Theoretical study of ternary indole-cation-anion complexes

Jorge A. Carrazana-Garcia, Enrique M. Cabaleiro-Lago,
Alba Campo-Cacharrón, Jesus Rodriguez-Otero

Supporting Information (SI)

Table SI-1. LMO-EDA results (in kcal/mol) of the E_{int} (M-X) (the **cation-anion** interaction) in the indole-cation-anion complexes studied. The level and other conditions of the calculations are the same of Tables 2 and 4 in the paper.

	Elec	Exch	Rep	Pol	Disp
INBz	-126,05	-10,4	25,02	-9,24	1,29
INBb	-129,54	-11,21	26,96	-9,35	1,56
INNz	-132,62	-9,97	24,18	-11,14	1,15
INNb	-140,18	-14,85	36,04	-12,15	1,98
INCz	-137,46	-13,61	34,03	-10,79	0,67
INCb	-140,11	-15,36	38,44	-11,01	0,80
INFz	-150,78	-11,71	28,65	-11,06	4,09
INFb	-152,71	-12,93	31,65	-11,36	4,28
IABz	-111,90	-21,49	41,53	-14,16	-3,28
IABb	-116,41	-25,49	49,44	-15,31	-3,56
IANz	-156,45	-97,95	191,55	-133,17	2,53
IANb	-159,02	-100,97	196,76	-140,65	3,63
IACz	-124,85	-37,56	72,85	-30,70	-4,86
IACb	-130,78	-49,34	96,16	-41,07	-5,40
IAFz	-168,58	-98,95	189,00	-155,53	13,26
IAFb	-173,75	-101,71	194,22	-157,74	13,97
IGBz	-100,98	-23,71	44,41	-14,13	-4,43
IGBb	-104,88	-27,79	51,98	-15,36	-5,14
IGNz	-112,36	-36,82	68,27	-21,91	-6,43
IGNb	-115,82	-42,58	79,47	-24,68	-6,89
IGCz	-115,79	-37,15	67,52	-20,78	-6,41
IGCb	-120,23	-45,79	83,94	-25,13	-7,26
IGFz	-132,25	-48,15	89,53	-29,29	-3,90
IGFb	-138,22	-57,64	107,97	-34,17	-4,26
ITBz	-84,04	-16,87	29,10	-8,42	-4,53
ITBb	-87,37	-20,73	35,90	-9,31	-5,17
ITNz	-86,97	-23,12	39,44	-10,10	-7,11
ITNb	-89,14	-26,92	46,12	-10,93	-7,62
ITCz	-97,30	-34,49	58,84	-15,01	-6,09
ITCb	-101,18	-41,80	71,78	-16,77	-6,69
ITFz	-94,14	-27,35	46,60	-14,30	-3,48
ITFb	-103,97	-36,12	62,24	-17,00	-4,10

Table SI-2. LMO-EDA results (in kcal/mol) of the E_{int} (M-I) (the **cation-π** interaction) in the indole-cation-anion complexes studied. The level and other conditions of the calculations are the same of Tables 2 and 4 in the paper.

	Elec	Exch	Rep	Pol	Disp
INBz	-15,27	-7,84	19,30	-18,84	1,34
INBb	-17,26	-5,44	13,56	-15,93	0,68
INNz	-18,40	-4,74	11,68	-16,55	1,62
INNb	-17,06	-5,04	12,56	-15,60	0,63
INCz	-11,26	-3,23	7,93	-15,39	1,10
INCb	-14,37	-3,81	9,49	-15,05	0,29
INFz	-7,83	-3,18	7,95	-13,58	0,74
INFb	-14,47	-3,58	8,91	-14,73	0,33
IABz	-13,14	-12,20	23,15	-13,63	-4,95
IABb	-16,58	-10,83	20,45	-12,48	-4,35
IANz	-10,50	-6,86	12,59	-9,30	-4,17
IANb	-13,38	-6,22	11,39	-8,87	-3,95
IACz	-11,06	-11,81	22,24	-12,87	-4,99
IACb	-15,76	-9,97	18,70	-11,12	-4,34
IAFz	-7,81	-7,19	13,08	-8,93	-4,56
IAFb	-12,94	-6,24	11,37	-8,46	-4,05
IGBz	-15,17	-22,68	40,15	-9,13	-10,86
IGBb	-16,18	-18,82	33,32	-8,07	-9,12
IGNz	-13,35	-19,97	35,23	-8,73	-9,95
IGNb	-14,94	-17,62	31,03	-7,32	-8,91
IGCz	-13,62	-23,65	41,84	-9,08	-11,19
IGCb	-14,87	-19,18	33,56	-6,91	-10,02
IGFz	-12,07	-20,06	35,38	-8,44	-9,97
IGFb	-14,54	-17,77	31,29	-6,99	-8,85
ITBz	-8,33	-15,34	26,45	-5,19	-8,39
ITBb	-10,37	-13,29	22,67	-4,81	-7,52
ITNz	-9,98	-17,59	30,02	-5,99	-9,13
ITNb	-11,61	-17,28	29,20	-5,84	-9,17
ITCz	-7,70	-16,18	27,76	-5,19	-8,79
ITCb	-10,01	-12,59	21,61	-4,40	-7,23
ITFz	-10,65	-20,47	35,11	-6,14	-10,17
ITFb	-11,50	-16,66	28,16	-5,52	-9,13

Table SI-3. LMO-EDA results (in kcal/mol) of the E_{int} (I-X) (the **indole-anion** interaction) in the indole-cation-anion complexes studied. The level and other conditions of the calculations are the same of Tables 2 and 4 in the paper.

	Elec	Exch	Rep	Pol	Disp
INBz	-17,86	-28,27	51,28	-12,02	-6,00
INBb	0,42	-7,17	11,62	-4,98	-2,60
INNz	-1,48	-9,83	15,78	-5,17	-4,95
INNb	1,69	-6,03	9,41	-4,66	-2,58
INCz	-11,56	-15,82	26,13	-7,73	-4,67
INCb	-0,07	-6,36	9,76	-5,28	-1,88
INFz	-15,08	-15,95	27,17	-9,90	-3,56
INFb	1,05	-5,07	7,79	-5,56	-1,56
IABz	-12,88	-15,01	26,32	-7,98	-4,54
IABb	2,56	-7,40	11,81	-5,04	-3,28
IANz	-7,40	-8,98	14,96	-5,39	-3,89
IANb	3,22	-9,11	14,28	-4,71	-5,00
IACz	-17,46	-21,29	36,15	-10,32	-5,21
IACb	2,32	-8,38	12,72	-5,60	-2,80
IAFz	-16,36	-13,4	23,26	-9,56	-2,99
IAFb	3,25	-6,08	9,28	-5,54	-2,72
IGBz	-14,61	-12,72	22,61	-7,54	-3,32
IGBb	-0,49	-4,70	7,66	-4,00	-1,40
IGNz	-13,54	-13,52	23,63	-7,52	-4,00
IGNb	0,24	-5,72	9,04	-4,44	-2,32
IGCz	-20,45	-22,62	39,05	-11,79	-5,05
IGCb	1,97	-10,21	15,63	-6,05	-3,15
IGFz	-17,74	-17,33	30,14	-10,68	-3,41
IGFb	0,07	-4,83	7,41	-5,37	-1,67
ITBz	-14,29	-12,18	21,48	-7,32	-3,38
ITBb	1,39	-5,81	9,37	-4,26	-2,24
ITNz	-17,23	-19,78	33,76	-9,14	-6,16
ITNb	-0,48	-10,62	16,92	-5,60	-3,86
ITCz	-20,15	-22,78	39,19	-11,78	-5,21
ITCb	0,06	-9,04	13,96	-5,96	-2,57
ITFz	-25,70	-28,86	51,46	-17,24	-4,50
ITFb	1,49	-8,83	13,76	-6,44	-2,68

