

Spiroaquilarenes A–E: unprecedented anti-inflammatory sesquiterpene polymers from agarwood of *Aquilaria sinensis*

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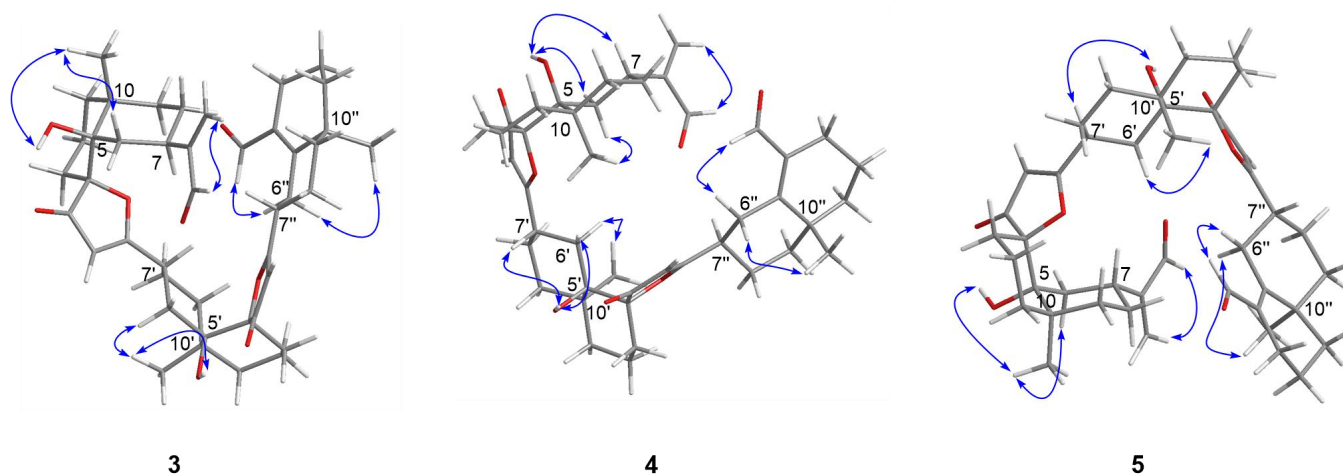
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Table S1. ^1H (600 MHz) and ^{13}C NMR (150 MHz) Data of **1** and **2** in pyridine- d_5 (δ in ppm, J in Hz)

		1		2	
no	δ_{H}	δ_{C}	δ_{H}	δ_{C}	
1	Ha: 2.11, m Hb: 1.07, overlap	34.1, t	Ha: 2.02, m Hb: 1.28, overlap	36.6, t	
2	Ha: 1.93, m Hb: 1.50, m	18.3 ^a , t	Ha: 1.91, m Hb: 1.52, overlap	18.4 ^b , t	
3	Ha: 2.46, overlap Hb: 1.46, overlap	31.1, t	Ha: 2.33, dt (13.3, 3.7) Hb: 1.45, overlap	32.9, t	
4		92.3, s		93.3, s	
5		75.9, s		75.0, s	
6	Ha: 2.06, t-like (12.8) Hb: 1.38, m	32.8, t	Ha: 1.65, m Hb: 1.62, m	39.7 ^c , t	
7	3.39, m	33.3, d	3.03, m	32.5, d	
8	Ha: 1.76, dt (13.3, 4.1) Hb: 1.58, m	26.8, t	Ha: 1.59, m Hb: 1.50, overlap	26.0, t	
9	Ha: 2.22, m Hb: 1.06, overlap	36.8, t	Ha: 2.42, m Hb: 1.14, m	33.2, t	
10		36.9, s		38.0, s	
11		154.9, s		155.1, s	
12	Ha: 6.18, s Hb: 5.85, s	134.4, t	Ha: 6.10, s Hb: 5.86, s	133.7, t	
13	9.53, s	195.1, d	9.42, s	195.3, d	
14		209.9, s		210.7, s	
15	1.37, s	20.8, q	1.20, s	23.8, q	
1'	Ha: 1.44, overlap Hb: 1.25, m	39.7, t	Ha: 1.46, overlap Hb: 1.28, overlap	39.7 ^c , t	
2'	Ha: 1.54, m Hb: 1.45, overlap	18.3 ^a , t	Ha: 1.52, overlap Hb: 1.52, overlap	18.3 ^b , t	
3'	Ha: 2.47, overlap Hb: 2.18, m	24.7, t	Ha: 2.52, m Hb: 2.18, m	24.7, t	
4'		134.3, s		134.5, s	
5'		160.1, s		160.4, s	
6'	Ha: 3.76, dd (13.9, 3.7) Hb: 2.39, t-like (13.9)	27.0, t	Ha: 4.08, brd (13.9) Hb: 2.45, m	26.8, t	
7'	2.70, m	41.7, d	2.70, m	42.1, d	
8'	1.90, m	26.0, t	Ha: 2.05, m Hb: 1.85, m	26.5, t	
9'	Ha: 1.60, m Hb: 1.44, overlap	40.9, t	Ha: 1.68, m Hb: 1.50, overlap	41.1, t	
10'		37.6, s		37.0, s	
11'		196.2, s		197.1, s	
12'	5.75, s	102.4, d	5.91, s	102.5, d	
13'	10.43, s	191.0, d	10.62, s	191.5, d	
14'	1.12, s	25.0, q	1.17, s	25.1, q	
5-OH	5.04, brs		5.67, brs		

