

SUPPORTING INFORMATION DOCUMENT

A Two-Step MM and QM/MM approach to model AIEE of Aryloxy Benzothiadiazole derivatives for Optoelectronic Applications

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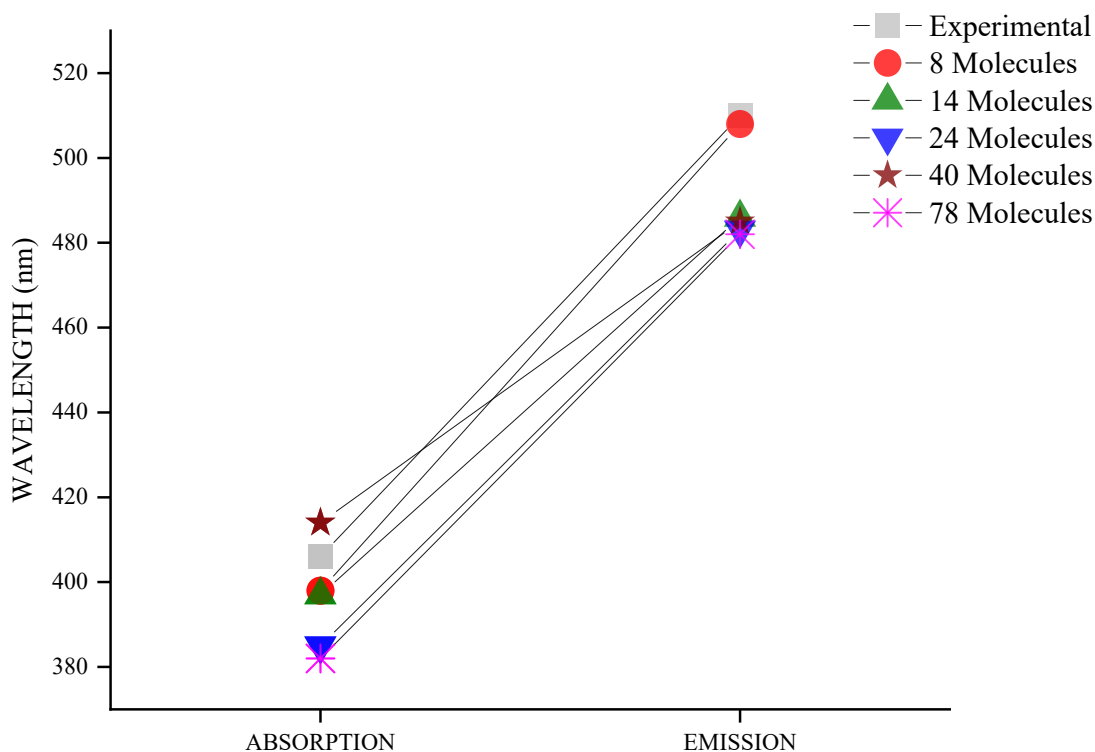


Figure 1: Comparison of cluster size with absorption and emission spectra for HB. 8 molecule clusters yields values closer to experimentally reported values.

Table 1: Selected bond parameters of derivatives in the individual molecules and in cluster (ONIOM)

Molecule	Structure	O2-C12	O2-C18	C9-C15	C7-C8	C8-C12	C7-C9	C12-C13	C9-C10	C10-C13	C12-O2-C18	C12-O2-C18-C21 (ϕ_1)	C7-C9-C15-C16 (ϕ_2)	C13-C12-O2-C18 (ϕ_3)
HB	CRYSTAL	1.364	1.399	1.482	1.434	1.426	1.429	1.362	1.373	1.424	119.67	120.26	39.65	1.82
	MONOMER	1.364	1.395	1.482	1.456	1.433	1.441	1.374	1.382	1.427	119.14	98.78	38.79	3.44
	CLUSTER	1.361	1.389	1.481	1.454	1.434	1.440	1.373	1.380	1.426	122.77	132.58	33.22	6.02
FB	MONOMER	1.359	1.397	1.483	1.457	1.431	1.441	1.374	1.377	1.428	120.61	148.76	43.36	54.26
	CLUSTER	1.354	1.399	1.480	1.456	1.435	1.442	1.372	1.375	1.429	122.44	115.90	35.14	10.11
CB	MONOMER	1.350	1.404	1.482	1.447	1.433	1.438	1.388	1.390	1.459	121.98	137.98	51.24	45.13
	CLUSTER	1.343	1.401	1.489	1.450	1.433	1.456	1.384	1.399	1.468	125.32	116.03	8.64	14.45
NB	MONOMER	1.347	1.403	1.484	1.447	1.435	1.439	1.382	1.377	1.435	122.62	144.38	55.86	46.61
	CLUSTER	1.339	1.398	1.487	1.450	1.432	1.456	1.381	1.385	1.438	124.19	137.99	16.25	5.39
CAB	MONOMER	1.374	1.410	1.489	1.446	1.430	1.440	1.381	1.384	1.450	119.83	142.14	58.21	125.35
	CLUSTER	1.356	1.394	1.499	1.454	1.438	1.454	1.385	1.388	1.460	126.29	135.60	13.07	5.18

Table 2: Occupancy numbers for selected bonds

Molecule	O2-C12	O2-C18	C9-C15	C7-C8	C7-C9	C8-C12	C9-C10	C10-C13	C12-C13
HB	0.0182	0.0163	0.0144	0.0259	0.0187	0.0198	0.1515	0.0067	0.1703
FB	0.0118	0.0176	0.0142	0.0263	0.0181	0.0203	0.1798	0.0207	0.1912
CB	0.0125	0.0184	0.0145	0.0259	0.0190	0.0208	0.1694	0.0164	0.1935
NB	0.0122	0.0187	0.0148	0.0259	0.0199	0.0209	0.1599	0.0129	0.1900
CAB	0.0153	0.0197	0.0150	0.0264	0.0185	0.0228	0.1399	0.0121	0.1702

Table 3 Percentage of p character in bonds connecting ArO, Btz, Ar and EWG groups

Molecule	C12-C13	C9-C10	C10-C13	O2-C12	O2-C18	C9-C15
HB	99.9	99.9	65	68	68	66
FB	99.9	99.9	64	68	68	65
CB	99.9	99.9	66	67	68	65
NB	99.9	99.9	63	67	68	65
CAB	99.9	99.9	66	68	68	66

SIT 4: List of NBO interactions

Type	Donor NBO (i)			Acceptor NBO (j)			E(2) kcal/mol
	NBO	Type	Bond	NBO	Type	Bond	
HB							
π-π*							
	8	BD	N4-C7	585	BD*	N6-C8	13.73
	12	BD	N6-C8	581	BD*	N4-C7	13.88
	12	BD	N6-C8	595	BD*	C12-C13	10.58
	17	BD	C9-C10	581	BD*	N4-C7	25.97
	17	BD	C9-C10	595	BD*	C12-C13	15.2
	22	BD	C12-C13	585	BD*	N6-C8	21.97
	22	BD	C12-C13	590	BD*	C9-C10	17.16
	25	BD	C15-C16	590	BD*	C9-C10	10.33
	25	BD	C15-C16	607	BD*	C19-C26	19.31
	25	BD	C15-C16	617	BD*	C27-C28	15.64
	30	BD	C18-C21	611	BD*	C23-C24	16.37
	30	BD	C18-C21	621	BD*	C29-C31	20.32
	34	BD	C19-C26	598	BD*	C15-C16	19.75
	34	BD	C19-C26	617	BD*	C27-C28	14.12
	38	BD	C23-C24	603	BD*	C18-C21	21.46
	38	BD	C23-C24	621	BD*	C29-C31	17.01

	44	BD	C27-C28	598	BD*	C15-C16	19.55
	44	BD	C27-C28	607	BD*	C19-C26	21.16
	48	BD	C29-C31	603	BD*	C18-C21	18.75
	48	BD	C29-C31	611	BD*	C23-C24	20.27
σ-σ^*							
	61	BD	C45-H48	633	BD*	C45-H47	11.52
n-π^*							
	95	LP	S1	581	BD*	N4-C7	19.46
	95	LP	S1	585	BD*	N6-C8	20.43
	97	LP	O2	595	BD*	C12-C13	31.2
	102	LP	O5	611	BD*	C23-C24	29.69
FB							
π-π^*							
	8	BD	N4-C7	613	BD*	N6-C8	13.78
	12	BD	N6-C8	609	BD*	N4-C7	13.83
	12	BD	N6-C8	623	BD*	C11-C12	10.7
	17	BD	C9-C10	609	BD*	N4-C7	23.22
	17	BD	C9-C10	623	BD*	C11-C12	15.99
	22	BD	C11-C12	613	BD*	N6-C8	21.62
	22	BD	C11-C12	618	BD*	C9-C10	15.9
	25	BD	C13-C14	618	BD*	C9-C10	10.47
	25	BD	C13-C14	635	BD*	C17-C24	19.48
	25	BD	C13-C14	645	BD*	C25-C26	20.2
	30	BD	C16-C19	639	BD*	C21-C22	17.57
	30	BD	C16-C19	649	BD*	C27-C29	20.03
	34	BD	C17-C24	626	BD*	C13-C14	19.84
	34	BD	C17-C24	645	BD*	C25-C26	19.97
	38	BD	C21-C22	631	BD*	C16-C19	20.8
	38	BD	C21-C22	649	BD*	C27-C29	18.22
	44	BD	C25-C26	626	BD*	C13-C14	20.53
	44	BD	C25-C26	635	BD*	C17-C24	20.34
	48	BD	C27-C29	631	BD*	C16-C19	19.32
	48	BD	C27-C29	639	BD*	C21-C22	19.5
n-π^*							
	97	LP	S1	609	BD*	N4-C7	20.17
	97	LP	S1	613	BD*	N6-C8	20.51
	99	LP	O2	623	BD*	C11-C12	15.19
	99	LP	O2	631	BD*	C16-C19	12.64
	104	LP	O5	639	BD*	C21-C22	29.49
	108	LP	F47	623	BD*	C11-C12	19.74

	111	LP	F48	618	BD*	C9-C10	18.98
CB							
π-π^*							
	8	BD	N4-C7	644	BD*	N6-C8	14.4
	8	BD	N4-C7	649	BD*	C9-C10	10.45
	12	BD	N6-C8	640	BD*	N4-C7	14.45
	12	BD	N6-C8	654	BD*	C11-C12	11.4
	17	BD	C9-C10	640	BD*	N4-C7	22.91
	17	BD	C9-C10	654	BD*	C11-C12	14.57
	17	BD	C9-C10	699	BD*	C48-N50	17.15
	22	BD	C11-C12	644	BD*	N6-C8	20.7
	22	BD	C11-C12	649	BD*	C9-C10	15.24
	26	BD	C13-C17	661	BD*	C14-C26	16.24
	26	BD	C13-C17	674	BD*	C24-C25	19.46
	29	BD	C14-C26	658	BD*	C13-C17	16.25
	29	BD	C14-C26	674	BD*	C24-C25	20.2
	31	BD	C16-C19	670	BD*	C21-C22	16.56
	31	BD	C16-C19	680	BD*	C27-C29	20.16
	38	BD	C21-C22	663	BD*	C16-C19	21.87
	38	BD	C21-C22	680	BD*	C27-C29	17.95
	42	BD	C24-C25	658	BD*	C13-C17	16.99
42	BD	C24-C25	661	BD*	C14-C26	16.15	
48	BD	C27-C29	663	BD*	C16-C19	18.93	
48	BD	C27-C29	670	BD*	C21-C22	19.68	
n-π*							
	105	LP	S1	640	BD*	N4-C7	19.99
	105	LP	S1	644	BD*	N6-C8	20.65
	107	LP	O2	654	BD*	C11-C12	23.91
	112	LP	O5	670	BD*	C21-C22	30.29
	114	LP	N49	655	BD*	C12-C47	13.1
	115	LP	N50	652	BD*	C10-C48	13.03
NB							
π-π^*							
	9	BD	N4-C7	673	BD*	S1-N6	13.15
	9	BD	N4-C7	687	BD*	C9-C10	10.45
	17	BD	C9-C10	679	BD*	N4-C7	21.65
	17	BD	C9-C10	692	BD*	C11-C12	15.72
	22	BD	C11-C12	687	BD*	C9-C10	16.77
	26	BD	C13-C17	699	BD*	C14-C26	18.69

	26	BD	C13-C17	712	BD*	C24-C25	19.25
	29	BD	C14-C26	696	BD*	C13-C17	20.6
	29	BD	C14-C26	712	BD*	C24-C25	20.24
	31	BD	C16-C19	708	BD*	C21-C22	16.66
	31	BD	C16-C19	718	BD*	C27-C29	20.02
	38	BD	C21-C22	701	BD*	C16-C19	22.04
	38	BD	C21-C22	718	BD*	C27-C29	17.47
	42	BD	C24-C25	696	BD*	C13-C17	20.52
	42	BD	C24-C25	699	BD*	C14-C26	19.97
	48	BD	C27-C29	701	BD*	C16-C19	19.21
	48	BD	C27-C29	708	BD*	C21-C22	19.6
σ-σ^*							
	20	BD	C10-N47	735	BD*	N48-O49	14.02
	64	BD	N47-O52	735	BD*	N48-O49	34.69
n-π^*							
	108	LP	O2	692	BD*	C11-C12	22.21
	113	LP	O5	708	BD*	C21-C22	30.28
	118	LP	O49	737	BD*	N48-O50	124.01
	125	LP	O52	733	BD*	N47-O51	29.75
n-σ^*							
	117	LP	O49	693	BD*	C12-N48	12.18
	117	LP	O49	736	BD*	N48-O50	17.8
	120	LP	O50	693	BD*	C12-N48	12.68
	122	LP	O51	690	BD*	C10-N47	13.11
	124	LP	O52	690	BD*	C10-N47	11.82
	124	LP	O52	732	BD*	N47-O51	18.02
CAB							
n-σ^*							
	5	BD	O3-C25	722	BD*	C27-C29	1008.87
	5	BD	O3-C25	725	BD*	C31-H33	22.89
	5	BD	O3-C25	739	BD*	O48-H53	33.12
	5	BD	O3-C25	742	BD*	O50-C52	43.85
	5	BD	O3-C25	743	BD*	O50-C52	470.19
	6	BD	O3-C31	743	BD*	O50-C52	24.47
	8	BD	N4-C7	686	BD*	N6-C8	14.69
	9	BD	O5-C21	722	BD*	C27-C29	31.34
	9	BD	O5-C21	743	BD*	O50-C52	29.27
	10	BD	O5-C43	725	BD*	C31-H33	15.74
	10	BD	O5-C43	739	BD*	O48-H53	23.97
	10	BD	O5-C43	742	BD*	O50-C52	29.58