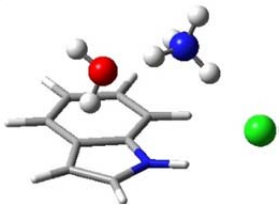
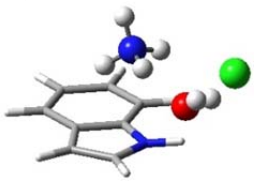
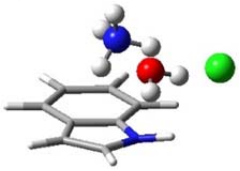
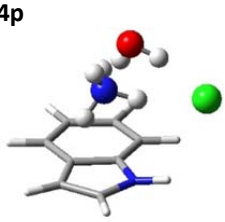
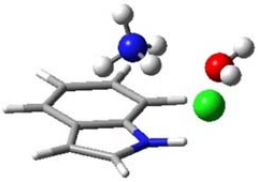
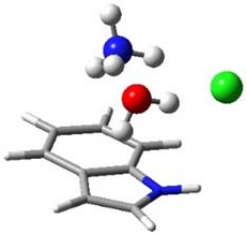
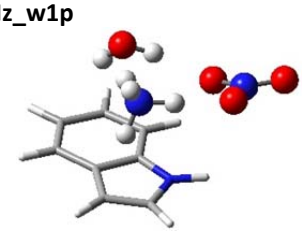
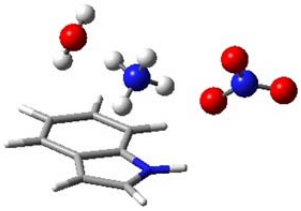
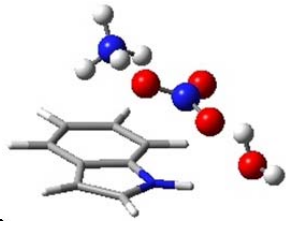
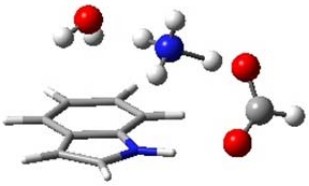
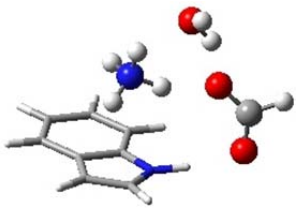
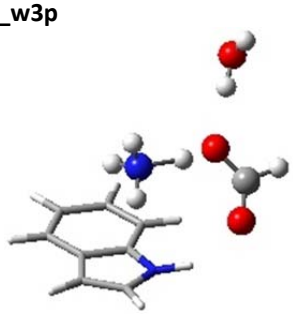
Table SI-4. LMO-EDA results (in kcal/mol) of the E_{int} (Thr) (the **three-body** interaction) in the indole-cation-anion complexes studied. The level and other conditions of the calculations are the same of Tables 2 and 4 in the paper.

	Elec	Exch	Rep	Pol	Disp
INBz	0.00	0.00	0.31	15.01	0.22
INBb	0.01	0.00	0.12	14.89	0.02
INNz	0.01	0.00	0.27	14.90	0.08
INNb	-0.01	0.00	0.11	15.71	-0.03
INCz	0.00	0.00	0.46	15.67	0.25
INCb	0.01	0.00	0.20	15.52	0.03
INFz	0.00	-0.01	0.35	16.40	0.11
INFb	0.00	0.00	0.11	16.42	-0.17
IABz	0.01	0.00	-0.16	11.67	0.54
IABb	0.00	0.00	-0.25	11.02	0.29
IANz	0.00	0.01	0.74	17.19	0.56
IANb	0.00	0.00	-0.32	14.51	0.46
IACz	0.00	0.00	-0.57	15.52	0.79
IACb	0.01	0.00	-0.83	13.85	0.22
IAFz	-0.01	-0.01	0.94	19.40	0.71
IAFb	0.00	0.00	0.00	15.62	0.02
IGBz	0.00	0.00	-0.26	7.51	0.46
IGBb	0.00	0.00	-0.34	7.21	0.14
IGNz	0.01	0.00	-0.52	9.41	0.60
IGNb	0.00	-0.01	-0.63	8.09	0.24
IGCz	0.00	0.00	-1.01	10.85	0.99
IGCb	0.00	0.01	-1.28	8.30	0.48
IGFz	0.00	0.01	-0.85	12.08	0.48
IGFb	-0.01	0.00	-0.81	10.09	-0.07
ITBz	0.00	0.00	-0.36	6.49	0.45
ITBb	-0.01	0.01	-0.47	5.39	0.21
ITNz	0.00	-0.01	-0.33	7.06	0.57
ITNb	0.00	0.00	-0.37	5.45	0.24
ITCz	0.00	0.00	-1.24	9.18	0.95
ITCb	0.00	0.00	-1.12	6.79	0.42
ITFz	0.01	0.00	-0.74	8.16	0.60
ITFb	0.00	0.01	-0.90	7.17	0.18

Table SI-5. Comparison of the results of the calculations at the M06-2X/6-31+G* level in the gas phase with the results at the same level in water (PCM) for the IACz complex as the anion is separated from the cation-indole fragment. The starting geometries correspond to the structure of the IACz complex optimized in gas phase and in water, respectively.

r IM-X	phase	Total	M-X	I-X	Thr
2.89	Gas	-150.34	-130.23	-16.01	15.48
3.13	Water (PCM)	-16.50	-8.99	-2.17	-2.24
3.30	Gas	-142.91	-118.63	-16.81	12.13
	Water (PCM)	-15.98	-8.29	-2.48	-2.06
3.70	Gas	-130.68	-104.28	-16.09	9.30
	Water (PCM)	-12.44	-5.09	-2.45	-1.67
4.00	Gas	-121.48	-94.53	-14.95	7.62
	Water (PCM)	-9.57	-2.94	-1.94	-1.41
4.50	Gas	-108.02	-81.35	-12.71	5.67
	Water (PCM)	-6.43	-1.21	-1.00	-0.90
4.70	Gas	-103.44	-77.11	-11.84	5.13
	Water (PCM)	-5.75	-0.87	-0.73	-0.82
4.80	Gas	-101.31	-75.16	-11.41	4.88
	Water (PCM)	-5.51	-0.76	-0.62	-0.81
4.90	Gas	-99.27	-73.32	-11.00	4.66
	Water (PCM)	-5.32	-0.68	-0.52	-0.80
5.00	Gas	-97.32	-71.57	-10.59	4.46
	Water (PCM)	-5.17	-0.61	-0.44	-0.79
5.50	Gas	-88.77	-64.01	-8.76	3.61
	Water (PCM)	-4.72	-0.39	-0.23	-0.75
6.00	Gas	-81.84	-58.02	-7.24	3.03
	Water (PCM)	-4.44	-0.27	-0.10	-0.71
7.00	Gas	-71.47	-49.29	-5.05	2.48
	Water (PCM)	-4.12	-0.11	0.07	-0.71
9.00	Gas	-58.73	-39.14	-2.74	2.76
	Water (PCM)	-3.89	0.03	0.18	-0.73

Fig. SI-1. Structures of the monohydrates included in the study of the influence of the solvent using a combination of PCM=water and the addition of one H_2O molecule. All the structures were optimized at the m062x/6-31+g* level of calculation in with PCM=water and are minima in their respective PES.