^{a, b, c} Signals with the same symbol might be interchangeable.

**Figure S1.** Key 2D NMR correlations of **3–5**.

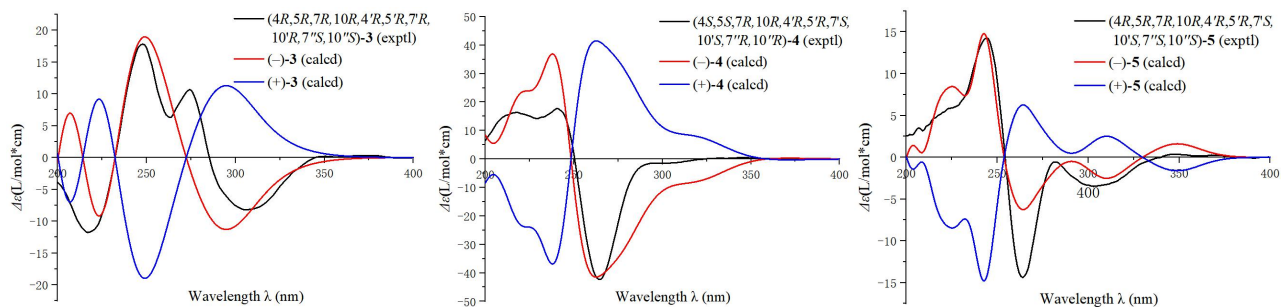


Figure S2. Calculated and experimental ECD spectra of **3–5**.