10	BD	O5-C43	743	BD*	O50-C52	397.34
12	BD	N6-C8	682	BD*	N4-C7	13.91
12	BD	N6-C8	696	BD*	C11-C12	10.79
14	BD	C7-C9	743	BD*	O50-C52	123.97
16	BD	C9-C10	743	BD*	O50-C52	219.79
17	BD	C9-C10	682	BD*	N4-C7	22.01
17	BD	C9-C10	696	BD*	C11-C12	15.05
17	BD	C9-C10	725	BD*	C31-H33	68.94
17	BD	C9-C10	739	BD*	O48-H53	50.75
17	BD	C9-C10	742	BD*	O50-C52	12.78
18	BD	C9-C13	725	BD*	C31-H33	17.65
18	BD	C9-C13	739	BD*	O48-H53	31.49
18	BD	C9-C13	742	BD*	O50-C52	33.41
19	BD	C10-C12	743	BD*	O50-C52	130.56
20	BD	C10-C52	706	BD*	C16-C29	13.86
20	BD	C10-C52	725	BD*	C31-H33	58.24
20	BD	C10-C52	739	BD*	O48-H53	19.12
20	BD	C10-C52	742	BD*	O50-C52	32.41
22	BD	C11-C12	686	BD*	N6-C8	22.26
22	BD	C11-C12	691	BD*	C9-C10	14.75
26	BD	C13-C17	703	BD*	C14-C26	21.28
26	BD	C13-C17	716	BD*	C24-C25	21.1
26	BD	C13-C17	739	BD*	O48-H53	20.14
27	BD	C14-H15	739	BD*	O48-H53	11.84
27	BD	C14-H15	742	BD*	O50-C52	10.96
28	BD	C14-C26	742	BD*	O50-C52	10.52
29	BD	C14-C26	700	BD*	C13-C17	19.25
29	BD	C14-C26	716	BD*	C24-C25	20.09
30	BD	C16-C19	743	BD*	O50-C52	190.49
31	BD	C16-C19	712	BD*	C21-C22	16.4
36	BD	C19-C22	743	BD*	O50-C52	77.35
37	BD	C21-C22	743	BD*	O50-C52	148.03
38	BD	C21-C22	705	BD*	C16-C19	22.54
39	BD	C21-C27	743	BD*	O50-C52	28.2
41	BD	C24-C25	743	BD*	O50-C52	1008.87
42	BD	C24-C25	700	BD*	C13-C17	20.18
42	BD	C24-C25	703	BD*	C14-C26	21.28
46	BD	C27-H28	706	BD*	C16-C29	17.97
46	BD	C27-H28	725	BD*	C31-H33	25.46
46	BD	C27-H28	739	BD*	O48-H53	31.15
46	BD	C27-H28	742	BD*	O50-C52	31.97

	47	BD	C27-C29	743	BD*	O50-C52	224.56
	48	BD	C27-C29	705	BD*	C16-C19	19.44
	48	BD	C27-C29	712	BD*	C21-C22	19.79
	64	BD	048-C51	738	BD*	048-C51	11.81
	64	BD	048-C51	743	BD*	O50-C52	15.4
	65	BD	048-H53	737	BD*	O47-C51	46.7
	65	BD	048-H53	738	BD*	048-C51	34.76
	65	BD	048-H53	743	BD*	O50-C52	372.04
	66	BD	049-C52	679	BD*	O3-C25	50.81
	66	BD	049-C52	680	BD*	O3-C31	20.89
	66	BD	049-C52	699	BD*	C13-C17	36.37
	66	BD	049-C52	706	BD*	C16-C29	79.11
	66	BD	049-C52	717	BD*	C24-C35	11
	66	BD	049-C52	718	BD*	C25-C26	34.2
	66	BD	049-C52	719	BD*	C26-C39	45.14
	66	BD	049-C52	721	BD*	C27-C29	18.26
	66	BD	049-C52	722	BD*	C27-C29	9004.68
	66	BD	049-C52	725	BD*	C31-H33	308.18
	66	BD	049-C52	727	BD*	C35-H36	13.36
	66	BD	049-C52	731	BD*	C39-H41	10.81
	66	BD	049-C52	733	BD*	C43-H44	14.55
	66	BD	049-C52	739	BD*	O48-H53	140.97
	66	BD	049-C52	742	BD*	O50-C52	436.64
	66	BD	049-C52	743	BD*	O50-C52	6898.72
	67	BD	049-H54	679	BD*	O3-C25	136.68
	67	BD	049-H54	680	BD*	O3-C31	49.15
	67	BD	049-H54	687	BD*	C7-C8	15.91
	67	BD	049-H54	690	BD*	C9-C10	11.45
	67	BD	049-H54	699	BD*	C13-C17	48.79
	67	BD	049-H54	706	BD*	C16-C29	109.3
	67	BD	049-H54	717	BD*	C24-C35	12.29
	67	BD	049-H54	718	BD*	C25-C26	33.37
	67	BD	049-H54	719	BD*	C26-C39	61.6
	67	BD	049-H54	721	BD*	C27-C29	38.71
	67	BD	049-H54	724	BD*	C31-H32	16.31
	67	BD	049-H54	725	BD*	C31-H33	1437.49
	67	BD	049-H54	727	BD*	C35-H36	38.87
	67	BD	049-H54	729	BD*	C35-H38	10.69
	67	BD	049-H54	731	BD*	C39-H41	18.47
	67	BD	049-H54	732	BD*	C39-H42	11.03
	67	BD	049-H54	733	BD*	C43-H44	28.22

	67	BD	049-H54	739	BD*	048-H53	2007.09
	67	BD	049-H54	742	BD*	050-C52	626.5
	68	BD	050-C52	722	BD*	C27-C29	19.03
	68	BD	050-C52	743	BD*	050-C52	12.13
n-π*							
	109	LP	S1	682	BD*	N4-C7	19.52
	109	LP	S1	686	BD*	N6-C8	19.84
	110	LP	02	679	BD*	03-C25	28.99
	110	LP	02	680	BD*	03-C31	10.81
	110	LP	02	699	BD*	C13-C17	14.13
	110	LP	02	706	BD*	C16-C29	57.48
	110	LP	02	718	BD*	C25-C26	10.57
	110	LP	02	719	BD*	C26-C39	15.44
	110	LP	02	721	BD*	C27-C29	12.7
	110	LP	02	725	BD*	C31-H33	142.27
	110	LP	02	739	BD*	048-H53	326.63
	110	LP	02	742	BD*	050-C52	194.22
	110	LP	02	743	BD*	050-C52	25981.84
	111	LP	02	705	BD*	C16-C19	10.23
	111	LP	02	739	BD*	048-H53	11.34
	112	LP	03	725	BD*	C31-H33	10.7
	116	LP	05	712	BD*	C21-C22	30.5
	118	LP	047	743	BD*	050-C52	269.43
	119	LP	047	697	BD*	C12-C51	19.85
	119	LP	047	739	BD*	048-H53	20.61
	120	LP	048	679	BD*	03-C25	19.54
	120	LP	048	706	BD*	C16-C29	19.23
	120	LP	048	719	BD*	C26-C39	10.18
	120	LP	048	725	BD*	C31-H33	100.25
	120	LP	048	737	BD*	047-C51	25.4
	120	LP	048	739	BD*	048-H53	103.58
	120	LP	048	742	BD*	050-C52	104.17
	122	LP	049	675	BD*	S1-N4	10
	122	LP	049	679	BD*	03-C25	64.11
	122	LP	049	680	BD*	03-C31	26.12
	122	LP	049	699	BD*	C13-C17	38.29
	122	LP	049	706	BD*	C16-C29	84.19
	122	LP	049	717	BD*	C24-C35	11.25
	122	LP	049	718	BD*	C25-C26	33.97
	122	LP	049	719	BD*	C26-C39	45.16
	122	LP	049	721	BD*	C27-C29	20.95

	122	LP	049	725	BD*	C31-H33	386.43
	122	LP	049	727	BD*	C35-H36	16.24
	122	LP	049	733	BD*	C43-H44	13.81
	122	LP	049	739	BD*	048-H53	240.31
	122	LP	049	742	BD*	050-C52	624.81
	125	LP	050	694	BD*	C10-C52	20.66
	109	LP	S1	682	BD*	N4-C7	19.52
	109	LP	S1	686	BD*	N6-C8	19.84
	110	LP	02	743	BD*	050-C52	25981.84
	111	LP	02	705	BD*	C16-C19	10.23
	116	LP	05	712	BD*	C21-C22	30.5
	118	LP	047	743	BD*	050-C52	269.43
	120	LP	048	737	BD*	047-C51	25.4
n-σ*							
	110	LP	02	679	BD*	03-C25	28.99
	110	LP	02	680	BD*	03-C31	10.81
	110	LP	02	699	BD*	C13-C17	14.13
	110	LP	02	706	BD*	C16-C29	57.48
	110	LP	02	718	BD*	C25-C26	10.57
	110	LP	02	719	BD*	C26-C39	15.44
	110	LP	02	721	BD*	C27-C29	12.7
	110	LP	02	725	BD*	C31-H33	142.27
	110	LP	02	739	BD*	048-H53	326.63
	110	LP	02	742	BD*	050-C52	194.22
	111	LP	02	739	BD*	048-H53	11.34
	112	LP	03	725	BD*	C31-H33	10.7
	119	LP	047	697	BD*	C12-C51	19.85
	119	LP	047	739	BD*	048-H53	20.61
	120	LP	048	679	BD*	03-C25	19.54
	120	LP	048	706	BD*	C16-C29	19.23
	120	LP	048	719	BD*	C26-C39	10.18
	120	LP	048	725	BD*	C31-H33	100.25
	120	LP	048	739	BD*	048-H53	103.58
	120	LP	048	742	BD*	050-C52	104.17
	122	LP	049	675	BD*	S1-N4	10
	122	LP	049	679	BD*	03-C25	64.11
	122	LP	049	680	BD*	03-C31	26.12
	122	LP	049	699	BD*	C13-C17	38.29
	122	LP	049	706	BD*	C16-C29	84.19
	122	LP	049	717	BD*	C24-C35	11.25
	122	LP	049	718	BD*	C25-C26	33.97

	122	LP	049	719	BD*	C26-C39	45.16
	122	LP	049	721	BD*	C27-C29	20.95
	122	LP	049	725	BD*	C31-H33	386.43
	122	LP	049	727	BD*	C35-H36	16.24
	122	LP	049	733	BD*	C43-H44	13.81
	122	LP	049	739	BD*	048-H53	240.31
	122	LP	049	742	BD*	050-C52	624.81
	125	LP	050	694	BD*	C10-C52	20.66
σ-π*							
	5	BD	03-C25	722	BD*	C27-C29	1008.87
	5	BD	03-C25	743	BD*	050-C52	470.19
	6	BD	03-C31	743	BD*	050-C52	24.47
	9	BD	05-C21	722	BD*	C27-C29	31.34
	9	BD	05-C21	743	BD*	050-C52	29.27
	10	BD	05-C43	743	BD*	050-C52	397.34
	14	BD	C7-C9	743	BD*	050-C52	123.97
	16	BD	C9-C10	743	BD*	050-C52	219.79
	19	BD	C10-C12	743	BD*	050-C52	130.56
	30	BD	C16-C19	743	BD*	050-C52	190.49
	36	BD	C19-C22	743	BD*	050-C52	77.35
	37	BD	C21-C22	743	BD*	050-C52	148.03
	39	BD	C21-C27	743	BD*	050-C52	28.2
	41	BD	C24-C25	743	BD*	050-C52	1008.87
	47	BD	C27-C29	743	BD*	050-C52	224.56
	64	BD	048-C51	743	BD*	050-C52	15.4
	65	BD	048-H53	737	BD*	047-C51	46.7
	65	BD	048-H53	743	BD*	050-C52	372.04
	66	BD	049-C52	722	BD*	C27-C29	9004.68
	66	BD	049-C52	743	BD*	050-C52	6898.72
	68	BD	050-C52	722	BD*	C27-C29	19.03
	68	BD	050-C52	743	BD*	050-C52	12.13
σ-σ*							
	5	BD	03-C25	725	BD*	C31-H33	22.89
	5	BD	03-C25	739	BD*	048-H53	33.12
	5	BD	03-C25	742	BD*	050-C52	43.85
	10	BD	05-C43	725	BD*	C31-H33	15.74
	10	BD	05-C43	739	BD*	048-H53	23.97
	10	BD	05-C43	742	BD*	050-C52	29.58
	18	BD	C9-C13	725	BD*	C31-H33	17.65
	18	BD	C9-C13	739	BD*	048-H53	31.49
	18	BD	C9-C13	742	BD*	050-C52	33.41