IACz_w1p 	**IACz_w2p** 	**IACz_w3p** 
IACz_w4p 	**IACz_w5p** 	**IACz_w6p** 
IANz_w1p 	**IANz_w2p** 	**IANz_w3p** 
IAFz_w1p 	**IAFz_w2p** 	**IAFz_w3p** 

Optimized structures of the indole-cation-anion complexes studied.

Level of calculation: M062X/6-31+G(d)

The labels use the following acronyms:
π-system: **I** = indole;
Cation: **A** = NH_4^+, **N** = Na^+, **G** = $C(NH_2)_3^+$, **T** = $N(CH_3)_4^+$;
Anion: **B** = BF_4^-, **C** = Cl^-, **F** = $HCOO^-$, **N** = NO_3^-;
Orientation: **z** = anion by the side of the N-H group of indole,
b = anion by the opposite side of the N-H group of indole.

IABz

C	0.468559	2.149690	-0.532901
C	1.591261	2.131166	0.258625
C	2.176279	0.824125	0.117460
C	3.269499	0.165648	0.711322
C	3.485996	-1.171020	0.417608
C	2.636674	-1.872407	-0.466874
C	1.561342	-1.249530	-1.080864
C	1.350473	0.104149	-0.784734
N	0.334548	0.943991	-1.175501
H	-0.265205	2.928262	-0.686762
H	1.966832	2.955647	0.848834
H	3.927279	0.697688	1.393666
H	4.323864	-1.691706	0.871468
H	2.832135	-2.920602	-0.671869
H	0.896695	-1.785781	-1.751930
H	-0.519505	0.633671	-1.624816
N	-0.345815	-0.219009	1.606502
H	-1.240799	-0.311630	2.109864
H	-0.467311	-0.763030	0.731775
H	-0.202902	0.765719	1.331322
H	0.459090	-0.557532	2.136436
B	-2.761485	-0.277040	-0.007055
F	-2.269056	1.045036	0.114130
F	-1.688095	-1.035118	-0.604019
F	-3.892568	-0.351894	-0.759892
F	-2.935212	-0.783726	1.304495

IABb

C	-1.536037	2.495032	-0.036388
C	-0.654366	1.745959	-0.762181
C	-1.124846	0.389697	-0.709947
C	-0.647485	-0.825405	-1.235543
C	-1.330364	-1.995985	-0.939737
C	-2.485922	-1.983560	-0.126034
C	-2.988195	-0.796891	0.397564
C	-2.301320	0.385180	0.087003
N	-2.526487	1.681722	0.485126
H	-1.541551	3.556258	0.169312
H	0.245434	2.091110	-1.250789
H	0.260834	-0.836034	-1.829715
H	-0.967602	-2.941401	-1.331315
H	-2.999599	-2.916849	0.086052
H	-3.883527	-0.788866	1.013434
H	-3.324702	2.003179	1.011657
N	0.165365	-0.886702	1.756087
H	0.908099	-1.299760	1.133452
H	0.362357	-1.100336	2.734120
H	-0.770992	-1.209393	1.480385
H	0.273292	0.125048	1.588335
B	2.636919	0.059762	-0.039030
F	3.994356	0.133193	0.106750
F	2.198222	-1.312472	0.177598
F	2.190005	0.460195	-1.289449
F	1.972131	0.826743	0.966580

IACz

C	-0.292414	2.192279	-0.474871
C	0.931991	2.163730	0.150463
C	1.434829	0.823950	0.009703
C	2.575959	0.145078	0.478603
C	2.683487	-1.216579	0.251286
C	1.676223	-1.925175	-0.444270
C	0.552473	-1.282803	-0.938541
C	0.453940	0.097542	-0.713087
N	-0.569658	0.962587	-1.016101
H	-0.995642	3.005889	-0.588467
H	1.425617	3.001305	0.623758
H	3.351237	0.679527	1.021013
H	3.555503	-1.754771	0.610982
H	1.788858	-2.994466	-0.596864
H	-0.236340	-1.818970	-1.457857
H	-1.500802	0.645673	-1.284486
N	-0.971004	-0.175261	1.825324
H	-1.338152	-0.198791	2.776930
H	-0.552939	0.743016	1.627152
H	-0.247991	-0.889651	1.705813
H	-1.820722	-0.378686	1.079423
Cl	-3.102525	-0.678794	-0.064569

IACb

C	-0.734829	2.457887	-0.208827
C	0.077070	1.617958	-0.916924
C	-0.454916	0.293180	-0.756185
C	-0.037783	-0.978314	-1.189624
C	-0.749158	-2.091739	-0.770865
C	-1.878894	-1.965255	0.069543
C	-2.318472	-0.723552	0.505330
C	-1.594805	0.398497	0.079971
N	-1.737791	1.729211	0.407426
H	-0.682313	3.529554	-0.076376
H	0.971905	1.887658	-1.459283
H	0.853772	-1.076946	-1.801338
H	-0.433425	-3.080751	-1.088561
H	-2.416627	-2.857549	0.376684
H	-3.185409	-0.628914	1.153705
H	-2.510805	2.125068	0.920851
N	1.025085	-0.415447	1.763883
H	0.384203	-1.132146	1.410780
H	1.946751	-0.282183	0.981230
H	1.377518	-0.678603	2.683380
H	0.519590	0.469705	1.821413
Cl	3.194971	-0.089601	-0.058598

IAFz

C	0.537027	2.377542	-0.246506
C	1.738660	1.994836	0.295243
C	1.868848	0.584466	0.055562
C	2.823269	-0.391904	0.396523
C	2.582263	-1.712732	0.057472
C	1.404869	-2.089267	-0.628430
C	0.452953	-1.150974	-0.991195
C	0.702966	0.183872	-0.645329
N	-0.080267	1.296518	-0.827141
H	0.071205	3.353112	-0.278802
H	2.448786	2.642334	0.790494
H	3.729288	-0.113386	0.928121
H	3.308973	-2.476394	0.318875
H	1.246390	-3.134466	-0.877456
H	-0.456790	-1.429006	-1.515506
H	-1.051987	1.244517	-1.122191
N	-0.794800	-0.085918	1.971697
H	-0.393308	0.810727	1.691724
H	-0.096267	-0.792592	1.739734
H	-0.894933	-0.073380	2.985082
H	-2.211351	-0.452800	1.222221
C	-3.441981	-0.382597	-0.310143
H	-4.430385	-0.752906	-0.618270
O	-2.759864	0.308818	-1.043683
O	-3.134810	-0.781243	0.896795