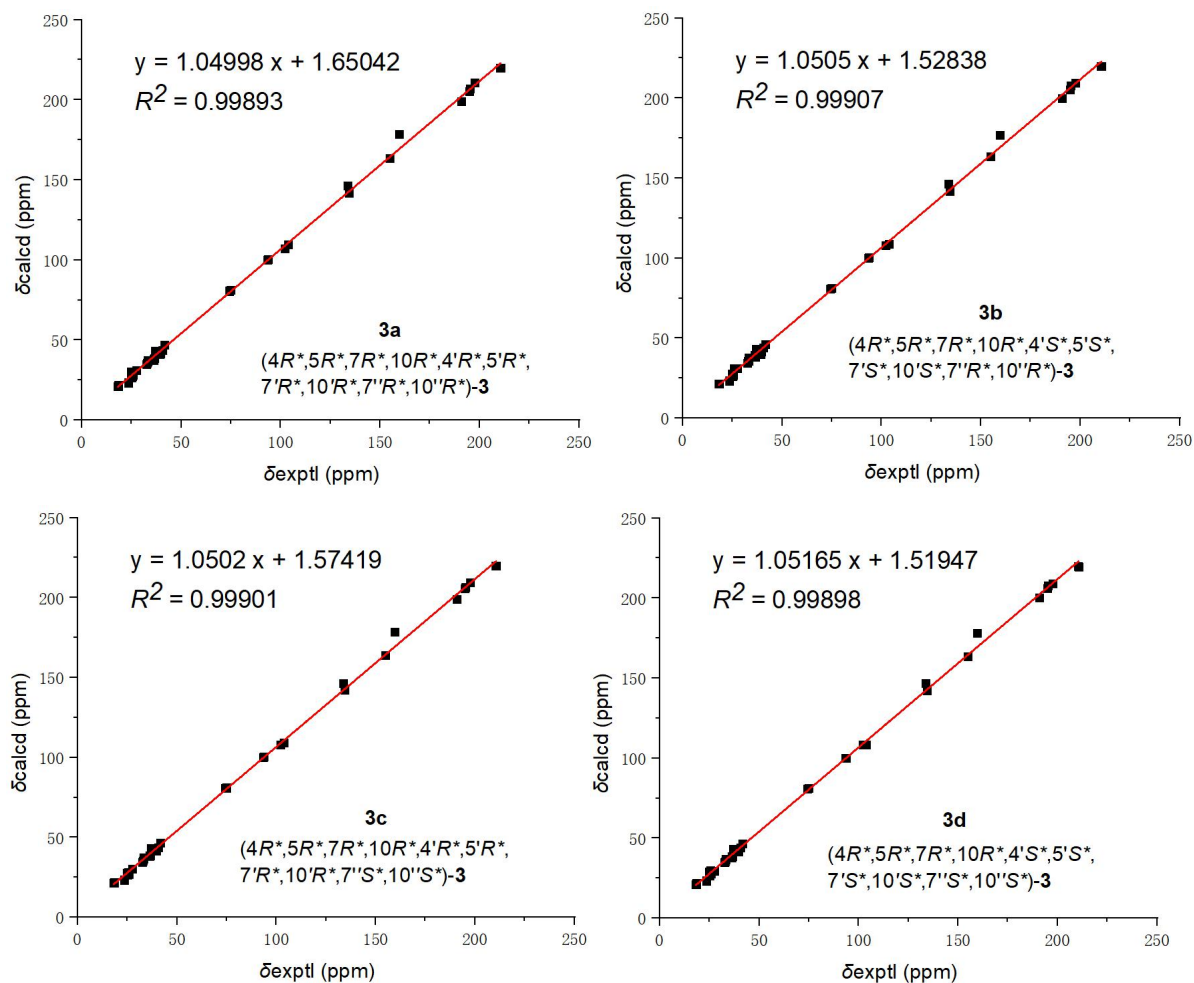


Figure S3. Regression analysis of experimental versus calculated ^{13}C NMR chemical shifts of **3a–3d** at the mPW1PW91/6-311+G(d,p) level