	20	BD	C10-C52	706	BD*	C16-C29	13.86
	20	BD	C10-C52	725	BD*	C31-H33	58.24
	20	BD	C10-C52	739	BD*	O48-H53	19.12
	20	BD	C10-C52	742	BD*	O50-C52	32.41
	27	BD	C14-H15	739	BD*	O48-H53	11.84
	27	BD	C14-H15	742	BD*	O50-C52	10.96
	28	BD	C14-C26	742	BD*	O50-C52	10.52
	46	BD	C27-H28	706	BD*	C16-C29	17.97
	46	BD	C27-H28	725	BD*	C31-H33	25.46
	46	BD	C27-H28	739	BD*	O48-H53	31.15
	46	BD	C27-H28	742	BD*	O50-C52	31.97
	64	BD	O48-C51	738	BD*	O48-C51	11.81
	65	BD	O48-H53	738	BD*	O48-C51	34.76
	66	BD	O49-C52	679	BD*	O3-C25	50.81
	66	BD	O49-C52	680	BD*	O3-C31	20.89
	66	BD	O49-C52	699	BD*	C13-C17	36.37
	66	BD	O49-C52	706	BD*	C16-C29	79.11
	66	BD	O49-C52	717	BD*	C24-C35	11
	66	BD	O49-C52	718	BD*	C25-C26	34.2
	66	BD	O49-C52	719	BD*	C26-C39	45.14
	66	BD	O49-C52	721	BD*	C27-C29	18.26
	66	BD	O49-C52	725	BD*	C31-H33	308.18
	66	BD	O49-C52	727	BD*	C35-H36	13.36
	66	BD	O49-C52	731	BD*	C39-H41	10.81
	66	BD	O49-C52	733	BD*	C43-H44	14.55
	66	BD	O49-C52	739	BD*	O48-H53	140.97
	66	BD	O49-C52	742	BD*	O50-C52	436.64
	67	BD	O49-H54	679	BD*	O3-C25	136.68
	67	BD	O49-H54	680	BD*	O3-C31	49.15
	67	BD	O49-H54	687	BD*	C7-C8	15.91
	67	BD	O49-H54	690	BD*	C9-C10	11.45
	67	BD	O49-H54	699	BD*	C13-C17	48.79
	67	BD	O49-H54	706	BD*	C16-C29	109.3
	67	BD	O49-H54	717	BD*	C24-C35	12.29
	67	BD	O49-H54	718	BD*	C25-C26	33.37
	67	BD	O49-H54	719	BD*	C26-C39	61.6
	67	BD	O49-H54	721	BD*	C27-C29	38.71
	67	BD	O49-H54	724	BD*	C31-H32	16.31
	67	BD	O49-H54	725	BD*	C31-H33	1437.49
	67	BD	O49-H54	727	BD*	C35-H36	38.87
	67	BD	O49-H54	729	BD*	C35-H38	10.69

	67	BD	049-H54	731	BD*	C39-H41	18.47
	67	BD	049-H54	732	BD*	C39-H42	11.03
	67	BD	049-H54	733	BD*	C43-H44	28.22
	67	BD	049-H54	739	BD*	O48-H53	2007.09
	67	BD	049-H54	742	BD*	O50-C52	626.5
π-π*							
	8	BD	N4-C7	686	BD*	N6-C8	14.69
	22	BD	C11-C12	686	BD*	N6-C8	22.26
	22	BD	C11-C12	691	BD*	C9-C10	14.75
	26	BD	C13-C17	703	BD*	C14-C26	21.28
	26	BD	C13-C17	716	BD*	C24-C25	21.1
	29	BD	C14-C26	700	BD*	C13-C17	19.25
	29	BD	C14-C26	716	BD*	C24-C25	20.09
	31	BD	C16-C19	712	BD*	C21-C22	16.4
	38	BD	C21-C22	705	BD*	C16-C19	22.54
	42	BD	C24-C25	700	BD*	C13-C17	20.18
	42	BD	C24-C25	703	BD*	C14-C26	21.28
	48	BD	C27-C29	705	BD*	C16-C19	19.44
	48	BD	C27-C29	712	BD*	C21-C22	19.79
π-σ*							
	17	BD	C9-C10	725	BD*	C31-H33	68.94
	17	BD	C9-C10	739	BD*	O48-H53	50.75
	17	BD	C9-C10	742	BD*	O50-C52	12.78
	12	BD	N6-C8	682	BD*	N4-C7	13.91
	12	BD	N6-C8	696	BD*	C11-C12	10.79
	17	BD	C9-C10	682	BD*	N4-C7	22.01
	17	BD	C9-C10	696	BD*	C11-C12	15.05

Table 5: Orbital Contribution from various fragments towards HOMO and LUMO for single molecule.

Molecule	HOMO (%)				LUMO (%)			
	Btz	Ar-O	Ar	EWG	Btz	Ar-O	Ar	EWG
HB	18.97	1.39	79.64	0	15.9	0.17	83.93	0
FB	50.52	0.18	29.98	19.31	20.12	0.15	45.22	34.52
CB	38.39	29.35	6.48	25.77	42.72	36.88	13.63	6.76
NB	6.78	74.58	13.21	5.43	46.85	40.31	11.12	1.72
CAB	15.84	53.96	20.97	9.23	32.17	52.66	9.74	5.43

Table 6: Energies (eV) of Frontier Molecular Orbitals in eV of Btz derivatives upon aggregation

Molecule	HOMO-1	HOMO	LUMO	LUMO+1	HOMO-LUMO Gap
HB	-6.01	-5.36	-2.12	-0.35	3.24
FB	-6.01	-5.60	-2.29	-0.52	3.31
CB	-6.18	-5.88	-3.02	-1.74	2.86
NB	-6.23	-5.82	-3.05	-2.31	2.78
CAB	-6.10	-5.52	-2.53	-1.12	2.99

SIT 7: Computer Absorption and Emission Spectra (λ_{\max} in nm), for HB in comparison with experimental findings using different functionals in cyclohexane solvent

Functional	Absorption (nm)	Emission (nm)
B3LYP	436	-
WB97XD	362	-
PBE0	417	-
M062X	389	466
BMK	382	509
CAM-B3LYP	372	483
Experiment	396	485

SIT 8: Computed Absorption Spectra (λ_{\max} in nm), oscillator strengths (f_o), electronic excitation energies (eV) and transitions in different solvents using TD-DFT method at CAM-B3LYP/6-31G(d). (*H* denotes HOMO and *L* denotes LUMO)

Molecule	Gas			Transition
	eV	λ_{\max} (nm)	f_o	
HB	3.379	366.89	0.2333	H→L=95%
FB	3.442	360.22	0.2659	H→L=81%; H-1→L=13%
CB	3.214	385.83	0.2108	H→L=77%; H-1→L=16%
NB	3.217	385.44	0.1543	H→L=79%; H→L+1=4%; H-1→L=7%
CAB	3.476	356.7	0.1903	H→L=83%; H-1→L=6%

Molecule	Toluene			Transition
	eV	λ_{\max} (nm)	f_o	
HB	3.320	373.39	0.2776	H→L=95%
FB	3.411	363.49	0.3220	H→L=79%; H-1→L=14%
CB	3.223	384.65	0.2675	H→L=73%; H-1→L=18%
NB	3.189	388.75	0.1640	H→L=77%; H→L+1=5%; H-1→L=6%
CAB	3.470	357.32	0.2282	H→L=72%; H-1→L=17%

Molecule	Dichloromethane			Transition
	eV	λ_{\max} (nm)	f_o	
HB	3.314	374.15	0.2661	H→L=95%
FB	3.424	362.15	0.3165	H→L=78%; H-1→L=15%
CB	3.264	379.83	0.2701	H→L=74%; H-1→L=18%
NB	3.181	389.79	0.1341	H→L=76%; H→L+1=8%; H-1→L=4%
CAB	3.487	355.6	0.2097	H→L=72%; H-1→L=18%

Molecule	Isopropanol			Transition
	eV	λ_{\max} (nm)	f_o	
HB	3.314	374.11	0.2612	H→L=95%
FB	3.428	361.64	0.3127	H→L=79%; H-1→L=15%
CB	3.276	378.52	0.2683	H→L=74%; H-1→L=18%
NB	3.178	390.08	0.1259	H→L=76%; H→L+1=8%; H-1→L=4%
CAB	3.491	355.16	0.2024	H→L=73%; H-1→L=17%

SIT 9: Computed bond parameters in excited state.

Molecule	Structure	O2-C12	O2-C18	C9-C15	C12-C13	C9-C10	C10-C13	C12-O2-C18	C12-O2-C18-C21 (ϕ_1)	C7-C9-C15-C16 (ϕ_2)	C13-C12-O2-C18 (ϕ_3)
HB	MONOMER	1.340	1.386	1.445	1.415	1.432	1.371	121.84	131.58	17.45	18.78
	ONIOM	1.336	1.381	1.447	1.410	1.423	1.373	124.94	137.92	27.92	9.11
FB	MONOMER	1.338	1.384	1.446	1.415	1.428	1.371	122.84	149.75	25.75	38.92
	ONIOM	1.332	1.374	1.451	1.414	1.421	1.375	128.01	150.59	27.93	22.17
CB	MONOMER	1.402	1.314	1.481	1.395	1.425	1.396	120.29	171.93	49.31	119.23
	ONIOM	1.328	1.388	1.421	1.412	1.441	1.414	126.86	121.02	7.93	6.60
NB	MONOMER	1.398	1.307	1.487	1.407	1.436	1.366	120.34	179.54	59.99	97.06
	ONIOM	1.384	1.318	1.489	1.374	1.382	1.442	121.87	161.86	14.97	37.59
CAB	MONOMER	1.356	1.391	1.452	1.423	1.432	1.393	123.26	149.45	37.63	141.60
	ONIOM	1.335	1.367	1.457	1.424	1.431	1.401	126.18	144.07	13.25	8.91

Optimized XYZ Coordinates:

SINGLE MOLECULE:

Ground State:

HB:

S	0.574622000000	3.966592000000	-0.449953000000
O	-2.982773000000	1.384558000000	-0.098801000000
O	6.533926000000	-1.542603000000	-0.079294000000
N	1.535188000000	2.638547000000	-0.343255000000
O	-7.254534000000	-2.055766000000	0.723687000000
N	-0.903347000000	3.259187000000	-0.337496000000
C	0.726910000000	1.577412000000	-0.211174000000
C	-0.681372000000	1.948046000000	-0.211567000000
C	1.133810000000	0.200027000000	-0.098517000000
C	0.102241000000	-0.712203000000	0.012924000000
H	0.349295000000	-1.762949000000	0.129218000000
C	-1.692703000000	0.940032000000	-0.091943000000
C	-1.282819000000	-0.367501000000	0.014221000000
H	-2.017975000000	-1.157698000000	0.113347000000
C	2.553915000000	-0.226652000000	-0.105160000000
C	3.552162000000	0.514884000000	0.546043000000
H	3.291047000000	1.449448000000	1.029353000000
C	-4.018290000000	0.467499000000	0.082666000000
C	2.931260000000	-1.411017000000	-0.760797000000
H	2.187691000000	-1.969852000000	-1.322698000000
C	-4.702085000000	-0.018342000000	-1.025053000000
H	-4.385716000000	0.276532000000	-2.020394000000
C	-6.200976000000	-1.232028000000	0.440617000000
C	-5.798424000000	-0.872759000000	-0.851899000000
H	-6.323926000000	-1.238905000000	-1.725515000000
C	4.249770000000	-1.874845000000	-0.750239000000
C	5.211477000000	-1.122712000000	-0.054462000000
C	4.883051000000	0.086002000000	0.581803000000
C	-5.506079000000	-0.729938000000	1.553251000000
H	-5.840368000000	-1.010881000000	2.546477000000
C	-4.419565000000	0.119453000000	1.375739000000
H	-3.884759000000	0.522054000000	2.229966000000
C	6.929694000000	-2.363898000000	1.021270000000
H	7.978954000000	-2.617995000000	0.856568000000
H	6.335274000000	-3.285307000000	1.065979000000
H	6.830973000000	-1.831048000000	1.975044000000
C	4.643373000000	-3.127151000000	-1.497469000000
H	5.501756000000	-2.941873000000	-2.150671000000
H	3.812189000000	-3.489413000000	-2.108751000000

H	4.931363000000	-3.936697000000	-0.816412000000
C	5.943066000000	0.913739000000	1.269939000000
H	5.584138000000	1.932247000000	1.440535000000
H	6.856075000000	0.960358000000	0.669136000000
H	6.219743000000	0.495036000000	2.245528000000
C	-8.015527000000	-2.582482000000	-0.356544000000
H	-8.793450000000	-3.195722000000	0.099576000000
H	-7.398136000000	-3.207983000000	-1.013609000000
H	-8.481274000000	-1.781882000000	-0.944774000000

FB:

S	0.330475000000	3.867240000000	-0.133662000000
O	-2.934573000000	0.970778000000	-1.035977000000
O	6.757327000000	-0.901096000000	0.391305000000
N	1.395066000000	2.617834000000	-0.088271000000
O	-7.167640000000	-1.520778000000	1.553396000000
N	-1.060950000000	3.046053000000	-0.428926000000
C	0.694890000000	1.497549000000	-0.304068000000
C	-0.724584000000	1.756354000000	-0.504454000000
C	1.242778000000	0.165322000000	-0.354061000000
C	0.309246000000	-0.814140000000	-0.608908000000
C	-1.634261000000	0.683202000000	-0.764623000000
C	-1.081928000000	-0.573130000000	-0.828852000000
C	2.683351000000	-0.122044000000	-0.150277000000
C	3.401607000000	0.510101000000	0.875817000000
H	2.901008000000	1.227356000000	1.516726000000
C	-3.965426000000	0.294494000000	-0.377394000000
C	3.363140000000	-1.015898000000	-0.993026000000
H	2.833212000000	-1.489960000000	-1.812927000000
C	-5.144055000000	0.110544000000	-1.089092000000
H	-5.198189000000	0.439186000000	-2.121576000000
C	-6.155964000000	-0.914516000000	0.858609000000
C	-6.246097000000	-0.493092000000	-0.473720000000
H	-7.155912000000	-0.629439000000	-1.045687000000
C	4.721151000000	-1.296292000000	-0.820154000000
C	5.399689000000	-0.668565000000	0.238892000000
C	4.759212000000	0.250981000000	1.086597000000
C	-4.961636000000	-0.717346000000	1.567380000000
H	-4.909036000000	-1.041677000000	2.601399000000
C	-3.869745000000	-0.108793000000	0.956585000000
H	-2.954035000000	0.051027000000	1.516483000000
C	7.096913000000	-1.953971000000	1.297674000000
H	8.186372000000	-2.026017000000	1.292459000000
H	6.667130000000	-2.910785000000	0.976218000000
H	6.752383000000	-1.733080000000	2.315303000000
C	5.451165000000	-2.225410000000	-1.760565000000

H	6.371558000000	-1.764193000000	-2.131627000000
H	4.820461000000	-2.483574000000	-2.615441000000
H	5.739472000000	-3.161425000000	-1.267962000000
C	5.521481000000	0.962128000000	2.179753000000
H	4.963135000000	1.832958000000	2.533399000000
H	6.499809000000	1.295642000000	1.821746000000
H	5.698714000000	0.311408000000	3.044904000000
C	-8.401585000000	-1.752644000000	0.886897000000
H	-9.047328000000	-2.241455000000	1.617375000000
H	-8.270052000000	-2.411707000000	0.019248000000
H	-8.865451000000	-0.811781000000	0.564030000000
F	-1.850975000000	-1.643170000000	-1.097462000000
F	0.666909000000	-2.114135000000	-0.663530000000

CB:

S	0.458256000000	3.959579000000	-0.371336000000
O	-2.865831000000	1.141761000000	-0.898584000000
O	6.807746000000	-0.711612000000	0.436570000000
N	1.498095000000	2.697860000000	-0.245864000000
O	-7.255659000000	-1.215060000000	1.541093000000
N	-0.956634000000	3.149513000000	-0.553594000000
C	0.764532000000	1.581077000000	-0.341824000000
C	-0.645564000000	1.850709000000	-0.525672000000
C	1.276494000000	0.238385000000	-0.283470000000
C	0.330865000000	-0.770960000000	-0.421004000000
C	-1.585965000000	0.779286000000	-0.668003000000
C	-1.088415000000	-0.516012000000	-0.643739000000
C	2.724689000000	-0.016461000000	-0.096258000000
C	3.428704000000	0.600642000000	0.950030000000
H	2.909764000000	1.276028000000	1.622258000000
C	-3.946292000000	0.486520000000	-0.286054000000
C	3.420168000000	-0.859345000000	-0.973945000000
H	2.899604000000	-1.309560000000	-1.813919000000
C	-5.056613000000	0.215465000000	-1.071851000000
H	-5.030019000000	0.440956000000	-2.132456000000
C	-6.203855000000	-0.651163000000	0.877311000000
C	-6.193528000000	-0.356146000000	-0.492057000000
H	-7.050151000000	-0.571117000000	-1.118796000000
C	4.785266000000	-1.117272000000	-0.814487000000
C	5.448576000000	-0.515521000000	0.268694000000
C	4.788975000000	0.359756000000	1.151076000000
C	-5.076634000000	-0.357617000000	1.660681000000
H	-5.104624000000	-0.584577000000	2.721057000000
C	-3.950282000000	0.218176000000	1.084390000000

H	-3.084928000000	0.455013000000	1.695104000000
C	7.171800000000	-1.895023000000	1.155772000000
H	8.261181000000	-1.888508000000	1.225314000000
H	6.846035000000	-2.800379000000	0.630596000000
H	6.740857000000	-1.892747000000	2.164578000000
C	5.522079000000	-2.003118000000	-1.790182000000
H	6.540594000000	-1.642019000000	-1.956042000000
H	5.000992000000	-2.036669000000	-2.750835000000
H	5.592201000000	-3.034787000000	-1.424170000000
C	5.545155000000	1.036150000000	2.269192000000
H	4.904038000000	1.751340000000	2.791169000000
H	6.420378000000	1.568768000000	1.884073000000
H	5.912572000000	0.314570000000	3.007543000000
C	-8.415958000000	-1.571265000000	0.798465000000
H	-9.105148000000	-2.012886000000	1.518942000000
H	-8.180012000000	-2.307869000000	0.020568000000
H	-8.883674000000	-0.690259000000	0.340967000000
C	-1.948510000000	-1.633729000000	-0.883966000000
C	0.729219000000	-2.145525000000	-0.309007000000
N	-2.614560000000	-2.559647000000	-1.114393000000
N	1.021492000000	-3.266488000000	-0.200685000000

NB:

S	0.458401000000	4.077623000000	-0.443751000000
O	-2.823176000000	1.201620000000	-0.938927000000
O	6.873618000000	-0.479282000000	0.463373000000
N	1.511407000000	2.834817000000	-0.253520000000
O	-7.226845000000	-0.935049000000	1.671636000000
N	-0.940962000000	3.244114000000	-0.633328000000
C	0.793725000000	1.707239000000	-0.329794000000
C	-0.614130000000	1.951286000000	-0.558923000000
C	1.321732000000	0.373643000000	-0.209564000000
C	0.381673000000	-0.626458000000	-0.324181000000
C	-1.542020000000	0.864821000000	-0.692234000000
C	-1.010535000000	-0.407354000000	-0.597586000000
C	2.777121000000	0.139071000000	-0.031792000000
C	3.467238000000	0.741154000000	1.029504000000
H	2.933028000000	1.380935000000	1.724538000000
C	-3.904453000000	0.598857000000	-0.278122000000
C	3.484852000000	-0.659725000000	-0.939419000000
H	2.970460000000	-1.095645000000	-1.791507000000
C	-5.061367000000	0.400528000000	-1.018882000000
H	-5.064336000000	0.636998000000	-2.077118000000
C	-6.172453000000	-0.425247000000	0.969111000000
C	-6.203478000000	-0.111219000000	-0.396311000000
H	-7.097387000000	-0.266838000000	-0.987628000000

C	4.856463000000	-0.891585000000	-0.790526000000
C	5.509449000000	-0.306932000000	0.307752000000
C	4.834219000000	0.527607000000	1.217292000000
C	-4.996485000000	-0.213248000000	1.704077000000
H	-4.989801000000	-0.456106000000	2.761189000000
C	-3.862751000000	0.304546000000	1.086174000000
H	-2.960598000000	0.477405000000	1.664212000000
C	7.264131000000	-1.663378000000	1.167316000000
H	8.353831000000	-1.639097000000	1.227341000000
H	6.948990000000	-2.568618000000	0.635303000000
H	6.842322000000	-1.679536000000	2.179758000000
C	5.611621000000	-1.729639000000	-1.794096000000
H	6.606269000000	-1.315694000000	-1.980922000000
H	5.068624000000	-1.780416000000	-2.741658000000
H	5.745597000000	-2.759443000000	-1.441084000000
C	5.579004000000	1.189138000000	2.351675000000
H	4.929883000000	1.890323000000	2.882626000000
H	6.452999000000	1.733872000000	1.981327000000
H	5.945841000000	0.456705000000	3.079649000000
C	-8.441110000000	-1.200112000000	0.978889000000
H	-9.124304000000	-1.609044000000	1.723935000000
H	-8.291145000000	-1.935918000000	0.179092000000
H	-8.869711000000	-0.281912000000	0.557682000000
N	0.837289000000	-2.036654000000	-0.226710000000
N	-1.890245000000	-1.579696000000	-0.749870000000
O	-1.860357000000	-2.418931000000	0.147572000000
O	-2.589197000000	-1.625550000000	-1.756400000000
O	1.295704000000	-2.408817000000	0.843524000000
O	0.731245000000	-2.714739000000	-1.247637000000

CAB:

S	0.853001000000	-2.894790000000	-1.428379000000
O	2.854716000000	1.111910000000	-0.952126000000
O	-6.678903000000	-1.392381000000	0.290038000000
N	-0.547346000000	-2.205885000000	-0.923859000000
O	7.177311000000	-1.365108000000	1.501267000000
N	1.859190000000	-1.600087000000	-1.332014000000
C	-0.274384000000	-0.922859000000	-0.653847000000
C	1.111810000000	-0.583901000000	-0.891804000000
C	-1.230744000000	0.071655000000	-0.241541000000
C	-0.742881000000	1.351604000000	-0.042435000000
C	1.560004000000	0.753841000000	-0.661142000000
C	0.654023000000	1.698539000000	-0.220608000000
C	-2.666317000000	-0.300484000000	-0.102833000000
C	-3.047624000000	-1.328915000000	0.772326000000
H	-2.288953000000	-1.862209000000	1.337715000000

C	3.925935000000	0.437108000000	-0.330523000000
C	-3.652532000000	0.345266000000	-0.859339000000
H	-3.368714000000	1.119337000000	-1.565601000000
C	5.051901000000	0.191303000000	-1.101531000000
H	5.051748000000	0.459612000000	-2.152613000000
C	6.145123000000	-0.767211000000	0.836380000000
C	6.171813000000	-0.410695000000	-0.518513000000
H	7.044806000000	-0.599270000000	-1.131185000000
C	-5.005010000000	0.005842000000	-0.737665000000
C	-5.355519000000	-1.000027000000	0.177802000000
C	-4.387431000000	-1.691340000000	0.929093000000
C	4.998010000000	-0.505941000000	1.601854000000
H	4.998218000000	-0.777932000000	2.651988000000
C	3.889656000000	0.103359000000	1.023313000000
H	3.010406000000	0.319313000000	1.621858000000
C	-7.465885000000	-0.632506000000	1.212563000000
H	-8.466734000000	-1.068254000000	1.194294000000
H	-7.522812000000	0.422123000000	0.918626000000
H	-7.058545000000	-0.697583000000	2.229271000000
C	-6.050302000000	0.693949000000	-1.582249000000
H	-6.820064000000	-0.011616000000	-1.906793000000
H	-5.594050000000	1.148847000000	-2.465366000000
H	-6.551896000000	1.496530000000	-1.027890000000
C	-4.790842000000	-2.815181000000	1.853239000000
H	-3.908631000000	-3.305802000000	2.273202000000
H	-5.385308000000	-3.564696000000	1.321220000000
H	-5.404907000000	-2.458067000000	2.687697000000
C	8.374968000000	-1.647497000000	0.786478000000
H	9.047974000000	-2.112457000000	1.507463000000
H	8.834407000000	-0.729516000000	0.399129000000
H	8.190921000000	-2.343707000000	-0.041321000000
O	0.451480000000	3.672785000000	1.075275000000
O	2.206221000000	3.597930000000	-0.287793000000
O	-2.332261000000	2.502541000000	1.430615000000
O	-2.031005000000	3.265380000000	-0.640480000000
C	1.088124000000	3.072144000000	0.236454000000
C	-1.730391000000	2.478868000000	0.224592000000
H	2.668224000000	2.931969000000	-0.831846000000
H	-1.916519000000	1.865833000000	2.030584000000

Excited State:

HB:

S	0.524772000000	3.963719000000	-0.080292000000
O	-2.912724000000	1.236206000000	-0.325406000000
O	6.501862000000	-1.549050000000	-0.129886000000
N	1.527062000000	2.610280000000	-0.080459000000

O	-7.205644000000	-2.035569000000	0.789386000000
N	-0.955907000000	3.179354000000	-0.169371000000
C	0.731738000000	1.544744000000	-0.147379000000
C	-0.666064000000	1.877499000000	-0.195794000000
C	1.151719000000	0.164489000000	-0.203836000000
C	0.114196000000	-0.819504000000	-0.281123000000
H	0.384853000000	-1.866381000000	-0.291223000000
C	-1.632504000000	0.845505000000	-0.257450000000
C	-1.220296000000	-0.507399000000	-0.300103000000
H	-1.963845000000	-1.291279000000	-0.361542000000
C	2.535125000000	-0.254391000000	-0.190798000000
C	3.574738000000	0.603833000000	0.235504000000
H	3.323800000000	1.614752000000	0.524314000000
C	-3.957759000000	0.365008000000	-0.063007000000
C	2.904867000000	-1.557953000000	-0.609917000000
H	2.156634000000	-2.233414000000	-1.006266000000
C	-4.998893000000	0.325191000000	-0.974312000000
H	-4.935275000000	0.920058000000	-1.878556000000
C	-6.172502000000	-1.225687000000	0.448834000000
C	-6.110868000000	-0.472662000000	-0.723672000000
H	-6.915825000000	-0.496255000000	-1.447059000000
C	4.213470000000	-1.994338000000	-0.587976000000
C	5.203710000000	-1.115389000000	-0.115148000000
C	4.896690000000	0.191221000000	0.286655000000
C	-5.119652000000	-1.165244000000	1.367963000000
H	-5.195043000000	-1.744858000000	2.281244000000
C	-4.016224000000	-0.370144000000	1.119981000000
H	-3.209682000000	-0.304883000000	1.842014000000
C	7.018975000000	-1.979182000000	1.126215000000
H	8.040057000000	-2.313603000000	0.940367000000
H	6.429701000000	-2.811149000000	1.527324000000
H	7.031491000000	-1.163718000000	1.855817000000
C	4.599630000000	-3.364875000000	-1.073390000000
H	5.339695000000	-3.303264000000	-1.876370000000
H	3.726266000000	-3.903550000000	-1.448301000000
H	5.048515000000	-3.963480000000	-0.274241000000
C	5.979039000000	1.135397000000	0.737565000000
H	5.680164000000	2.171286000000	0.562268000000
H	6.912452000000	0.944297000000	0.202785000000
H	6.185062000000	1.032541000000	1.809019000000
C	-8.307186000000	-2.122686000000	-0.094435000000
H	-9.010795000000	-2.814184000000	0.368631000000
H	-8.005353000000	-2.514007000000	-1.072639000000
H	-8.790978000000	-1.148432000000	-0.227595000000