IAFb

C	1.640930	-2.298746	0.006044
C	0.604413	-1.769316	-0.711004
C	0.767647	-0.342316	-0.682224
C	0.019961	0.733728	-1.191284
C	0.434278	2.026898	-0.919258
C	1.589713	2.274827	-0.146106
C	2.352139	1.234604	0.364083
C	1.927435	-0.070666	0.085792
N	2.441706	-1.282240	0.488511
H	1.882060	-3.330293	0.222362
H	-0.201654	-2.313037	-1.182170
H	-0.879281	0.540929	-1.768221
H	-0.140267	2.867331	-1.297003
H	1.888272	3.300241	0.051621
H	3.240822	1.428053	0.958912
H	3.277531	-1.410081	1.037906
N	-0.988223	0.279027	1.872204
H	-2.415811	0.591063	1.090930
H	-0.989747	0.179924	2.884442
H	-0.257092	0.943712	1.617741
H	-0.725979	-0.617553	1.459051
C	-3.355959	-0.297715	-0.325772
H	-4.285356	-0.244095	-0.913085
O	-3.283714	0.680478	0.551351
O	-2.522688	-1.163163	-0.497491

IANz

C	0.586147	2.258454	-0.613976
C	1.771155	2.114680	0.062505
C	2.113722	0.719567	0.007679
C	3.157913	-0.060019	0.538753
C	3.133374	-1.431198	0.349392
C	2.085647	-2.051817	-0.367764
C	1.048931	-1.312449	-0.913977
C	1.082884	0.075257	-0.721603
N	0.177926	1.038483	-1.097400
H	-0.000639	3.146321	-0.805411
H	2.338592	2.909723	0.525934
H	3.964828	0.408786	1.095565
H	3.931016	-2.045120	0.756950
H	2.095123	-3.130259	-0.495093
H	0.233094	-1.782898	-1.454598
H	-0.725419	0.831388	-1.503729
N	-0.525765	0.008626	1.887058
H	-0.448769	-0.080739	2.898834
H	-0.040541	-0.783297	1.462062
H	-0.005555	0.844297	1.608998
H	-1.925833	0.047914	1.411874
N	-3.136261	-0.327903	-0.087672
O	-4.260100	-0.349421	-0.515714
O	-2.979369	0.103917	1.156909
O	-2.123760	-0.663925	-0.698862

IANb

C	2.048201	-2.219789	-0.095135
C	0.914833	-1.797210	-0.732726
C	0.939449	-0.360920	-0.715950
C	0.061124	0.636928	-1.174430
C	0.366910	1.965393	-0.930044
C	1.544295	2.327249	-0.239692
C	2.439489	1.367438	0.210776
C	2.121885	0.025776	-0.036171
N	2.778366	-1.127766	0.329038
H	2.405326	-3.221857	0.097787
H	0.140428	-2.424700	-1.150191
H	-0.843338	0.366674	-1.713698
H	-0.311818	2.742346	-1.267887
H	1.757210	3.377622	-0.064062
H	3.348224	1.647104	0.737051
H	3.669562	-1.170778	0.799181
N	-0.435625	0.282319	2.063566
H	0.285326	0.948399	1.781957
H	-0.150356	-0.636012	1.720496
H	-0.472245	0.253815	3.079869
H	-1.751673	0.552177	1.326291
N	-2.820398	-0.314207	-0.028969
O	-2.626936	0.747405	0.756514
O	-2.113199	-1.292468	0.160537
O	-3.678635	-0.203235	-0.868554

IGBz

C	-0.496603	2.376583	-0.646325
C	-1.774122	2.107829	-1.083174
C	-2.292973	1.080461	-0.222627
C	-3.510535	0.376518	-0.141454
C	-3.647673	-0.619756	0.813360
C	-2.592856	-0.931337	1.703709
C	-1.388732	-0.244640	1.662368
C	-1.258614	0.766536	0.700352
N	-0.196553	1.588369	0.429964
H	0.237546	3.075326	-1.023797
H	-2.292728	2.614289	-1.885585
H	-4.331774	0.615015	-0.812881
H	-4.586527	-1.160529	0.893492
H	-2.739274	-1.707530	2.449809
H	-0.571211	-0.470694	2.340880
H	0.737274	1.453578	0.807609
C	-0.075899	-1.567076	-1.104592
N	-1.379564	-1.875580	-1.306236
N	0.672112	-2.365001	-0.356063
N	0.462311	-0.523433	-1.728667
H	1.435140	-0.281182	-1.538630
H	-0.139790	0.256887	-1.979424
H	-1.936469	-1.153238	-1.749432
H	-1.865579	-2.273366	-0.508416
H	0.294911	-3.224271	0.014203
H	1.626603	-2.083156	-0.122412
B	2.958207	0.179014	0.360750
F	2.501855	1.206529	-0.499160
F	1.934487	-0.048868	1.317073
F	4.152790	0.475157	0.944502
F	3.039838	-1.010307	-0.434843

IGBb

C	-1.779489	2.587641	0.367563
C	-0.870893	1.896762	-0.385256
C	-1.482479	0.638722	-0.720300
C	-1.053714	-0.485561	-1.448059
C	-1.909916	-1.571719	-1.560330
C	-3.190509	-1.560505	-0.962270
C	-3.639955	-0.463261	-0.240365
C	-2.772531	0.631239	-0.131281
N	-2.922136	1.824915	0.539180
H	-1.716032	3.576552	0.800583
H	0.122436	2.216261	-0.669506
H	-0.061836	-0.493547	-1.890653
H	-1.600951	-2.442793	-2.131362
H	-3.842716	-2.421218	-1.081034
H	-4.628591	-0.453120	0.210842
H	-3.772058	2.146058	0.978269
C	0.255383	-1.088224	1.434333
N	1.048513	-1.963231	0.837278
N	-1.022567	-1.450730	1.721497
N	0.715890	0.090188	1.843031
H	0.055948	0.858614	1.880101
H	1.676117	0.361585	1.593264
H	1.943675	-1.681332	0.413397
H	0.713501	-2.900366	0.666567
H	-1.514373	-1.953554	0.986303
H	-1.598355	-0.734089	2.145494
B	3.155761	0.290505	-0.439933
F	4.070238	0.904251	-1.245613
F	3.210023	0.790912	0.894758
F	3.377417	-1.115424	-0.359204
F	1.828006	0.470244	-0.891465

IGCz

C	-0.012091	2.482559	0.449863
C	1.218166	2.141560	0.964298
C	1.674089	1.005921	0.211403
C	2.828473	0.198627	0.234019
C	2.917437	-0.870839	-0.643832
C	1.878131	-1.152915	-1.561964
C	0.739008	-0.364692	-1.622478
C	0.655113	0.717493	-0.735965
N	-0.341579	1.646073	-0.582541
H	-0.687723	3.276196	0.739853
H	1.748881	2.664877	1.747835
H	3.639943	0.415614	0.924439
H	3.808932	-1.491813	-0.645130
H	1.988391	-1.986659	-2.250199
H	-0.063396	-0.563861	-2.327936
H	-1.295473	1.508595	-0.936511
C	-0.722237	-1.388016	1.090705
N	0.483448	-1.874699	1.471843
N	-1.480034	-2.070608	0.243131
N	-1.202355	-0.273939	1.644045
H	-2.047324	0.105818	1.190102
H	-0.534162	0.423128	1.962274
H	1.075986	-1.231549	1.984133
H	1.003820	-2.372107	0.756668
H	-1.135859	-2.926264	-0.167751
H	-2.244164	-1.549816	-0.225901
Cl	-3.207691	0.301287	-0.735500

