.08094	0.1666	0.16215
SI21	0.19976	0.12344	0.30268
SI22	0.23348	0.16917	0.51918
SI23	0.38828	0.17067	0.51033
SI24	0.43983	0.12246	0.30131
SI25	0.32295	0.16002	0.16804
SI26	0.57625	0.55281	0.34713
SI27	0.69278	0.5242	0.19411
SI28	0.71204	0.55929	0.98081
SI29	0.87172	0.5606	0.97489
SI30	0.93118	0.52489	0.18513
SI31	0.81743	0.54836	0.32678
SI32	0.57789	0.32606	0.33708
SI33	0.69887	0.36983	0.19791
SI34	0.72707	0.3181	0.98831
SI35	0.88151	0.32157	0.99191
SI36	0.9386	0.36767	0.19705
SI37	0.92517	0.43465	0.84812
SI38	0.77195	0.43463	0.47818
SI39	0.61513	0.43278	0.48571
SI40	0.57223	0.46715	0.70335
SI41	0.67407	0.43272	0.85843
SI42	0.91611	0.67136	0.82462
SI43	0.80192	0.62867	0.68967
SI44	0.76716	0.66122	0.46796
SI45	0.61165	0.66757	0.48054
SI46	0.56441	0.62474	0.69905
SI47	0.6809	0.67301	0.8207
SI48	0.57721	0.9379	0.36247
SI49	0.69683	0.96487	0.22192
SI50	0.72205	0.93261	-0.00225
SI51	0.88159	0.92976	0.9969
SI52	0.93259	0.96529	0.20674
SI53	0.82357	0.94093	0.36091
SI54	0.5833	0.17013	0.3353
SI55	0.69812	0.12038	0.19836
SI56	0.7332	0.16182	0.97811
SI57	0.88712	0.16818	0.98837
SI58	0.93775	0.12298	0.20065
SI59	0.81973	0.16333	0.32884
SI60	0.92546	0.05016	0.8591

SI61	0.80383	0.02052	0.71213
SI62	0.78332	0.06112	0.49494
SI63	0.62366	0.06389	0.49132
SI64	0.56989	0.02447	0.70047
SI65	0.67983	0.04637	0.85217
SI66	0.92167	0.82456	0.83913
SI67	0.802	0.86527	0.69608
SI68	0.77024	0.8189	0.48073
SI69	0.61577	0.82119	0.49638
SI70	0.56597	0.86702	0.70439
SI71	0.68169	0.82932	0.83717
SI72	0.42566	0.44272	0.63833
SI73	0.30574	0.4684	0.78876
SI74	0.28678	0.42525	0.00627
SI75	0.12884	0.42734	0.00548
SI76	0.07479	0.46664	0.79776
SI77	0.18381	0.44411	0.6446
SI78	0.42348	0.66659	0.65545
SI79	0.30054	0.62442	0.79212
SI80	0.2697	0.66846	0.00616
SI81	0.11532	0.66779	0.00094
SI82	0.06189	0.62523	0.79267
SI83	0.17838	0.66265	0.65864
SI84	0.07737	0.54992	0.13529
SI85	0.20093	0.52467	0.27499
SI86	0.22372	0.56272	0.49925
SI87	0.38403	0.56494	0.49823
SI88	0.43325	0.52516	0.28521
SI89	0.3271	0.54899	0.13325
SI90	0.08334	0.32175	0.15497
SI91	0.20109	0.36495	0.2965
SI92	0.23296	0.32625	0.51814
SI93	0.38767	0.32506	0.50763
SI94	0.4362	0.36672	0.29051
SI95	0.32168	0.31832	0.16363
O96	0.35997	0.0584	0.71783
O97	0.30089	0.05826	0.89305
O98	0.2019	0.04851	0.02744
O99	0.10424	0.0609	0.89294
O100	0.10342	0.05525	0.69531
O101	0.23049	0.03054	0.73292
O102	0.36034	0.82032	0.74958
O103	0.30622	0.8426	0.92444
O104	0.19109	0.84764	0.02077