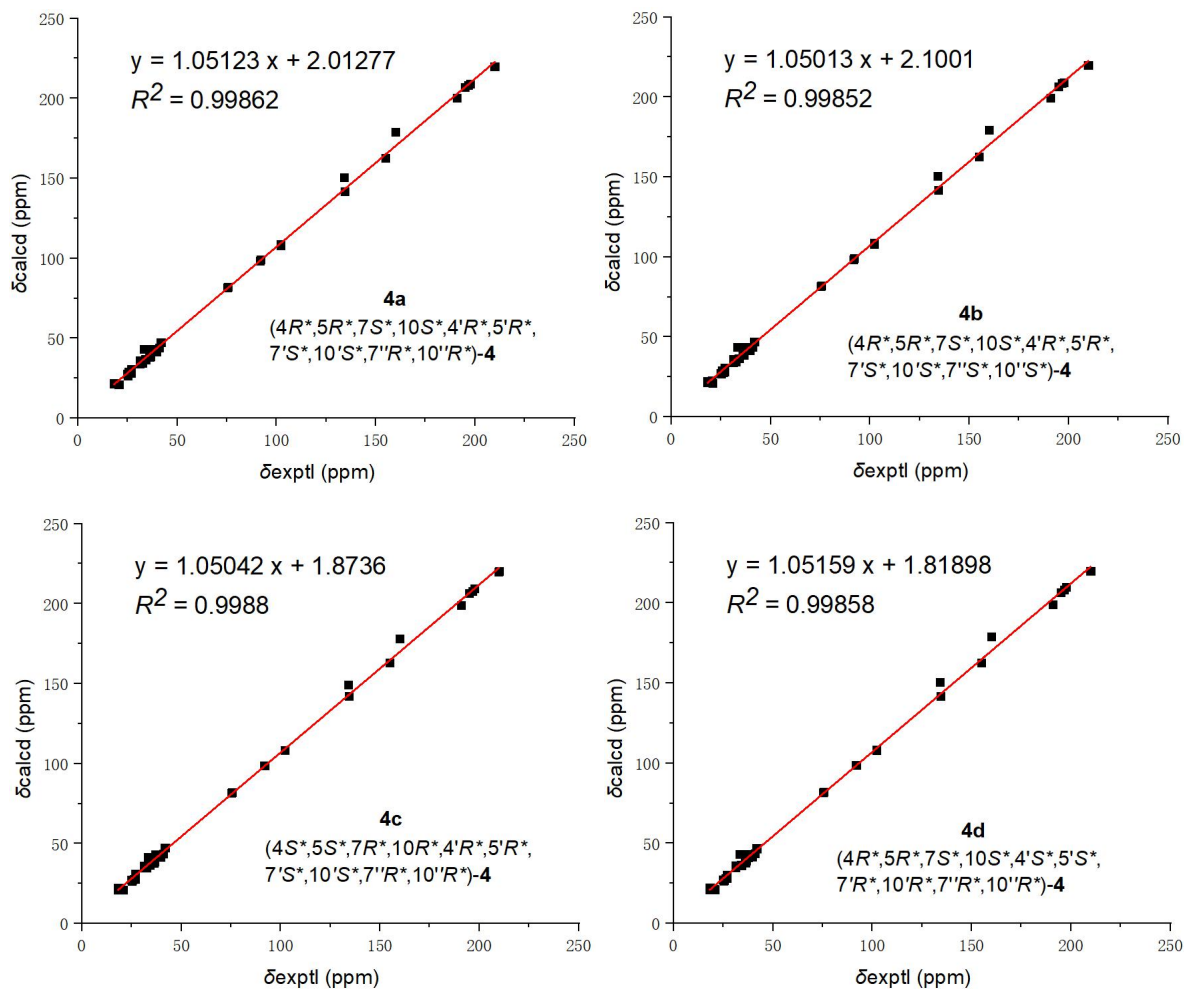
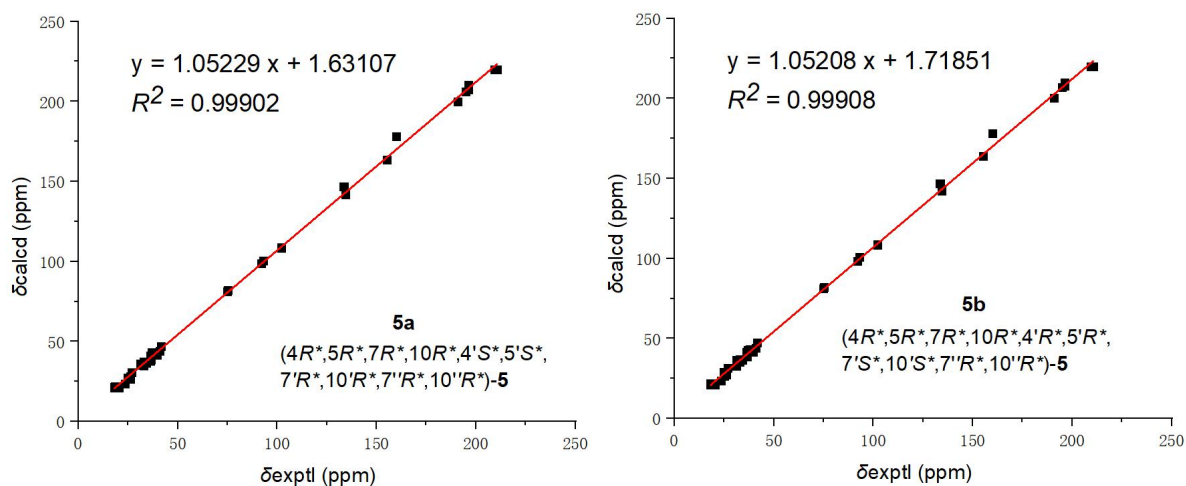