IGCb

C	0.711683	-1.788079	-1.830948
C	0.007043	-0.636087	-2.011032
C	0.602121	0.356103	-1.154809
C	0.323522	1.710149	-0.902406
C	1.112795	2.394071	0.008954
C	2.175695	1.751580	0.682740
C	2.470074	0.413659	0.453332
C	1.671588	-0.269225	-0.472756
N	1.694162	-1.596924	-0.862203
H	0.591385	-2.758458	-2.293282
H	-0.864196	-0.496729	-2.635793
H	-0.519891	2.187679	-1.391306
H	0.913172	3.441926	0.213163
H	2.786689	2.319702	1.379105
H	3.299280	-0.075630	0.960042
H	2.498879	-2.199144	-0.759378
C	-0.727590	-0.826784	1.573319
N	-0.990989	0.460211	1.790774
N	0.303001	-1.436267	2.228023
N	-1.528238	-1.534298	0.799470
H	-1.371053	-2.520280	0.653450
H	-2.193410	-1.000527	0.191017
H	-1.714581	0.865906	1.165962
H	-0.217371	1.068951	2.031699
H	0.975289	-0.808671	2.652249
H	0.747118	-2.187547	1.713281
Cl	-3.021085	0.722438	-0.567707

IGFz

C	0.863533	2.554182	0.467180
C	2.028010	1.936382	0.855471
C	2.125103	0.726689	0.086007
C	3.056909	-0.327231	0.008255
C	2.797158	-1.391767	-0.841647
C	1.622841	-1.430190	-1.627646
C	0.697642	-0.398626	-1.588752
C	0.969804	0.682133	-0.740194
N	0.239481	1.819665	-0.508144
H	0.427755	3.483665	0.808169
H	2.743689	2.317159	1.570989
H	3.966928	-0.303351	0.602635
H	3.513867	-2.204703	-0.918233
H	1.451201	-2.276185	-2.287620
H	-0.207759	-0.419676	-2.189244
H	-0.747646	1.914869	-0.760019
C	-0.718230	-1.221842	1.217811
N	0.441040	-1.824812	1.597823
N	-1.644426	-1.892196	0.553341
N	-0.961250	0.030590	1.600099
H	-1.647370	0.560171	1.017023
H	-0.184139	0.570409	1.966342
H	1.242593	-1.206974	1.683835
H	0.680416	-2.676500	1.106407
H	-1.427674	-2.808427	0.188510
H	-2.506340	-1.393140	0.181953
C	-3.463955	0.630752	-0.756249
O	-2.484217	1.295981	-0.312005
O	-3.706658	-0.574332	-0.531251
H	-4.175330	1.173868	-1.407951

IGFb

C	-1.773487	2.466739	0.440706
C	-0.726537	1.998627	-0.301884
C	-1.052585	0.646509	-0.665754
C	-0.385478	-0.347059	-1.402404
C	-0.995138	-1.582166	-1.564934
C	-2.260835	-1.852230	-1.000865
C	-2.939906	-0.894102	-0.260867
C	-2.320733	0.353394	-0.102971
N	-2.732274	1.477743	0.578785
H	-1.923484	3.434737	0.898713
H	0.192789	2.516951	-0.542098
H	0.598628	-0.143182	-1.817777
H	-0.496319	-2.355162	-2.143425
H	-2.719386	-2.824598	-1.158366
H	-3.918521	-1.100165	0.164950
H	-3.636049	1.602236	1.009367
C	0.971568	-1.034705	1.310652
N	1.928905	-1.676646	0.661841
N	-0.134558	-1.701218	1.757250
N	1.131546	0.250873	1.608471
H	0.335239	0.741679	1.994100
H	1.723896	0.814201	0.932188
H	2.718375	-1.116597	0.200113
H	1.746782	-2.609309	0.319715
H	-0.318355	-2.590377	1.309291
H	-0.977589	-1.139774	1.817426
C	3.431621	0.953707	-0.813063
O	2.440071	1.560088	-0.329084
O	3.752290	-0.244586	-0.617651
H	4.088827	1.537794	-1.486444

IGNz

C	-0.883168	2.511207	-0.728623
C	-2.122301	1.983243	-1.002931
C	-2.307388	0.882474	-0.098102
C	-3.343103	-0.043911	0.136845
C	-3.159736	-1.025953	1.099052
C	-1.959040	-1.107473	1.841086
C	-0.928228	-0.201669	1.644510
C	-1.122906	0.798238	0.682572
N	-0.291265	1.816018	0.293526
H	-0.372374	3.349466	-1.182799
H	-2.830346	2.362869	-1.726564
H	-4.274506	0.017702	-0.420601
H	-3.956311	-1.737204	1.298681
H	-1.850357	-1.883286	2.593951
H	-0.004059	-0.252654	2.213546
H	0.696762	1.867120	0.541025
C	0.197001	-1.465965	-1.165926
N	-1.031088	-2.021491	-1.314833
N	1.151163	-2.102916	-0.506447
N	0.477870	-0.312352	-1.771100
H	1.281241	0.199443	-1.375845
H	-0.294425	0.257681	-2.101433
H	-1.799259	-1.367117	-1.430955
H	-1.268733	-2.765249	-0.671076
H	0.937144	-2.947930	0.002329
H	2.088306	-1.663589	-0.361948
N	3.353340	0.295219	0.375933
O	4.156184	0.911796	1.048623
O	2.256933	0.837227	0.014921
O	3.561881	-0.891491	0.015360

IGNb

C	1.691487	2.534086	-0.718745
C	0.700553	2.036252	0.079132
C	1.189243	0.796049	0.617472
C	0.641413	-0.168579	1.480354
C	1.404307	-1.278735	1.811981
C	2.706992	-1.451744	1.295271
C	3.270595	-0.521337	0.432421
C	2.495343	0.598859	0.100855
N	2.769858	1.665312	-0.727691
H	1.725813	3.446912	-1.297373
H	-0.275407	2.468276	0.257048
H	-0.366142	-0.033564	1.864955
H	1.002710	-2.021959	2.495503
H	3.287303	-2.322036	1.589064
H	4.277882	-0.649880	0.044852
H	3.662983	1.856585	-1.156576
C	-0.411387	-1.378615	-1.254142
N	0.792805	-1.964729	-1.487671
N	-0.677694	-0.182360	-1.774640
N	-1.363015	-2.018842	-0.595960
H	-2.272953	-1.528720	-0.404358
H	-1.135236	-2.842221	-0.058304
H	1.000000	-2.791925	-0.942739
H	1.585851	-1.332410	-1.526542
H	0.085709	0.341793	-2.181579
H	-1.378447	0.372112	-1.244494
N	-3.371675	0.512651	0.384229
O	-2.213653	0.984477	0.163029
O	-3.635618	-0.643236	-0.054892
O	-4.198642	1.153183	1.004996