FB:

S	0.407127000000	3.960504000000	0.338421000000
O	-2.882826000000	1.148213000000	-0.537777000000
O	6.697162000000	-1.029122000000	0.116629000000
N	1.461615000000	2.650988000000	0.290543000000
O	-7.182212000000	-1.880957000000	1.092730000000
N	-1.021451000000	3.141174000000	0.023612000000
C	0.726762000000	1.573123000000	0.035369000000
C	-0.677947000000	1.862563000000	-0.112292000000
C	1.234538000000	0.233478000000	-0.144517000000
C	0.245508000000	-0.761091000000	-0.410676000000
C	-1.598424000000	0.817425000000	-0.361700000000
C	-1.094571000000	-0.494433000000	-0.524828000000
C	2.639562000000	-0.099243000000	-0.070471000000
C	3.533043000000	0.695504000000	0.684751000000
H	3.149151000000	1.567498000000	1.194663000000
C	-3.928658000000	0.335835000000	-0.136729000000
C	3.181730000000	-1.209754000000	-0.766326000000
H	2.542259000000	-1.816606000000	-1.391116000000
C	-5.092556000000	0.413478000000	-0.883939000000
H	-5.115870000000	1.046502000000	-1.763760000000
C	-6.154349000000	-1.126273000000	0.634158000000
C	-6.209744000000	-0.320916000000	-0.504169000000
H	-7.110778000000	-0.255644000000	-1.100287000000
C	4.524497000000	-1.521125000000	-0.706219000000
C	5.364468000000	-0.724816000000	0.092442000000
C	4.880437000000	0.393840000000	0.785474000000
C	-4.977008000000	-1.180029000000	1.389198000000
H	-4.961431000000	-1.796601000000	2.280894000000
C	-3.866573000000	-0.451017000000	1.011999000000
H	-2.963771000000	-0.474650000000	1.612389000000
C	7.147638000000	-1.737785000000	1.268478000000
H	8.212506000000	-1.918961000000	1.120299000000
H	6.624398000000	-2.695110000000	1.367077000000
H	7.002548000000	-1.152900000000	2.181734000000
C	5.102838000000	-2.671754000000	-1.483528000000
H	5.902759000000	-2.334002000000	-2.148585000000
H	4.332102000000	-3.157118000000	-2.086391000000
H	5.538669000000	-3.426394000000	-0.820873000000
C	5.805725000000	1.262861000000	1.594551000000
H	5.412701000000	2.279680000000	1.663679000000
H	6.799675000000	1.301465000000	1.142584000000
H	5.922151000000	0.887543000000	2.617580000000
C	-8.404371000000	-1.853965000000	0.379441000000
H	-9.080483000000	-2.519289000000	0.915859000000
H	-8.276315000000	-2.217462000000	-0.646398000000
H	-8.831092000000	-0.844898000000	0.356289000000

F	-1.925773000000	-1.500414000000	-0.811862000000
F	0.592862000000	-2.049302000000	-0.538446000000

CB:

S	-0.621806000000	2.917509000000	0.328505000000
O	-2.921672000000	-0.457030000000	-1.513296000000
O	6.697653000000	-0.135595000000	0.742627000000
N	0.729870000000	1.938307000000	0.271085000000
O	-7.016924000000	0.148772000000	1.954737000000
N	-1.741246000000	1.850693000000	-0.322409000000
C	0.352699000000	0.778895000000	-0.245219000000
C	-1.053170000000	0.739281000000	-0.589777000000
C	1.191742000000	-0.361406000000	-0.479986000000
C	0.592271000000	-1.504629000000	-1.010932000000
C	-1.577844000000	-0.441332000000	-1.114449000000
C	-0.790564000000	-1.568810000000	-1.347524000000
C	2.637651000000	-0.303389000000	-0.163674000000
C	3.077763000000	0.163432000000	1.078218000000
H	2.350739000000	0.504671000000	1.806522000000
C	-3.878387000000	-0.312231000000	-0.624667000000
C	3.590740000000	-0.697029000000	-1.103232000000
H	3.270672000000	-1.020599000000	-2.088834000000
C	-5.187976000000	-0.165106000000	-1.163676000000
H	-5.295119000000	-0.174713000000	-2.240994000000
C	-6.055497000000	-0.002484000000	1.068616000000
C	-6.260367000000	-0.008271000000	-0.336848000000
H	-7.251903000000	0.111184000000	-0.751308000000
C	4.954233000000	-0.663966000000	-0.821764000000
C	5.353428000000	-0.220493000000	0.440186000000
C	4.428950000000	0.209133000000	1.397743000000
C	-4.752667000000	-0.169399000000	1.606618000000
H	-4.645225000000	-0.168660000000	2.684024000000
C	-3.677596000000	-0.318159000000	0.783470000000
H	-2.682828000000	-0.448628000000	1.182038000000
C	7.266045000000	-1.344622000000	1.224078000000
H	8.311972000000	-1.131119000000	1.451041000000
H	7.215425000000	-2.139902000000	0.472109000000
H	6.760737000000	-1.687225000000	2.134622000000
C	5.968696000000	-1.074471000000	-1.855469000000
H	6.879414000000	-0.477427000000	-1.767886000000
H	5.564978000000	-0.953599000000	-2.863919000000
H	6.254048000000	-2.127031000000	-1.744448000000
C	4.902647000000	0.724849000000	2.730243000000
H	4.066743000000	1.125664000000	3.308587000000
H	5.647324000000	1.515602000000	2.603097000000
H	5.375373000000	-0.062923000000	3.326768000000

C	-8.375935000000	0.329035000000	1.536557000000
H	-8.946924000000	0.433246000000	2.455848000000
H	-8.720271000000	-0.544574000000	0.979297000000
H	-8.469582000000	1.234085000000	0.932981000000
C	-1.381830000000	-2.746889000000	-1.875141000000
C	1.350413000000	-2.708819000000	-1.194418000000
N	-1.901222000000	-3.691575000000	-2.303175000000
N	1.921802000000	-3.704040000000	-1.343322000000

NB:

S	-0.340877000000	3.420459000000	-1.236339000000
O	-2.857146000000	-0.221309000000	-1.343761000000
O	6.781531000000	0.705715000000	0.630327000000
N	0.938679000000	2.460315000000	-0.813733000000
O	-7.184159000000	0.515864000000	1.787296000000
N	-1.528827000000	2.263624000000	-1.278966000000
C	0.482654000000	1.232910000000	-0.692015000000
C	-0.934646000000	1.116082000000	-0.959322000000
C	1.265164000000	0.065670000000	-0.364030000000
C	0.591956000000	-1.119995000000	-0.285124000000
C	-1.547886000000	-0.137582000000	-0.859502000000
C	-0.819988000000	-1.284050000000	-0.492388000000
C	2.722443000000	0.207785000000	-0.105298000000
C	3.163507000000	1.026080000000	0.936272000000
H	2.436973000000	1.549060000000	1.549993000000
C	-3.871634000000	-0.037053000000	-0.540067000000
C	3.663578000000	-0.430483000000	-0.909201000000
H	3.331101000000	-1.045030000000	-1.738710000000
C	-5.155486000000	-0.136770000000	-1.147869000000
H	-5.197338000000	-0.360369000000	-2.206162000000
C	-6.163052000000	0.328712000000	0.979120000000
C	-6.284806000000	0.040597000000	-0.405373000000
H	-7.257964000000	-0.040624000000	-0.869519000000
C	5.030433000000	-0.289681000000	-0.675374000000
C	5.436225000000	0.512218000000	0.392306000000
C	4.517076000000	1.187950000000	1.202173000000
C	-4.881849000000	0.432198000000	1.585628000000
H	-4.839545000000	0.648963000000	2.645603000000
C	-3.753536000000	0.250199000000	0.848081000000
H	-2.773096000000	0.311219000000	1.297022000000
C	7.384999000000	-0.298012000000	1.434307000000
H	8.427698000000	-0.005939000000	1.569726000000
H	7.345558000000	-1.279177000000	0.948506000000
H	6.898621000000	-0.369082000000	2.414062000000
C	6.040244000000	-0.970251000000	-1.560127000000
H	6.942794000000	-0.363110000000	-1.660690000000

H	5.624769000000	-1.150506000000	-2.554765000000
H	6.341403000000	-1.942520000000	-1.153284000000
C	4.998466000000	2.078523000000	2.315779000000
H	4.162495000000	2.615093000000	2.770888000000
H	5.722420000000	2.810996000000	1.947935000000
H	5.498164000000	1.506832000000	3.105045000000
C	-8.529002000000	0.426536000000	1.299415000000
H	-9.160294000000	0.618449000000	2.163485000000
H	-8.723897000000	-0.573989000000	0.908293000000
H	-8.704820000000	1.182950000000	0.531917000000
N	1.398150000000	-2.292312000000	0.113634000000
N	-1.455715000000	-2.497714000000	-0.210808000000
O	-0.772069000000	-3.530717000000	-0.088619000000
O	-2.702720000000	-2.502466000000	-0.086925000000
O	1.528140000000	-2.483515000000	1.308165000000
O	1.929400000000	-2.932002000000	-0.774377000000

CAB:

S	0.941136000000	-2.948260000000	-1.077315000000
O	2.797119000000	1.154496000000	-0.650097000000
O	-6.629709000000	-1.466788000000	0.115969000000
N	-0.521931000000	-2.214879000000	-0.709480000000
O	7.303256000000	-1.469475000000	1.116050000000
N	1.927219000000	-1.601323000000	-0.959814000000
C	-0.262297000000	-0.936258000000	-0.472866000000
C	1.127232000000	-0.592834000000	-0.617025000000
C	-1.249779000000	0.076507000000	-0.214649000000
C	-0.783030000000	1.419075000000	-0.037366000000
C	1.519656000000	0.751138000000	-0.440566000000
C	0.564351000000	1.759399000000	-0.131518000000
C	-2.651299000000	-0.292248000000	-0.130764000000
C	-3.032059000000	-1.514578000000	0.476984000000
H	-2.266219000000	-2.154042000000	0.893126000000
C	3.905415000000	0.435429000000	-0.214549000000
C	-3.674323000000	0.515231000000	-0.679938000000
H	-3.411217000000	1.415601000000	-1.219408000000
C	5.051581000000	0.542298000000	-0.982060000000
H	5.025642000000	1.109800000000	-1.905667000000
C	6.225244000000	-0.818461000000	0.620586000000
C	6.219340000000	-0.087852000000	-0.568295000000
H	7.109239000000	-0.002705000000	-1.178330000000
C	-5.006276000000	0.155123000000	-0.617646000000
C	-5.338936000000	-1.044004000000	0.043034000000
C	-4.353969000000	-1.893424000000	0.580237000000
C	5.058058000000	-0.903557000000	1.390934000000
H	5.090110000000	-1.464850000000	2.317890000000

C	3.898526000000	-0.278915000000	0.980034000000
H	2.997902000000	-0.336085000000	1.580161000000
C	-7.488848000000	-0.767704000000	1.017392000000
H	-8.463476000000	-1.249114000000	0.939974000000
H	-7.582570000000	0.288282000000	0.752838000000
H	-7.117568000000	-0.853792000000	2.043702000000
C	-6.059876000000	0.995577000000	-1.286616000000
H	-6.877703000000	0.375309000000	-1.661006000000
H	-5.630336000000	1.548443000000	-2.124927000000
H	-6.486204000000	1.733263000000	-0.597907000000
C	-4.759564000000	-3.179135000000	1.245830000000
H	-3.881628000000	-3.722268000000	1.601605000000
H	-5.306843000000	-3.823362000000	0.551625000000
H	-5.420349000000	-2.998341000000	2.099382000000
C	8.514363000000	-1.418770000000	0.384133000000
H	9.234877000000	-2.004083000000	0.954686000000
H	8.878325000000	-0.389864000000	0.286559000000
H	8.396270000000	-1.858986000000	-0.612175000000
O	0.223797000000	3.851016000000	0.916694000000
O	2.126961000000	3.633852000000	-0.176043000000
O	-2.317745000000	2.520214000000	1.486294000000
O	-2.196703000000	3.256610000000	-0.598839000000
C	0.954285000000	3.156881000000	0.245503000000
C	-1.789250000000	2.512835000000	0.254998000000
H	2.632401000000	2.934834000000	-0.632365000000
H	-1.802935000000	1.947617000000	2.077277000000

CLUSTER:

GROUND STATE:

HB:

S	-0.294540000000	0.728179000000	-3.499401000000
S	0.542586000000	-0.757611000000	3.421548000000
O	3.290282000000	-0.934385000000	-1.602968000000
O	-3.092177000000	0.880428000000	1.693204000000
O	2.288114000000	7.128863000000	0.976961000000
O	-2.347908000000	-7.119415000000	-0.951491000000
N	-1.237322000000	-0.152058000000	-2.481004000000
N	1.439187000000	0.145393000000	2.433117000000
O	-2.192047000000	5.192752000000	-1.026560000000
O	2.132254000000	-5.183304000000	1.052029000000
N	1.194060000000	0.246949000000	-2.999851000000
N	-0.941890000000	-0.313490000000	2.973190000000
C	-0.412020000000	-0.863473000000	-1.702930000000
C	0.584896000000	0.865630000000	1.677871000000
C	0.989305000000	-0.612843000000	-2.000697000000
C	-0.785937000000	0.583587000000	1.988543000000

C	-0.797797000000	-1.797820000000	-0.677121000000
C	0.930669000000	1.807016000000	0.659974000000
C	0.248133000000	-2.341081000000	0.041525000000
C	-0.131180000000	2.351210000000	-0.018697000000
H	0.021075000000	-3.055032000000	0.827018000000
H	0.054475000000	2.946911000000	-0.708302000000
C	2.019159000000	-1.247507000000	-1.230808000000
C	-1.840939000000	1.218599000000	1.269370000000
C	1.626067000000	-2.064780000000	-0.199936000000
C	-1.497909000000	2.066122000000	0.260215000000
H	2.369959000000	-2.533230000000	0.432732000000
H	-2.164302000000	2.462332000000	-0.252721000000
C	-2.204140000000	-2.194804000000	-0.439055000000
C	2.332061000000	2.199874000000	0.383118000000
C	-3.125037000000	-2.284754000000	-1.495461000000
C	3.246278000000	2.396787000000	1.416348000000
H	-2.823134000000	-1.992859000000	-2.493533000000
H	2.986828000000	2.221430000000	2.291787000000
C	4.408747000000	-1.524450000000	-1.028338000000
C	-4.210338000000	1.462654000000	1.085490000000
C	-2.641605000000	-2.556665000000	0.844057000000
C	2.756840000000	2.422632000000	-0.921359000000
H	-1.963090000000	-2.464440000000	1.686915000000
H	2.159273000000	2.278971000000	-1.619344000000
C	5.424903000000	-0.660565000000	-0.638418000000
C	-5.105007000000	0.619516000000	0.483375000000
H	5.270610000000	0.405378000000	-0.735869000000
H	-4.920753000000	-0.290025000000	0.426883000000
C	1.544387000000	4.155641000000	4.806534000000
C	-1.604068000000	-4.146191000000	-4.781151000000
C	6.633841000000	-1.157420000000	-0.152715000000
C	-6.288778000000	1.123416000000	-0.043040000000
H	7.409239000000	-0.459235000000	0.138719000000
H	-6.903619000000	0.552111000000	-0.444448000000
C	-3.939824000000	-3.010739000000	1.085567000000
C	4.044895000000	2.851860000000	-1.217043000000
C	-4.820979000000	-3.109248000000	-0.002982000000
C	4.913344000000	3.093559000000	-0.153313000000
C	-4.427815000000	-2.743417000000	-1.299669000000
C	4.541449000000	2.851015000000	1.168346000000
C	0.631132000000	3.316375000000	4.196012000000
C	-0.690861000000	-3.306857000000	-4.170573000000
H	0.802475000000	2.402786000000	4.147218000000
H	-0.862220000000	-2.393406000000	-4.121804000000
C	-0.532789000000	3.826803000000	3.659277000000
C	0.472996000000	-3.817355000000	-3.633808000000

H	-1.138618000000	3.263470000000	3.235132000000
H	1.078873000000	-3.254089000000	-3.209717000000
C	2.187202000000	5.721141000000	1.150297000000
C	-2.246996000000	-5.711693000000	-1.124828000000
H	1.273746000000	5.485083000000	1.329678000000
H	-1.333540000000	-5.475634000000	-1.304209000000
H	2.739128000000	5.449260000000	1.887806000000
H	-2.798874000000	-5.439879000000	-1.862392000000
H	2.481514000000	5.278103000000	0.350335000000
H	-2.541195000000	-5.268652000000	-0.324951000000
C	-4.392176000000	-3.359802000000	2.482655000000
C	4.498323000000	2.989461000000	-2.648960000000
H	3.087522000000	7.349243000000	3.225681000000
H	-3.147267000000	-7.339863000000	-3.200266000000
H	-3.747741000000	-2.885784000000	3.229689000000
H	4.437350000000	2.138442000000	-3.087589000000
H	-4.359359000000	-4.442755000000	2.663897000000
H	3.937646000000	3.624168000000	-3.102215000000
C	-5.396920000000	-2.839294000000	-2.453075000000
C	5.499685000000	3.074508000000	2.311982000000
H	-4.995154000000	-2.338215000000	-3.338754000000
H	5.066539000000	2.852238000000	3.139746000000
H	-6.359878000000	-2.384517000000	-2.199514000000
H	6.273079000000	2.517759000000	2.195503000000
H	-5.599021000000	-3.882950000000	-2.728264000000
H	5.768166000000	3.996877000000	2.328917000000
C	-1.286753000000	5.985841000000	-0.285367000000
C	1.227008000000	-5.976460000000	0.310781000000
H	-0.547810000000	5.443892000000	0.001650000000
H	0.488081000000	-5.434374000000	0.023789000000
H	-1.734303000000	6.349740000000	0.481418000000
H	1.674573000000	-6.340221000000	-0.455980000000
H	-0.963167000000	6.701550000000	-0.837207000000
H	0.903373000000	-6.692102000000	0.862676000000
C	3.581772000000	7.552006000000	0.710151000000
C	-3.641517000000	-7.542626000000	-0.684736000000
C	-3.312973000000	5.808359000000	-1.518095000000
C	3.253292000000	-5.798909000000	1.543479000000
C	4.596862000000	-2.908730000000	-0.945429000000
C	-4.467881000000	2.808725000000	1.181770000000
C	1.288048000000	5.512133000000	4.884009000000
O	2.665313000000	3.540034000000	5.298070000000
O	-2.725106000000	-3.530586000000	-5.272601000000
C	-1.347842000000	-5.502684000000	-4.858539000000
C	6.824592000000	-2.539467000000	-0.052094000000
C	-6.544993000000	2.479957000000	0.034482000000

O	-6.136575000000	-3.490351000000	0.210528000000
O	6.207061000000	3.516682000000	-0.420045000000
C	-0.790316000000	5.173013000000	3.755581000000
C	0.730587000000	-5.163494000000	-3.730142000000
H	-5.422874000000	-3.035069000000	2.653441000000
H	5.407653000000	3.296302000000	-2.668765000000
C	3.953775000000	7.794462000000	-0.611485000000
C	4.450221000000	7.793706000000	1.773881000000
C	-4.510014000000	-7.784257000000	-1.748412000000
C	-4.013456000000	-7.785012000000	0.636869000000
C	-4.226228000000	4.969093000000	-2.128618000000
C	-3.569312000000	7.164851000000	-1.440621000000
C	3.509518000000	-7.155402000000	1.466090000000
C	4.166499000000	-4.959574000000	2.154057000000
H	3.814576000000	-3.587195000000	-1.266966000000
C	5.797245000000	-3.407623000000	-0.450668000000
C	-5.631738000000	3.319223000000	0.645004000000
H	-3.862052000000	3.372059000000	1.605915000000
C	0.104277000000	6.016033000000	4.357594000000
H	1.902953000000	6.083508000000	5.285386000000
C	3.570607000000	4.333123000000	6.039263000000
C	-3.630352000000	-4.323743000000	-6.013848000000
H	-1.962683000000	-6.073989000000	-5.259948000000
C	-0.164022000000	-6.006653000000	-4.332180000000
O	7.964900000000	-3.128346000000	0.413193000000
O	-7.665983000000	3.095494000000	-0.457023000000
C	-6.361964000000	-4.896291000000	0.178685000000
C	6.307973000000	4.924404000000	-0.593381000000
O	-1.908494000000	5.755101000000	3.147843000000
O	1.848749000000	-5.745720000000	-3.122428000000
C	2.995490000000	7.571037000000	-1.755066000000
C	5.248897000000	8.248758000000	-0.859433000000
C	5.738336000000	8.222913000000	1.478274000000
C	3.996793000000	7.656104000000	3.205798000000
C	-4.056538000000	-7.646724000000	-3.180384000000
C	-5.798081000000	-8.213533000000	-1.452860000000
C	-5.308578000000	-8.239308000000	0.884816000000
C	-3.055171000000	-7.561587000000	1.780450000000
C	-5.390150000000	5.479521000000	-2.665352000000
H	-4.054885000000	4.055504000000	-2.177411000000
C	-4.753083000000	7.668751000000	-1.967035000000
H	-2.954407000000	7.736226000000	-1.039243000000
H	2.894678000000	-7.726707000000	1.064682000000
C	4.693338000000	-7.659370000000	1.992450000000
H	3.995140000000	-4.046123000000	2.202826000000
C	5.330356000000	-5.470072000000	2.690822000000

H	5.963617000000	-4.476064000000	-0.367633000000
H	-5.803205000000	4.232763000000	0.693751000000
H	-0.079977000000	6.925573000000	4.414086000000
H	3.894194000000	5.048833000000	5.487423000000
H	4.309550000000	3.791174000000	6.326280000000
H	3.123058000000	4.697022000000	6.806048000000
H	-4.369279000000	-3.781656000000	-6.300841000000
H	-3.182787000000	-4.687503000000	-6.780610000000
H	-3.953987000000	-5.039384000000	-5.461953000000
H	0.020232000000	-6.916193000000	-4.388672000000
C	9.025769000000	-2.278808000000	0.821184000000
C	-8.571337000000	2.302426000000	-1.198294000000
H	-6.046030000000	-5.330483000000	-0.778336000000
H	-7.437338000000	-5.045534000000	0.303772000000
H	-5.831625000000	-5.406008000000	0.992663000000
H	5.756095000000	5.196217000000	-1.330945000000
H	7.221429000000	5.160462000000	-0.772762000000
H	6.013661000000	5.367442000000	0.206581000000
C	-3.159731000000	5.416929000000	3.571677000000
C	3.099938000000	-5.407481000000	-3.546207000000
H	3.428636000000	7.793307000000	-2.582830000000
H	2.222097000000	8.127787000000	-1.638587000000
H	2.727010000000	6.648668000000	-1.772001000000
H	5.508288000000	8.424136000000	-1.734949000000
C	6.163115000000	8.445671000000	0.173797000000
H	6.335902000000	8.366574000000	2.176260000000
H	4.057825000000	8.507103000000	3.644505000000
H	4.557577000000	7.021309000000	3.659076000000
H	-4.617259000000	-7.011859000000	-3.633692000000
H	-4.117619000000	-8.497655000000	-3.619035000000
H	-6.395648000000	-8.357194000000	-2.150846000000
C	-6.222844000000	-8.436152000000	-0.148359000000
H	-5.568081000000	-8.414687000000	1.760418000000
H	-2.281826000000	-8.118268000000	1.664026000000
H	-2.786739000000	-6.639150000000	1.797439000000
H	-3.488381000000	-7.783927000000	2.608245000000
H	-5.995978000000	4.916187000000	-3.089498000000
C	-5.647677000000	6.825731000000	-2.569049000000
H	-4.937337000000	8.578291000000	-1.910544000000
C	5.587947000000	-6.816212000000	2.594487000000
H	4.877592000000	-8.568911000000	1.935958000000
H	5.936233000000	-4.906807000000	3.114912000000
H	9.388698000000	-1.660321000000	-0.010367000000
H	9.830738000000	-2.933272000000	1.157568000000
H	8.722554000000	-1.625920000000	1.650272000000
H	-9.310204000000	2.844492000000	-1.485209000000

H	-8.123712000000	1.938644000000	-1.964977000000
H	-8.894864000000	1.586696000000	-0.646376000000
C	-4.214733000000	6.051941000000	2.852503000000
C	-3.502697000000	4.569477000000	4.580801000000
C	3.443016000000	-4.560026000000	-4.555418000000
C	4.154940000000	-6.042492000000	-2.827034000000
C	7.564555000000	8.838461000000	-0.103113000000
C	-7.624236000000	-8.829010000000	0.128497000000
O	-6.765854000000	7.407818000000	-3.176787000000
O	6.706109000000	-7.398438000000	3.202201000000
N	-4.058716000000	6.949088000000	1.867826000000
C	-5.585566000000	5.769898000000	3.163176000000
H	-2.836368000000	4.173196000000	5.093767000000
C	-4.869491000000	4.284318000000	4.859744000000
C	4.809745000000	-4.274938000000	-4.834329000000
H	2.776575000000	-4.163748000000	-5.068298000000
C	5.525773000000	-5.760450000000	-3.137707000000
N	3.999035000000	-6.939638000000	-1.842442000000
C	7.910328000000	9.779847000000	-1.121010000000
C	8.626355000000	8.294335000000	0.575613000000
C	-8.686085000000	-8.284816000000	-0.550174000000
C	-7.970073000000	-9.770467000000	1.146424000000
C	-8.017092000000	7.069647000000	-2.752953000000
C	7.957298000000	-7.060199000000	2.778422000000
N	-6.439853000000	6.490226000000	2.407822000000
C	-5.931339000000	4.828512000000	4.181073000000
H	-5.055081000000	3.688687000000	5.549318000000
H	4.995400000000	-3.679237000000	-5.523935000000
C	5.871546000000	-4.819063000000	-4.155603000000
N	6.380124000000	-6.480707000000	-2.382383000000
N	7.055977000000	10.500104000000	-1.876334000000
C	9.281161000000	10.061890000000	-1.431683000000
C	9.993085000000	8.579424000000	0.296701000000
H	8.440701000000	7.698634000000	1.265218000000
H	-8.500494000000	-7.689186000000	-1.239749000000
C	-10.052830000000	-8.570043000000	-0.271287000000
C	-9.340906000000	-10.052509000000	1.457097000000
N	-7.115722000000	-10.490724000000	1.901748000000
C	-9.072093000000	7.704659000000	-3.472126000000
C	-8.360057000000	6.222195000000	-1.743828000000
C	8.300376000000	-6.212744000000	1.769212000000
C	9.012300000000	-7.695210000000	3.497596000000
C	-7.332731000000	4.435654000000	4.457928000000
C	7.272986000000	-4.426274000000	-4.432514000000
N	9.437066000000	10.959035000000	-2.416274000000
C	10.336163000000	9.426878000000	-0.712509000000