Figure S4. Regression analysis of experimental versus calculated ^{13}C NMR chemical shifts of **4a–4d** at the mPW1PW91/6-311+G(d,p) level



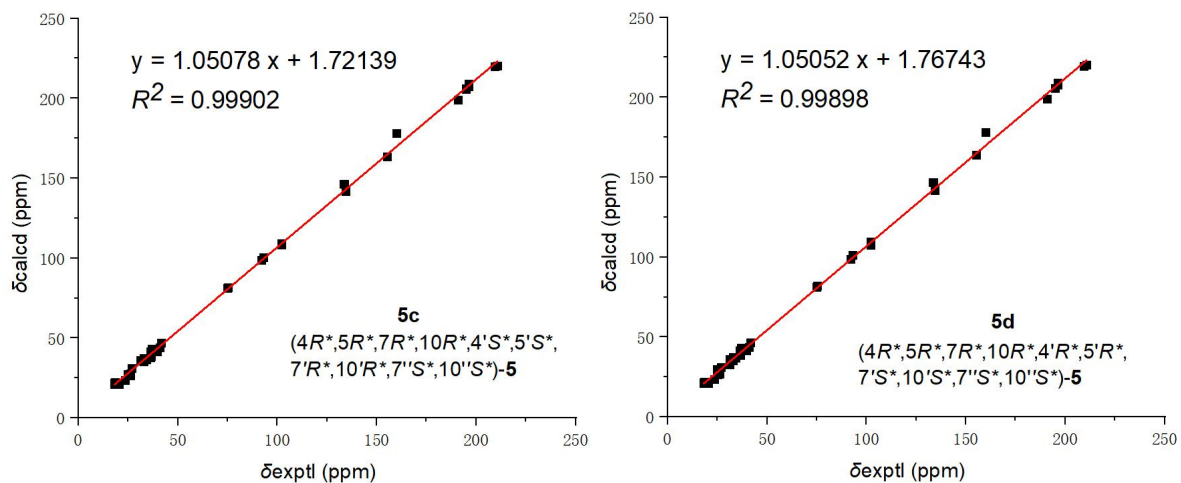


Figure S5. Regression analysis of experimental versus calculated ^{13}C NMR chemical shifts of **5a–5d** at the mPW1PW91/6-311+G(d,p) level