INBz

C	-0.288061	1.999788	0.749408
C	-1.430781	2.119667	-0.005899
C	-2.048281	0.817351	-0.035331
C	-3.206331	0.285451	-0.640509
C	-3.475063	-1.062760	-0.493335
C	-2.611638	-1.907792	0.241854
C	-1.471872	-1.418360	0.853126
C	-1.212156	-0.045939	0.720359
N	-0.152922	0.703871	1.183994
H	0.462838	2.735593	1.002394
H	-1.808199	3.031887	-0.447012
H	-3.872946	0.926987	-1.210280
H	-4.363332	-1.486326	-0.952029
H	-2.846374	-2.964590	0.323275
H	-0.795366	-2.063322	1.405127
H	0.689705	0.332585	1.621579
Na	0.322297	0.391590	-1.366046
B	2.607510	-0.373596	-0.065108
F	2.340026	0.886710	-0.707914
F	2.491844	-0.196273	1.318354
F	3.811326	-0.878881	-0.445240
F	1.521959	-1.211984	-0.500422

INBb

C	-0.948593	2.333557	-0.314511
C	-0.386239	1.215868	-0.870910
C	-1.301520	0.130452	-0.620493
C	-1.281766	-1.251460	-0.908167
C	-2.332418	-2.039158	-0.465089
C	-3.413811	-1.481763	0.252187
C	-3.464269	-0.128903	0.545874
C	-2.396935	0.666027	0.107121
N	-2.154335	2.010397	0.270335
H	-0.581419	3.349952	-0.287658
H	0.565704	1.167185	-1.385423
H	-0.450583	-1.678276	-1.463690
H	-2.332376	-3.103087	-0.681280
H	-4.224130	-2.126837	0.577757
H	-4.299025	0.297806	1.094843
H	-2.770393	2.664143	0.730336
Na	0.494765	-0.431769	1.146749
B	2.914559	-0.150833	-0.015907
F	2.898223	0.915086	-0.893222
F	2.500147	0.310452	1.291937
F	4.111512	-0.800220	0.060799
F	1.857970	-1.070625	-0.389294

INCz

C	-0.543862	2.020237	-0.596418
C	0.596643	2.149248	0.158137
C	1.288268	0.887285	0.083090
C	2.473564	0.372760	0.647264
C	2.801153	-0.951938	0.417811
C	1.971434	-1.788442	-0.363480
C	0.809887	-1.310557	-0.946282
C	0.494822	0.040365	-0.735264
N	-0.597486	0.766144	-1.156657
H	-1.337717	2.730350	-0.782574
H	0.923442	3.043453	0.670783
H	3.112917	1.006026	1.256166
H	3.710000	-1.362073	0.847502
H	2.250017	-2.827746	-0.507769
H	0.160661	-1.947816	-1.538872
H	-1.468440	0.329391	-1.458731
Na	-1.024733	-0.078776	1.375468
Cl	-3.014580	-0.822460	0.146518

INCb

C	-0.645547	2.411821	-0.268005
C	0.190088	1.440374	-0.750357
C	-0.484415	0.182591	-0.548455
C	-0.144159	-1.160394	-0.819499
C	-1.033956	-2.156455	-0.449543
C	-2.263878	-1.846586	0.171822
C	-2.628275	-0.537525	0.441722
C	-1.725922	0.469579	0.075078
N	-1.795939	1.835338	0.227943
H	-0.517332	3.484983	-0.240981
H	1.167746	1.581023	-1.193489
H	0.807633	-1.392213	-1.293044
H	-0.787768	-3.194857	-0.648958
H	-2.939174	-2.652555	0.442695
H	-3.576589	-0.303629	0.917363
H	-2.577187	2.340439	0.618787
Na	1.386196	-0.127817	1.239737
Cl	3.421322	-0.242647	-0.055980

INFz

C	-0.714711	2.456137	0.057366
C	-1.806567	1.961189	-0.607159
C	-1.880952	0.562331	-0.292473
C	-2.730719	-0.494045	-0.670939
C	-2.479117	-1.768604	-0.190084
C	-1.398933	-2.020119	0.685157
C	-0.552477	-0.999231	1.096670
C	-0.801892	0.287646	0.589926
N	-0.115367	1.460318	0.790636
H	-0.307069	3.457550	0.067793
H	-2.476905	2.525238	-1.240052
H	-3.568949	-0.311005	-1.337760
H	-3.125566	-2.590911	-0.481215
H	-1.239519	-3.027080	1.059618
H	0.272643	-1.173734	1.782534
H	0.826648	1.483298	1.177452
Na	1.195770	-0.708963	-0.891336
C	3.427448	-0.022913	0.095832
H	4.409847	0.274018	0.509850
O	2.398489	0.277924	0.768576
O	3.412823	-0.632343	-1.000295

INFb

C	-0.961803	2.408669	-0.263390
C	-0.183884	1.456326	-0.866193
C	-0.808014	0.185445	-0.596561
C	-0.487011	-1.147959	-0.928265
C	-1.311724	-2.161558	-0.467244
C	-2.456455	-1.878733	0.310322
C	-2.798424	-0.579378	0.647330
C	-1.960871	0.445087	0.187282
N	-2.028703	1.807549	0.369343
H	-0.846234	3.483297	-0.235988
H	0.722410	1.615411	-1.435903
H	0.399684	-1.357402	-1.521848
H	-1.080078	-3.193779	-0.711517
H	-3.082432	-2.698132	0.650592
H	-3.680399	-0.364362	1.244051
H	-2.754776	2.294141	0.873480
Na	1.340843	-0.054909	0.910882
C	3.610279	-0.204113	-0.127290
H	4.619924	-0.271798	-0.578417
O	2.625429	-0.150228	-0.913147
O	3.537194	-0.187139	1.129961

INNz

C	-1.252996	2.482275	-0.097833
C	-2.054582	1.698766	-0.883546
C	-1.962555	0.364081	-0.359223
C	-2.465024	-0.891222	-0.758373
C	-2.084321	-2.025718	-0.054064
C	-1.217717	-1.937134	1.060962
C	-0.717239	-0.714291	1.486501
C	-1.095325	0.427264	0.765815
N	-0.700096	1.731312	0.911935
H	-1.027183	3.536580	-0.175414
H	-2.641093	2.028648	-1.729176
H	-3.135244	-0.968813	-1.610306
H	-2.462491	-2.997846	-0.355487
H	-0.936840	-2.841782	1.591129
H	-0.029939	-0.644174	2.324104
H	0.130360	1.999888	1.425566
Na	0.491829	-0.830343	-0.985575
N	2.824249	0.022453	-0.119733
O	3.894695	0.373755	0.334642
O	1.770403	0.715264	0.057467
O	2.700128	-1.048920	-0.784101