H	10.659526000000	8.183145000000	0.809581000000
H	-10.719207000000	-8.173694000000	-0.784198000000
C	-10.395844000000	-9.417428000000	0.737893000000
N	-9.496859000000	-10.949586000000	2.441744000000
N	-8.916076000000	8.601806000000	-4.456804000000
C	-10.442927000000	7.422616000000	-3.161453000000
H	-7.693728000000	5.825914000000	-1.230862000000
C	-9.726851000000	5.937036000000	-1.464886000000
C	9.667106000000	-5.927655000000	1.490300000000
H	7.633935000000	-5.816465000000	1.256332000000
C	10.383133000000	-7.413167000000	3.186923000000
N	8.856395000000	-8.592355000000	4.482187000000
C	-8.246949000000	4.238741000000	3.424699000000
C	-7.757558000000	4.212965000000	5.762461000000
C	7.697765000000	-4.203516000000	-5.736991000000
C	8.187203000000	-4.229361000000	-3.399284000000
O	11.587352000000	9.765118000000	-1.136288000000
O	-11.647081000000	-9.755599000000	1.161727000000
N	-11.297213000000	8.142944000000	-3.916808000000
C	-10.788759000000	6.481250000000	-2.143635000000
H	-9.912441000000	5.341405000000	-0.775311000000
H	9.852760000000	-5.331955000000	0.800695000000
C	10.728965000000	-6.471802000000	2.169104000000
N	11.237484000000	-8.133425000000	3.942247000000
H	-7.987494000000	4.414189000000	2.549151000000
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C	3.291216000000	0.014707000000	-1.171884000000
C	-1.146481000000	-5.244765000000	-1.226396000000

H	2.652979000000	0.126845000000	-0.307898000000
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C	-4.549154000000	-3.153541000000	-3.425279000000
C	5.880695000000	-1.336597000000	0.927310000000
H	-4.349726000000	-4.057258000000	-3.979228000000
H	5.561400000000	-0.326686000000	0.964177000000
C	-5.672655000000	0.591701000000	3.237259000000
C	2.313577000000	1.591140000000	-5.478822000000
C	-5.791533000000	-2.982105000000	-2.823555000000
C	7.231764000000	-1.646492000000	0.723709000000
H	-6.523289000000	-3.778592000000	-2.885332000000
H	7.902844000000	-0.919003000000	0.316296000000
C	4.396893000000	0.860303000000	-1.242252000000
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C	5.304470000000	0.681565000000	-2.294814000000
C	-3.344557000000	-6.093652000000	-0.717755000000
C	5.138062000000	-0.357216000000	-3.219920000000
C	-3.226440000000	-5.584791000000	0.581347000000
C	-4.308420000000	0.515255000000	2.897964000000
C	1.430730000000	0.778289000000	-4.778979000000
H	-3.948127000000	-0.312664000000	2.322821000000
H	1.756652000000	-0.167660000000	-4.405028000000
C	-3.414025000000	1.519710000000	3.326673000000
C	0.097726000000	1.223731000000	-4.574302000000
H	-2.370787000000	1.440658000000	3.095307000000
H	-0.493655000000	0.872831000000	-3.748699000000
C	-0.317957000000	-3.370003000000	7.805852000000
C	1.858424000000	3.936526000000	-2.340710000000
H	0.577816000000	-3.918661000000	8.017943000000
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H	-2.634461000000	-4.537857000000	9.825150000000
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C	7.655082000000	-2.878973000000	1.076551000000
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S	-8.511231000000	-3.636026000000	4.051618000000
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S	-5.845027000000	3.453747000000	-3.718302000000
S	5.583225000000	11.137068000000	1.469234000000
S	-11.934610000000	4.845580000000	1.511585000000
C	0.542013000000	0.266500000000	-0.977754000000
C	-1.908939000000	-1.185576000000	-0.930107000000
C	9.813819000000	8.152447000000	-2.116928000000
C	7.507158000000	6.770960000000	-2.541851000000
C	-7.720877000000	1.827720000000	-2.055158000000
C	-10.032912000000	0.486276000000	-2.510252000000
C	-1.619500000000	0.472797000000	-7.306053000000
C	-3.917786000000	-0.909954000000	-7.731597000000
C	3.726878000000	-4.000223000000	-0.749422000000
C	1.424781000000	-5.377996000000	-1.175831000000
C	11.465753000000	-4.438827000000	1.460633000000
C	9.041770000000	-5.840749000000	0.604423000000
C	-5.592020000000	0.625839000000	7.860588000000
C	-8.227954000000	1.945524000000	7.091696000000
C	2.017092000000	4.252448000000	4.363227000000
C	-0.694335000000	5.323270000000	3.979110000000
O	10.928586000000	8.783304000000	-1.979681000000
O	9.711428000000	7.144297000000	-2.935320000000
O	8.612569000000	6.402756000000	-3.185893000000
O	6.424581000000	6.143953000000	-2.763584000000
O	0.483764000000	0.267171000000	0.360133000000
O	0.659561000000	1.280255000000	-1.613182000000
O	-2.633825000000	-2.265786000000	-0.570622000000
O	-2.079258000000	-0.097864000000	-0.424704000000
O	-6.566619000000	2.366611000000	-1.874961000000
O	-7.830041000000	0.848672000000	-2.914673000000
O	-8.931652000000	0.122366000000	-3.170344000000
O	-11.141667000000	-0.165310000000	-2.729043000000
O	-0.504424000000	1.103722000000	-7.172474000000
O	-1.718711000000	-0.535097000000	-8.128648000000
O	-2.814456000000	-1.280299000000	-8.374262000000
O	-5.032275000000	-1.560795000000	-7.960195000000
O	4.844213000000	-3.370249000000	-0.611680000000
O	3.627503000000	-5.007811000000	-1.573759000000

O	2.529572000000	-5.750476000000	-1.819973000000
O	0.311682000000	-6.030554000000	-1.403354000000
O	12.542397000000	-3.796907000000	1.820368000000
O	10.305679000000	-4.091935000000	1.939266000000
O	3.381026000000	3.938372000000	4.618998000000
O	1.741858000000	5.282911000000	3.693681000000
O	8.990523000000	-4.822837000000	1.417883000000
O	7.950459000000	-6.453700000000	0.247223000000
O	-4.474834000000	0.000946000000	8.487811000000
O	-5.815055000000	1.845337000000	8.083783000000
O	-7.605597000000	2.382325000000	8.306326000000
O	-9.121559000000	2.645215000000	6.546736000000
H	8.818882000000	5.507810000000	-2.913034000000
H	10.992690000000	9.271644000000	-1.193246000000
H	0.416694000000	1.206008000000	0.619944000000
H	-3.311080000000	-1.940153000000	0.052352000000
H	-6.460319000000	2.938755000000	-1.147353000000
H	-8.730610000000	-0.773679000000	-2.897719000000
H	-2.609758000000	-2.174334000000	-8.099736000000
H	-0.427506000000	1.585953000000	-6.381084000000
H	2.732579000000	-6.644158000000	-1.544808000000
H	4.897804000000	-2.879324000000	0.175651000000
H	-4.300832000000	0.463681000000	9.316975000000
H	-7.692790000000	3.331315000000	8.394532000000
H	12.481760000000	-3.059261000000	2.432379000000
H	8.147005000000	-4.513640000000	1.753852000000
O	-1.954802000000	5.776134000000	3.482864000000
O	0.323910000000	6.064663000000	3.910021000000
H	3.886654000000	4.759593000000	4.607641000000
H	-1.985440000000	6.733280000000	3.498088000000

Excited State:

HB:

S	-0.173834000000	0.681432000000	-3.538547000000
S	0.523975000000	-0.755819000000	3.416198000000
O	3.349549000000	-0.978476000000	-1.538830000000
O	-3.113030000000	0.875770000000	1.686473000000
O	2.254792000000	7.135761000000	0.977641000000
O	-2.350477000000	-7.120877000000	-0.962679000000
N	-1.132991000000	-0.229198000000	-2.489461000000
N	1.419356000000	0.149649000000	2.428917000000
O	-2.220035000000	5.191632000000	-1.030029000000
O	2.124353000000	-5.176746000000	1.044990000000
N	1.345989000000	0.215762000000	-2.977598000000
N	-0.961122000000	-0.314492000000	2.967137000000
C	-0.279585000000	-0.895378000000	-1.703551000000

C	0.564074000000	0.868586000000	1.673554000000
C	1.093308000000	-0.635861000000	-1.975274000000
C	-0.806376000000	0.583516000000	1.983148000000
C	-0.645710000000	-1.800766000000	-0.646633000000
C	0.908568000000	1.811316000000	0.656467000000
C	0.403945000000	-2.344013000000	0.146321000000
C	-0.153958000000	2.353733000000	-0.022566000000
H	0.164730000000	-3.005603000000	0.968153000000
H	0.030918000000	2.950245000000	-0.711680000000
C	2.093835000000	-1.274309000000	-1.192246000000
C	-1.862216000000	1.216790000000	1.263673000000
C	1.731515000000	-2.106939000000	-0.113170000000
C	-1.520278000000	2.065647000000	0.255269000000
H	2.484508000000	-2.559058000000	0.514622000000
H	-2.187150000000	2.460795000000	-0.257861000000
C	-2.014244000000	-2.198230000000	-0.396771000000
C	2.309326000000	2.207243000000	0.380778000000
C	-2.971637000000	-2.227988000000	-1.433989000000
C	3.222454000000	2.405406000000	1.414732000000
H	-2.689710000000	-1.893400000000	-2.421922000000
H	2.962792000000	2.228969000000	2.289891000000
C	4.477223000000	-1.577385000000	-1.012639000000
C	-4.231994000000	1.456059000000	1.078383000000
C	-2.421457000000	-2.610328000000	0.889513000000
C	2.734501000000	2.431687000000	-0.923281000000
H	-1.726832000000	-2.543126000000	1.718265000000
H	2.137693000000	2.287224000000	-1.621748000000
C	5.525531000000	-0.718604000000	-0.725842000000
C	-5.124521000000	0.611445000000	0.475157000000
H	5.390669000000	0.346407000000	-0.865244000000
H	-4.938349000000	-0.297678000000	0.418224000000
C	1.514699000000	4.158635000000	4.804883000000
C	-1.610270000000	-4.143747000000	-4.790008000000
C	6.733399000000	-1.222534000000	-0.265304000000
C	-6.308985000000	1.113222000000	-0.051726000000
H	7.534699000000	-0.530780000000	-0.040980000000
H	-6.922379000000	0.540895000000	-0.453892000000
C	-3.716616000000	-3.021268000000	1.152799000000
C	4.021860000000	2.863762000000	-1.217850000000
C	-4.620693000000	-3.082000000000	0.079520000000
C	4.889107000000	3.106597000000	-0.153399000000
C	-4.256125000000	-2.694238000000	-1.219019000000
C	4.516846000000	2.862465000000	1.167864000000
C	0.603584000000	3.317860000000	4.193240000000
C	-0.699203000000	-3.302905000000	-4.178309000000
H	0.776848000000	2.404658000000	4.143994000000

H	-0.872484000000	-2.389840000000	-4.129088000000
C	-0.561036000000	3.826213000000	3.656054000000
C	0.465355000000	-3.811327000000	-3.641094000000
H	-1.165421000000	3.261891000000	3.231162000000
H	1.069786000000	-3.247071000000	-3.216255000000
C	2.156679000000	5.727727000000	1.150039000000
C	-2.252363000000	-5.712840000000	-1.135079000000
H	1.243596000000	5.489669000000	1.328672000000
H	-1.339278000000	-5.474782000000	-1.313712000000
H	2.708682000000	5.456530000000	1.887744000000
H	-2.804316000000	-5.441711000000	-1.872838000000
H	2.452434000000	5.285794000000	0.349998000000
H	-2.548003000000	-5.270905000000	-0.335122000000
C	-4.148452000000	-3.352027000000	2.555707000000
C	4.475944000000	3.003188000000	-2.649383000000
H	3.052265000000	7.356400000000	3.227023000000
H	-3.147898000000	-7.341583000000	-3.212116000000
H	-3.547123000000	-2.795321000000	3.277972000000
H	4.417020000000	2.152316000000	-3.088578000000
H	-4.030965000000	-4.418599000000	2.780175000000
H	3.914253000000	3.637015000000	-3.102615000000
C	-5.251112000000	-2.777429000000	-2.344769000000
C	5.473865000000	3.087230000000	2.312269000000
H	-4.777479000000	-2.513064000000	-3.292510000000
H	5.040635000000	2.863552000000	3.139610000000
H	-6.100893000000	-2.108509000000	-2.174500000000
H	6.248485000000	2.532155000000	2.195956000000
H	-5.661043000000	-3.787931000000	-2.441263000000
H	5.740426000000	4.010142000000	2.329952000000
C	-1.316871000000	5.986131000000	-0.287749000000
C	1.221238000000	-5.971313000000	0.302655000000
H	-0.576997000000	5.445533000000	-0.000581000000
H	0.481380000000	-5.430578000000	0.015512000000
H	-1.765677000000	6.348628000000	0.478966000000
H	1.670058000000	-6.333672000000	-0.464036000000
H	-0.994404000000	6.702850000000	-0.838933000000
H	0.898720000000	-6.687964000000	0.853894000000
C	3.547748000000	7.561745000000	0.711945000000
C	-3.643382000000	-7.546927000000	-0.697038000000
C	-3.341909000000	5.805223000000	-1.521922000000
C	3.246338000000	-5.790336000000	1.536798000000
C	4.629284000000	-2.956505000000	-0.877001000000
C	-4.492385000000	2.801534000000	1.175326000000
C	1.255504000000	5.514545000000	4.883028000000
O	2.636573000000	3.545042000000	5.296777000000
O	-2.732256000000	-3.530157000000	-5.281816000000