O105	0.08658	0.82917	0.90233
O106	0.10414	0.83125	0.70601
O107	0.23001	0.8467	0.76235
O108	0.32041	0.94271	0.79519
O109	0.08708	0.94471	0.80448
O110	0.43269	0.12442	0.58485
O111	0.41774	0.99317	0.56459
O112	0.39842	0.86103	0.5688
O113	0.19423	0.12608	0.60322
O114	0.17845	0.99597	0.55795
O115	0.19653	0.8624	0.57001
O116	0.9911	0.03768	0.79066
O117	0.98526	0.85998	0.78377
O118	0.14262	0.93368	0.21984
O119	0.19912	0.92384	0.39629
O120	0.29795	0.94396	0.5281
O121	0.39696	0.92467	0.39727
O122	0.39722	0.94095	0.20005
O123	0.27099	0.9637	0.24123
O124	0.14591	0.16259	0.23413
O125	0.19793	0.15923	0.41137
O126	0.31089	0.14471	0.51362
O127	0.416	0.16675	0.39686
O128	0.40014	0.14869	0.20238
O129	0.27409	0.12946	0.25458
O130	0.1793	0.04488	0.31475
O131	0.42174	0.04429	0.32231
O132	0.06883	0.8646	0.09241
O133	0.08399	0.9949	0.06413
O134	0.09626	0.1276	0.05829
O135	0.30507	0.86224	0.12046
O136	0.31741	0.98797	0.05801
O137	0.30989	0.12226	0.06249
O138	0.51046	0.94583	0.29498
O139	0.51969	0.1316	0.28451
O140	0.64355	0.55211	0.28093
O141	0.68552	0.57086	0.09476
O142	0.79245	0.54544	0.98002
O143	0.90359	0.56344	0.08616
O144	0.89372	0.55121	0.28546
O145	0.76926	0.53181	0.23277
O146	0.64605	0.33681	0.27619
O147	0.6965	0.32136	0.10012
O148	0.80401	0.34655	0.98606

O149	0.90974	0.32174	0.10522
O150	0.90658	0.34297	0.30064
O151	0.77251	0.37174	0.24388
O152	0.67511	0.4462	0.16876
O153	0.92023	0.44516	0.16898
O154	0.5679	0.62623	0.39889
O155	0.57679	0.49665	0.43599
O156	0.58291	0.36292	0.44562
O157	0.79956	0.62111	0.37454
O158	0.81073	0.48937	0.41028
O159	0.79975	0.35766	0.44418
O160	0.01021	0.54167	0.20111
O161	0.02013	0.36139	0.20135
O162	0.87628	0.42251	0.75105
O163	0.79117	0.43913	0.59233
O164	0.69311	0.43786	0.45297
O165	0.60691	0.43374	0.60547
O166	0.60148	0.43203	0.8025
O167	0.73481	0.44131	0.78332
O168	0.85947	0.67703	0.73871
O169	0.80615	0.63996	0.56914
O170	0.68854	0.64099	0.47883
O171	0.58078	0.65738	0.59099
O172	0.60294	0.66588	0.78673
O173	0.72806	0.65447	0.72568
O174	0.81522	0.55248	0.72175
O175	0.58867	0.54718	0.70243
O176	0.92705	0.37117	0.92327
O177	0.90822	0.50229	0.90874
O178	0.88752	0.63224	0.92209
O179	0.67928	0.36096	0.91566
O180	0.67238	0.49464	0.9384
O181	0.69659	0.62656	0.91688
O182	0.4919	0.45611	0.70352
O183	0.48391	0.63057	0.71717
O184	0.64103	0.92689	0.28943
O185	0.70278	0.9271	0.11492
O186	0.8021	0.94237	0.98212
O187	0.90011	0.92347	0.11438
O188	0.89751	0.94345	0.31107
O189	0.76897	0.96196	0.27689
O190	0.64613	0.16763	0.25914
O191	0.69657	0.1436	0.08264
O192	0.8112	0.13866	0.98646

O193	0.91627	0.16453	0.10141
O194	0.89796	0.14914	0.29885
O195	0.77291	0.12567	0.24522
O196	0.6737	0.04249	0.2069
O197	0.92101	0.04425	0.18274
O198	0.56854	0.87238	0.4338
O199	0.58496	0.00399	0.43296
O200	0.60357	0.13532	0.4413
O201	0.81061	0.86519	0.40123
O202	0.8211	0.9945	0.45325
O203	0.80746	0.12897	0.43909
O204	0.01193	0.94957	0.21772
O205	0.01761	0.13322	0.2205
O206	0.86028	0.04932	0.78703
O207	0.80196	0.0709	0.61429
O208	0.70347	0.05042	0.48198
O209	0.60224	0.06657	0.60812
O210	0.6051	0.04529	0.80528
O211	0.73132	0.02156	0.76542
O212	0.85736	0.83182	0.76758
O213	0.80374	0.8254	0.59088
O214	0.69326	0.84563	0.48715
O215	0.59266	0.82032	0.61288
O216	0.60434	0.84522	0.80659
O217	0.72887	0.85959	0.74823
O218	0.81997	0.94431	0.67677
O219	0.58124	0.9451	0.67726
O220	0.93244	0.12301	0.91282
O221	0.92107	0.99224	0.9448
O222	0.90567	0.86002	0.9457
O223	0.69765	0.12215	0.8865
O224	0.68378	0.99673	0.94848
O225	0.69856	0.86385	0.94384
O226	0.491	0.04173	0.71248
O227	0.48599	0.8573	0.72048
O228	0.36181	0.44073	0.71275
O229	0.30467	0.42163	0.88808
O230	0.20779	0.44063	0.02499
O231	0.11505	0.42792	0.88571
O232	0.10725	0.44597	0.68907
O233	0.23292	0.46305	0.73577
O234	0.3545	0.65699	0.71705
O235	0.30037	0.66876	0.8937
O236	0.19264	0.64191	0.00297