INNb

C	-1.060093	2.415049	-0.352051
C	-0.373037	1.391054	-0.946037
C	-1.100531	0.183479	-0.652443
C	-0.895637	-1.178125	-0.961593
C	-1.791210	-2.113451	-0.467409
C	-2.897521	-1.723328	0.320194
C	-3.128045	-0.393810	0.634037
C	-2.217630	0.551432	0.141826
N	-2.167515	1.917099	0.301297
H	-0.850432	3.475489	-0.340458
H	0.539112	1.467026	-1.522029
H	-0.041629	-1.473991	-1.565793
H	-1.647934	-3.165185	-0.695513
H	-3.582811	-2.481597	0.686418
H	-3.981586	-0.097877	1.237237
H	-2.842725	2.472604	0.805081
Na	0.826636	-0.310521	1.026423
N	3.229715	-0.159549	0.043713
O	2.242109	-0.497003	-0.682219
O	2.991558	0.067564	1.271056
O	4.349062	-0.055232	-0.415064

ITBz

C	-1.107975	-1.444014	2.082395
C	-2.310429	-0.779601	2.084398
C	-2.655967	-0.551808	0.709359
C	-3.719035	0.094065	0.047667
C	-3.722809	0.135341	-1.337128
C	-2.690245	-0.469610	-2.090618
C	-1.627884	-1.108057	-1.472408
C	-1.616983	-1.124452	-0.070398
N	-0.692127	-1.653214	0.794105
H	-0.502379	-1.788394	2.909726
H	-2.883518	-0.501651	2.958223
H	-4.529539	0.543604	0.616024
H	-4.541920	0.623572	-1.857379
H	-2.735888	-0.437562	-3.175529
H	-0.822192	-1.570221	-2.036073
H	0.214231	-2.008029	0.500038
N	0.698082	2.259856	0.149352
C	0.437043	1.437227	-1.077194
H	-0.642406	1.399378	-1.238503
H	0.945704	1.907267	-1.921093
H	0.832643	0.433552	-0.923134
C	2.173545	2.410001	0.360502
H	2.601053	2.897051	-0.517697
H	2.327825	3.022691	1.251277
H	2.607618	1.417779	0.481295
C	0.096514	1.567762	1.335312
H	0.241613	2.201839	2.212925
H	-0.966984	1.408156	1.144999
H	0.605156	0.610700	1.458608
C	0.072934	3.600137	-0.018685
H	0.281413	4.201679	0.867921
H	0.497047	4.078116	-0.903728
H	-1.004130	3.471927	-0.141581
B	2.659552	-1.212761	-0.293129
F	2.197009	-0.707220	0.965209
F	1.520458	-1.774464	-0.931451
F	3.643827	-2.148886	-0.109855
F	3.101256	-0.113439	-1.051023

ITBb

C	-2.048676	-2.380196	-1.294869
C	-1.358121	-2.197042	-0.131035
C	-1.872264	-0.997843	0.468772
C	-1.559516	-0.282424	1.636895
C	-2.232681	0.901980	1.898600
C	-3.218556	1.394529	1.014513
C	-3.554947	0.704438	-0.141768
C	-2.874903	-0.492433	-0.398981
N	-2.963089	-1.356843	-1.464344
H	-1.958738	-3.158640	-2.039531
H	-0.551059	-2.809191	0.244481
H	-0.785102	-0.651919	2.302619
H	-2.009983	1.458708	2.805390
H	-3.735630	2.320216	1.251713
H	-4.318591	1.079113	-0.818359
H	-3.615297	-1.280108	-2.229530
N	1.132479	2.088101	-0.498804
C	0.639271	3.465408	-0.770613
H	0.505080	3.587371	-1.847158
H	-0.315060	3.603096	-0.258295
H	1.372872	4.184556	-0.401368
C	0.123457	1.095574	-1.000291
H	0.043315	1.214136	-2.083377
H	0.464772	0.088863	-0.751402
H	-0.830885	1.312955	-0.516341
C	1.310537	1.908238	0.979615
H	1.678155	0.899020	1.168077
H	2.030838	2.651553	1.327792
H	0.338054	2.052664	1.453976
C	2.442332	1.873040	-1.193637
H	3.162823	2.590280	-0.795584
H	2.775698	0.852086	-1.004476
H	2.290348	2.038894	-2.262002
B	2.494651	-1.430035	0.293807
F	2.996487	-2.686302	0.531760
F	3.409822	-0.414004	0.664612
F	1.298402	-1.207140	1.029043
F	2.186823	-1.243877	-1.078396

ITCz

C	1.338379	1.513177	1.911725
C	2.023305	0.330451	2.059311
C	2.170240	-0.223692	0.742565
C	2.737519	-1.401949	0.217291
C	2.691376	-1.617555	-1.150735
C	2.097519	-0.674305	-2.022044
C	1.527110	0.490936	-1.538323
C	1.561117	0.695174	-0.151774
N	1.073694	1.743312	0.587164
H	1.018094	2.225084	2.660722
H	2.392946	-0.080883	2.988691
H	3.214706	-2.124099	0.875286
H	3.133143	-2.518443	-1.567348
H	2.092768	-0.868461	-3.090950
H	1.046732	1.216893	-2.188866
H	0.374327	2.392650	0.213941
N	-2.090761	-1.109484	0.256035
C	-2.260563	-2.503954	0.742188
H	-2.867994	-2.493342	1.649154
H	-2.755600	-3.092265	-0.032887
H	-1.274793	-2.921430	0.956338
C	-3.423986	-0.500975	-0.055159
H	-4.022923	-0.499391	0.857898
H	-3.248351	0.520747	-0.410727
H	-3.907874	-1.107638	-0.823573
C	-1.248779	-1.107728	-0.985992
H	-1.159706	-0.069824	-1.321492
H	-0.266132	-1.518453	-0.740020
H	-1.749421	-1.724839	-1.736015
C	-1.409844	-0.285230	1.309393
H	-1.335016	0.735967	0.924114
H	-2.018872	-0.322145	2.215615
H	-0.416762	-0.702665	1.493074
Cl	-1.644127	2.366449	-0.899766

ITCb

C	2.547018	1.648598	-1.380396
C	1.787715	1.815053	-0.256998
C	1.735881	0.536678	0.396391
C	1.101865	0.070802	1.560657
C	1.216201	-1.271753	1.888863
C	1.948531	-2.166076	1.076557
C	2.589733	-1.731159	-0.074615
C	2.478375	-0.372822	-0.398159
N	2.964587	0.332282	-1.474942
H	2.829261	2.362330	-2.142082
H	1.276170	2.712514	0.063327
H	0.510410	0.759252	2.159070
H	0.741896	-1.647033	2.792339
H	2.023830	-3.210917	1.365507
H	3.160743	-2.417225	-0.694965
H	3.568722	-0.037059	-2.192589
N	-2.352608	-0.780679	-0.543170
C	-2.697007	-2.107362	-1.117371
H	-2.748724	-2.020894	-2.204485
H	-1.921969	-2.823043	-0.835829
H	-3.663459	-2.427056	-0.722398
C	-1.014504	-0.336516	-1.062403
H	-1.072885	-0.295550	-2.152740
H	-0.806513	0.651180	-0.635916
H	-0.263681	-1.063765	-0.741776
C	-2.292663	-0.878785	0.953234
H	-2.033639	0.115461	1.337539
H	-3.274264	-1.198696	1.310413
H	-1.526005	-1.611294	1.213255
C	-3.389179	0.232510	-0.927133
H	-4.355161	-0.105514	-0.545718
H	-3.097162	1.189470	-0.476755
H	-3.414112	0.298259	-2.017036
Cl	-1.546418	2.427844	0.899757