C	-1.351188000000	-5.499657000000	-4.868066000000
C	6.890310000000	-2.597596000000	-0.103583000000
C	-6.568057000000	2.469182000000	0.026466000000
O	-5.923813000000	-3.449099000000	0.294630000000
O	6.182122000000	3.532560000000	-0.419017000000
C	-0.821412000000	5.171826000000	3.753021000000
C	0.725792000000	-5.156870000000	-3.738090000000
H	-5.199779000000	-3.097251000000	2.707903000000
H	5.384650000000	3.311921000000	-2.668399000000
C	3.920117000000	7.805789000000	-0.609295000000
C	4.414995000000	7.804580000000	1.776396000000
C	-4.510678000000	-7.789695000000	-1.761436000000
C	-4.015689000000	-7.790901000000	0.624171000000
C	-4.253024000000	4.964449000000	-2.133565000000
C	-3.601105000000	7.161133000000	-1.443777000000
C	3.505420000000	-7.146248000000	1.458738000000
C	4.157406000000	-4.949492000000	2.148496000000
H	3.815592000000	-3.632078000000	-1.115348000000
C	5.837680000000	-3.459300000000	-0.420373000000
C	-5.656942000000	3.309957000000	0.638109000000
H	-3.888001000000	3.365857000000	1.600218000000
C	0.071040000000	6.016321000000	4.356145000000
H	1.868962000000	6.086941000000	5.285164000000
C	3.539736000000	4.339541000000	6.039056000000
C	-3.635371000000	-4.324724000000	-6.024150000000
H	-1.964581000000	-6.071984000000	-5.270234000000
C	-0.166674000000	-6.001504000000	-4.341239000000
O	8.037407000000	-3.180061000000	0.352345000000
O	-7.689994000000	3.082704000000	-0.465396000000
C	-6.150491000000	-4.848425000000	0.408305000000
C	6.280235000000	4.940594000000	-0.591415000000
O	-1.940392000000	5.751977000000	3.144907000000
O	1.844757000000	-5.737159000000	-3.130000000000
C	2.963048000000	7.581092000000	-1.753645000000
C	5.214460000000	8.262916000000	-0.856109000000
C	5.702415000000	8.236633000000	1.481904000000
C	3.960911000000	7.665153000000	3.207929000000
C	-4.056545000000	-7.650336000000	-3.193023000000
C	-5.798048000000	-8.221816000000	-1.466998000000
C	-5.310030000000	-8.248028000000	0.870984000000
C	-3.058620000000	-7.566204000000	1.768521000000
C	-5.417646000000	5.472801000000	-2.670750000000
H	-4.079760000000	4.051246000000	-2.182811000000
C	-4.785569000000	7.662911000000	-1.970660000000
H	-2.987646000000	7.733530000000	-1.041641000000
H	2.892028000000	-7.718574000000	1.056572000000

C	4.689934000000	-7.648092000000	1.985566000000
H	3.984125000000	-4.036428000000	2.197717000000
C	5.321962000000	-5.457915000000	2.685712000000
H	5.975693000000	-4.528869000000	-0.307461000000
H	-5.830330000000	4.223110000000	0.687308000000
H	-0.115133000000	6.925443000000	4.413078000000
H	3.862205000000	5.056262000000	5.487873000000
H	4.279610000000	3.798945000000	6.326225000000
H	3.090932000000	4.702040000000	6.805771000000
H	-4.375229000000	-3.783989000000	-6.311294000000
H	-3.186550000000	-4.687083000000	-6.790841000000
H	-3.957888000000	-5.041375000000	-5.472911000000
H	0.019498000000	-6.910625000000	-4.398172000000
C	9.060153000000	-2.318530000000	0.810677000000
C	-8.593218000000	2.288224000000	-1.207754000000
H	-5.850463000000	-5.367600000000	-0.507902000000
H	-7.221852000000	-4.980254000000	0.564210000000
H	-5.607830000000	-5.276796000000	1.256385000000
H	5.728280000000	5.211723000000	-1.329175000000
H	7.193318000000	5.178652000000	-0.770048000000
H	5.984481000000	5.382527000000	0.208626000000
C	-3.191204000000	5.410955000000	3.567707000000
C	3.095522000000	-5.396070000000	-3.552745000000
H	3.396279000000	7.804770000000	-2.580986000000
H	2.188430000000	8.136168000000	-1.637332000000
H	2.696489000000	6.658179000000	-1.771328000000
H	5.474063000000	8.439373000000	-1.731345000000
C	6.127588000000	8.461079000000	0.177845000000
H	6.299222000000	8.381097000000	2.180372000000
H	4.019895000000	8.516005000000	3.647202000000
H	4.522709000000	7.031239000000	3.661184000000
H	-4.618280000000	-7.016351000000	-3.646308000000
H	-4.115577000000	-8.501120000000	-3.632241000000
H	-6.394858000000	-8.366280000000	-2.165466000000
C	-6.223208000000	-8.446122000000	-0.162915000000
H	-5.569746000000	-8.424486000000	1.746306000000
H	-2.284049000000	-8.121212000000	1.652263000000
H	-2.792107000000	-6.643224000000	1.786258000000
H	-3.491913000000	-7.789952000000	2.595893000000
H	-6.022028000000	4.908478000000	-3.095644000000
C	-5.678020000000	6.818415000000	-2.573784000000
H	-4.971741000000	8.572032000000	-1.913727000000
C	5.582401000000	-6.803459000000	2.588714000000
H	4.876107000000	-8.557215000000	1.928633000000
H	5.926395000000	-4.893661000000	3.110550000000
H	9.469117000000	-1.708622000000	-0.003702000000

H	9.850620000000	-2.952621000000	1.212148000000
H	8.698561000000	-1.657222000000	1.605796000000
H	-9.333016000000	2.828939000000	-1.494821000000
H	-8.144338000000	1.925844000000	-1.974367000000
H	-8.915626000000	1.571485000000	-0.656492000000
C	-4.247045000000	6.044230000000	2.848231000000
C	-3.533081000000	4.562171000000	4.576080000000
C	3.437509000000	-4.547282000000	-4.561206000000
C	4.151362000000	-6.029344000000	-2.833270000000
C	7.528395000000	8.856937000000	-0.097898000000
C	-7.623965000000	-8.842050000000	0.112774000000
O	-6.796999000000	7.398566000000	-3.181899000000
O	6.701365000000	-7.383748000000	3.196805000000
N	-4.092236000000	6.942308000000	1.864212000000
C	-5.617495000000	5.759160000000	3.157826000000
H	-2.866269000000	4.166950000000	5.089240000000
C	-4.899465000000	4.274013000000	4.853946000000
C	4.803829000000	-4.259195000000	-4.839040000000
H	2.770588000000	-4.152065000000	-5.074279000000
C	5.521813000000	-5.744275000000	-3.142865000000
N	3.996667000000	-6.927420000000	-1.849336000000
C	7.872889000000	9.799667000000	-1.114985000000
C	8.590872000000	8.314588000000	0.581190000000
C	-8.686491000000	-8.299632000000	-0.566259000000
C	-7.968524000000	-9.784850000000	1.129891000000
C	-8.047814000000	7.057545000000	-2.759099000000
C	7.952130000000	-7.042658000000	2.774059000000
N	-6.472774000000	6.478187000000	2.402355000000
C	-5.961989000000	4.816431000000	4.174913000000
H	-5.084276000000	3.677572000000	5.543029000000
H	4.988705000000	-3.662684000000	-5.528154000000
C	5.866308000000	-4.801543000000	-4.159951000000
N	6.377155000000	-6.463231000000	-2.387424000000
N	7.017548000000	10.518624000000	-1.870426000000
C	9.243340000000	10.084738000000	-1.424580000000
C	9.957193000000	8.602676000000	0.303355000000
H	8.405997000000	7.718077000000	1.270304000000
H	-8.501680000000	-7.703192000000	-1.255343000000
C	-10.052826000000	-8.587858000000	-0.288450000000
C	-9.338975000000	-10.069919000000	1.439486000000
N	-7.113181000000	-10.503806000000	1.885332000000
C	-9.103653000000	7.690819000000	-3.478574000000
C	-8.389689000000	6.208760000000	-1.750724000000
C	8.294118000000	-6.193871000000	1.765600000000
C	9.007970000000	-7.675933000000	3.493535000000
C	-7.362748000000	4.420504000000	4.450601000000

C	7.267114000000	-4.405685000000	-4.435695000000
N	9.398037000000	10.982813000000	-2.408513000000
C	10.299180000000	9.451463000000	-0.705104000000
H	10.624114000000	8.207459000000	0.816429000000
H	-10.719684000000	-8.192570000000	-0.801554000000
C	-10.394751000000	-9.436575000000	0.719980000000
N	-9.493719000000	-10.967928000000	2.423475000000
N	-8.948844000000	8.588898000000	-4.462593000000
C	-10.474105000000	7.405750000000	-3.168978000000
H	-7.722878000000	5.813540000000	-1.237564000000
C	-9.756073000000	5.920601000000	-1.472859000000
C	9.660439000000	-5.905783000000	1.487765000000
H	7.627196000000	-5.798653000000	1.252526000000
C	10.378421000000	-7.390862000000	3.183940000000
N	8.853274000000	-8.574009000000	4.477468000000
C	-8.275877000000	4.222341000000	3.416648000000
C	-7.787971000000	4.196127000000	5.754716000000
C	7.692289000000	-4.181241000000	-5.739754000000
C	8.180241000000	-4.207523000000	-3.401741000000
O	11.549945000000	9.792553000000	-1.127849000000
O	-11.645564000000	-9.777596000000	1.142780000000
N	-11.329382000000	8.124776000000	-3.924450000000
C	-10.818658000000	6.463039000000	-2.151971000000
H	-9.940883000000	5.324161000000	-0.783775000000
H	9.845314000000	-5.309273000000	0.798651000000
C	10.722974000000	-6.448154000000	2.166932000000
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C	5.268855000000	1.807734000000	6.314620000000
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C	-4.462469000000	-3.255183000000	-3.360698000000
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H	-2.324318000000	-2.080927000000	1.760057000000
C	-4.393095000000	-1.568851000000	1.628876000000
C	6.760363000000	4.300037000000	-1.665931000000
H	5.899927000000	6.118218000000	-0.901010000000
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H	-5.396409000000	1.927143000000	-4.748801000000
C	-5.486962000000	1.355437000000	-0.804396000000
C	6.092581000000	-5.678150000000	1.437178000000
H	4.016837000000	-7.182114000000	1.477825000000
C	1.960433000000	-6.706153000000	1.138789000000

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C	6.199056000000	-3.257747000000	-1.919327000000
C	-4.325222000000	3.705309000000	6.450539000000
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C	-1.528863000000	6.571822000000	0.092439000000
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H	5.945392000000	-3.861786000000	-1.045340000000
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C	4.940725000000	4.568028000000	0.773355000000
C	3.136278000000	-0.098028000000	-0.950088000000

C	-0.591976000000	2.026029000000	5.039095000000
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H	0.338429000000	1.609062000000	5.396773000000
C	-3.952644000000	-0.784287000000	3.825742000000
C	5.208510000000	3.241374000000	0.823541000000
H	-3.693874000000	-0.502486000000	4.834027000000
H	4.781804000000	2.627190000000	1.604592000000
C	-4.703417000000	2.129282000000	-2.963964000000
C	4.180146000000	-5.245075000000	0.387429000000
C	-5.249703000000	-0.662186000000	3.369401000000
C	6.093024000000	2.658630000000	-0.108452000000
H	-5.998492000000	-0.259619000000	4.037843000000
H	6.301849000000	1.603774000000	-0.021354000000
C	4.194899000000	-0.461178000000	-1.753701000000
C	-1.797381000000	1.588855000000	5.604704000000
C	5.316239000000	-1.051966000000	-1.147311000000
C	-3.012675000000	2.146480000000	5.148116000000
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C	-3.500418000000	2.335661000000	-2.266628000000
C	3.272025000000	-4.226961000000	0.069767000000
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C	-2.320189000000	2.621948000000	-2.955773000000
C	1.899010000000	-4.501933000000	-0.006188000000
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H	-0.017482000000	-3.783895000000	-2.355182000000
C	4.135607000000	-0.275712000000	-3.244702000000
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H	-1.088289000000	0.875250000000	7.509870000000
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H	6.630652000000	-1.624718000000	1.954983000000

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C	0.733446000000	-4.954124000000	2.844178000000
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O	0.621516000000	4.470623000000	6.339401000000
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