O237	0.08869	0.66962	0.88631
O238	0.10098	0.64921	0.69171
O239	0.22669	0.62658	0.74086
O240	0.31903	0.54664	0.81828
O241	0.07864	0.54661	0.81546
O242	0.43263	0.37093	0.58155
O243	0.41672	0.50039	0.5536
O244	0.41462	0.6335	0.54512
O245	0.19382	0.36762	0.60528
O246	0.19322	0.49551	0.55218
O247	0.19115	0.62959	0.54911
O248	0.99845	0.43923	0.79349
O249	0.98212	0.63412	0.77845
O250	0.14075	0.55723	0.2102
O251	0.2035	0.56241	0.38235
O252	0.30374	0.56288	0.51521
O253	0.40164	0.5643	0.38068
O254	0.4	0.55527	0.18436
O255	0.27159	0.53524	0.21925
O256	0.14541	0.32512	0.2328
O257	0.19667	0.33961	0.41162
O258	0.3102	0.3512	0.51273
O259	0.41354	0.32958	0.39334
O260	0.39878	0.33139	0.19603
O261	0.27495	0.34966	0.25196
O262	0.18673	0.44509	0.29137
O263	0.41595	0.44562	0.29664
O264	0.07026	0.61738	0.06767
O265	0.08609	0.48595	0.06029
O266	0.10625	0.35454	0.04837
O267	0.31266	0.61902	0.07649
O268	0.32897	0.48628	0.05568
O269	0.30606	0.35358	0.05653
O270	0.51273	0.53813	0.2753
O271	0.51593	0.35821	0.27382
O272	0.43953	0.74538	0.63878
O273	0.19478	0.74202	0.65022
O274	0.27376	0.74397	0.05087
O275	0.10995	0.74278	0.04761
O276	0.06472	0.24388	0.13409
O277	0.30691	0.23891	0.15143
O278	0.22801	0.24784	0.54972
O279	0.39232	0.24816	0.54699
O280	0.56338	0.24726	0.35821

O281	0.80379	0.24127	0.33378
O282	0.72702	0.2405	0.95164
O283	0.88867	0.24523	0.94987
O284	0.93789	0.74626	0.86034
O285	0.69456	0.75013	0.85312
O286	0.77416	0.74129	0.44492
O287	0.60789	0.7464	0.45045
O288	0.93053	0.18067	0.61159
O289	0.82336	0.20854	0.68965
O290	0.87539	0.2931	0.55935
O291	0.92158	0.28714	0.72588
O292	0.02657	0.20798	0.45724
O293	0.03276	0.32922	0.63597
GA29	0.93139	0.37056	0.64006
H295	0.9623	0.18908	0.55736
H296	0.82268	0.3299	0.49894
H297	0.81422	0.16369	0.66038
H298	0.08707	0.56141	0.51834
H299	0.04306	0.57743	0.40848
H300	0.97199	0.60846	0.56063
H301	1.06635	0.36559	0.63804
H302	0.89305	0.52248	0.60003
H303	1.01332	0.37409	0.43648
H304	0.09295	0.46026	0.39704
H305	0.90171	0.42137	0.4823
H306	0.03906	0.30185	0.69584
AL30	0.8228	0.32485	0.3209
AL30	0.80075	0.46693	0.71339
P309	0.88746	0.24336	0.6461
C310	0.93774	0.50865	0.55879
C311	0.043	0.54473	0.47549
C312	0.98166	0.55704	0.53591
C313	1.0065	0.42448	0.4671
C314	0.9452	0.43778	0.5261
C315	0.05041	0.47298	0.44409
C316	0.04917	0.24633	0.40312