ITFz

C	1.391363	1.089794	2.145319
C	2.093509	-0.091677	2.048119
C	2.185788	-0.393230	0.648806
C	2.749423	-1.437475	-0.112604
C	2.650870	-1.390958	-1.494180
C	2.003382	-0.315200	-2.148030
C	1.433517	0.722059	-1.430024
C	1.522900	0.665154	-0.031535
N	1.050272	1.546088	0.903412
H	1.110016	1.652359	3.025762
H	2.511174	-0.656682	2.870432
H	3.268320	-2.258226	0.376868
H	3.092900	-2.184339	-2.090786
H	1.957515	-0.304047	-3.233448
H	0.919139	1.547213	-1.914547
H	0.380254	2.312578	0.665837
N	-1.899663	-1.476507	0.198053
C	-1.362625	-0.558882	1.258573
H	-0.338046	-0.858432	1.491565
H	-1.386206	0.454871	0.848879
H	-2.000741	-0.653462	2.140600
C	-3.297259	-1.066446	-0.144706
H	-3.257675	-0.036212	-0.510710
H	-3.676390	-1.744970	-0.912047
H	-3.908936	-1.141666	0.757074
C	-1.041072	-1.362776	-1.027748
H	-0.018984	-1.646309	-0.763763
H	-1.443770	-2.039387	-1.785552
H	-1.077976	-0.321972	-1.356487
C	-1.879698	-2.877668	0.693848
H	-2.271423	-3.536724	-0.083584
H	-0.848735	-3.147990	0.929840
H	-2.499608	-2.945470	1.590058
C	-1.740452	2.787083	-0.686707
H	-2.426940	3.491915	-1.205055
O	-0.837862	3.305112	0.008401
O	-1.961641	1.558790	-0.866648

ITFb

C	1.805570	-0.800837	2.327685
C	1.333435	-1.599061	1.326462
C	1.658478	-0.947856	0.087447
C	1.452745	-1.282422	-1.261986
C	1.925594	-0.422045	-2.239787
C	2.581968	0.781887	-1.899832
C	2.782166	1.146272	-0.575969
C	2.321362	0.261060	0.409543
N	2.376715	0.342553	1.785937
H	1.767964	-0.930304	3.400622
H	0.772869	-2.517501	1.426162
H	0.898154	-2.182712	-1.507100
H	1.779889	-0.665887	-3.288160
H	2.939690	1.436175	-2.690062
H	3.296435	2.068492	-0.316750
H	2.913968	1.019955	2.305542
N	-1.675636	1.481785	0.122801
C	-1.125817	2.851266	0.293973
H	-1.523359	3.279829	1.216438
H	-0.036622	2.785219	0.346173
H	-1.422574	3.461423	-0.561526
C	-1.265065	0.624444	1.283853
H	-1.751091	1.015238	2.181109
H	-1.564808	-0.404676	1.065943
H	-0.179326	0.683342	1.378573
C	-1.126843	0.875521	-1.135986
H	-1.432144	-0.174234	-1.163759
H	-1.520208	1.442014	-1.983419
H	-0.038659	0.949109	-1.098320
C	-3.170344	1.533216	0.043836
H	-3.444191	2.159634	-0.808108
H	-3.523552	0.503392	-0.083175
H	-3.545373	1.975258	0.969828
C	-2.481040	-2.353799	-0.306565
H	-2.875797	-3.387667	-0.439960
O	-1.235758	-2.229095	-0.220156
O	-3.335752	-1.432449	-0.258251

ITNz

C	-1.394131	-1.348231	2.225294
C	-2.408505	-0.450620	1.994011
C	-2.512599	-0.307492	0.568218
C	-3.321903	0.456296	-0.297617
C	-3.145425	0.330288	-1.666016
C	-2.176779	-0.550707	-2.202657
C	-1.356218	-1.303893	-1.380686
C	-1.532701	-1.164380	0.003009
N	-0.873640	-1.784526	1.034529
H	-1.001112	-1.720951	3.161504
H	-3.019343	0.027665	2.747277
H	-4.083925	1.120325	0.103088
H	-3.771410	0.905343	-2.342513
H	-2.073578	-0.632913	-3.280901
H	-0.586778	-1.961613	-1.773502
H	0.014228	-2.264906	0.900991
N	0.966739	2.082648	0.166011
C	0.850495	1.099745	1.292737
H	-0.195307	0.796295	1.374938
H	1.475190	0.238378	1.050166
H	1.177196	1.595075	2.210041
C	0.054030	3.231392	0.414509
H	0.346745	3.722294	1.344902
H	0.130938	3.931581	-0.419802
H	-0.967058	2.851396	0.492392
C	2.381045	2.559296	0.066428
H	3.011813	1.689626	-0.127085
H	2.444967	3.281407	-0.750078
H	2.651074	3.036438	1.010838
C	0.574572	1.402857	-1.113209
H	-0.488182	1.161541	-1.056898
H	0.766005	2.094953	-1.936480
H	1.168268	0.489715	-1.204010
N	2.799302	-1.505703	-0.302521
O	3.516941	-2.494702	-0.253278
O	1.537286	-1.612030	-0.241526
O	3.281045	-0.347754	-0.407087

ITNb

C	-2.177389	0.054206	-2.348966
C	-1.540984	-1.004870	-1.769910
C	-1.676922	-0.845993	-0.346331
C	-1.246235	-1.602306	0.758092
C	-1.584960	-1.168276	2.030799
C	-2.330530	0.013595	2.228774
C	-2.745901	0.794285	1.157941
C	-2.411878	0.346199	-0.127589
N	-2.678051	0.896139	-1.365897
H	-2.309419	0.302645	-3.393133
H	-1.000993	-1.794906	-2.271640
H	-0.631687	-2.485873	0.609712
H	-1.259555	-1.742500	2.893119
H	-2.584283	0.321484	3.239445
H	-3.324064	1.702254	1.311965
H	-3.313250	1.661617	-1.534388
N	1.510981	1.755043	0.114931
C	0.891694	3.096559	0.291393
H	1.157400	3.724335	-0.561213
H	-0.192130	2.971504	0.345871
H	1.264801	3.541208	1.215914
C	1.022867	1.160881	-1.176192
H	1.365373	1.806202	-1.988774
H	1.429429	0.152462	-1.287287
H	-0.067185	1.133682	-1.144843
C	1.108032	0.880734	1.267614
H	1.602150	-0.087793	1.176144
H	1.420842	1.377936	2.189008
H	0.023354	0.765979	1.247620
C	3.001603	1.878915	0.080137
H	3.332314	2.311061	1.026992
H	3.414629	0.877907	-0.058575
H	3.273474	2.535510	-0.748960
N	2.024398	-1.930345	-0.187018
O	2.993142	-1.132717	-0.331337
O	1.816905	-2.451268	0.920353
O	1.257593	-2.134032	-1.148474