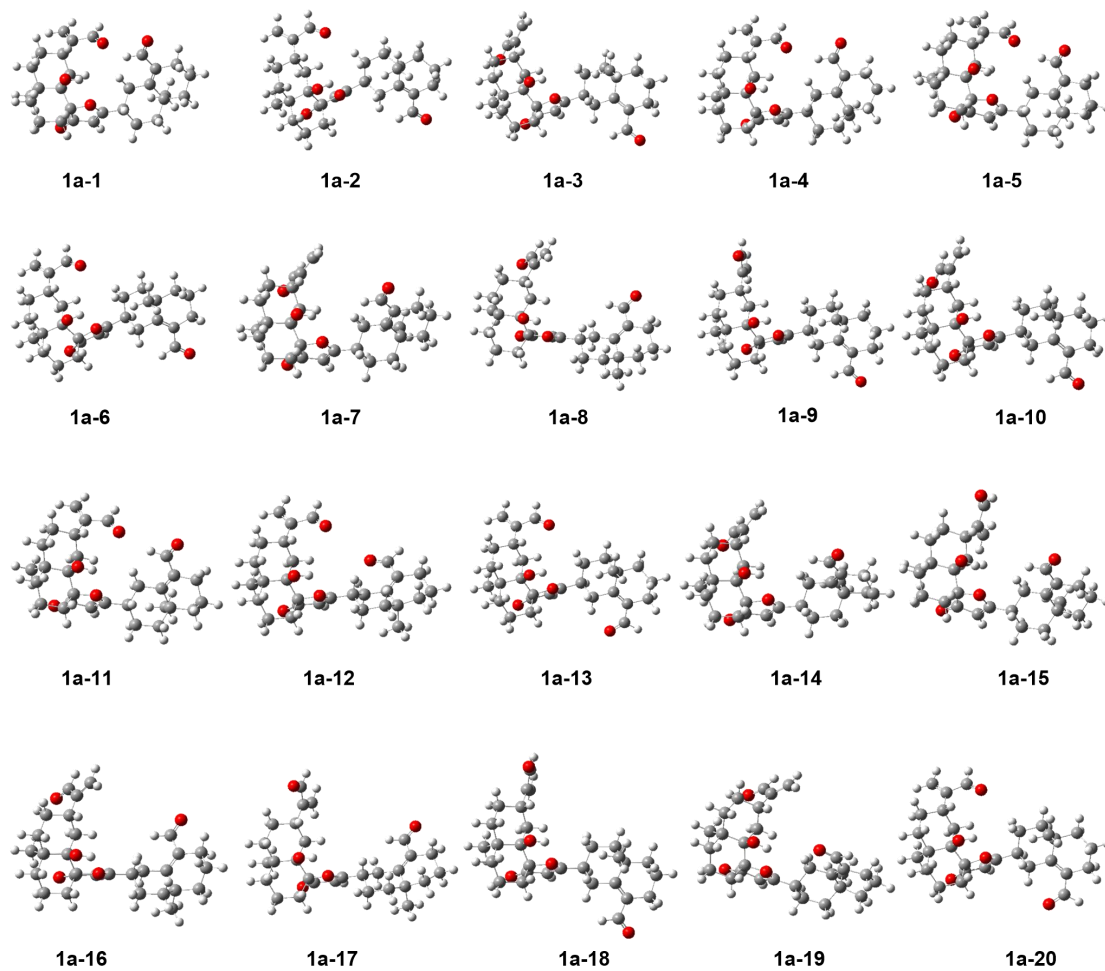
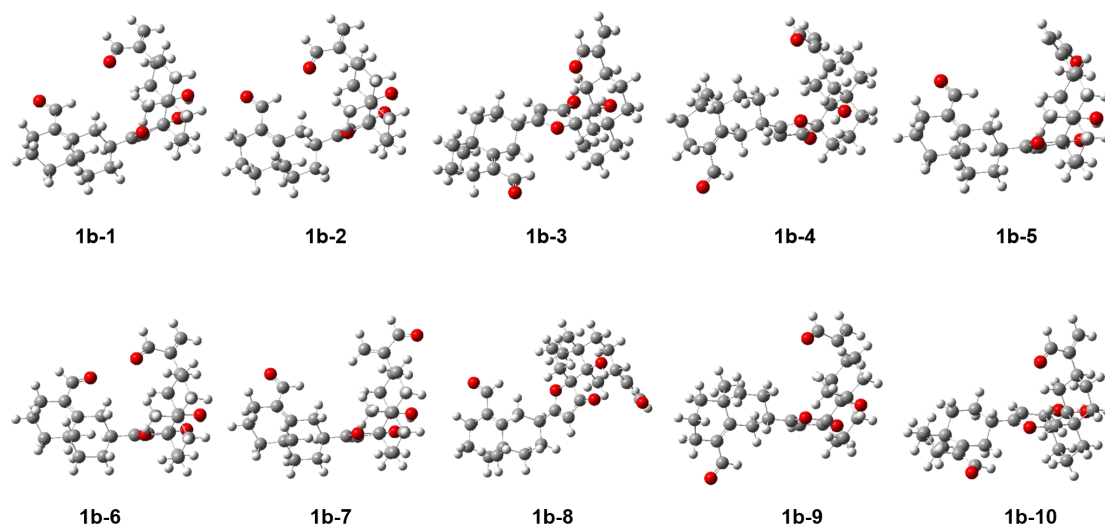


Figure S6. Optimized geometries of predominant conformers for **1a** at the B3LYP/6-31G (d,p) level



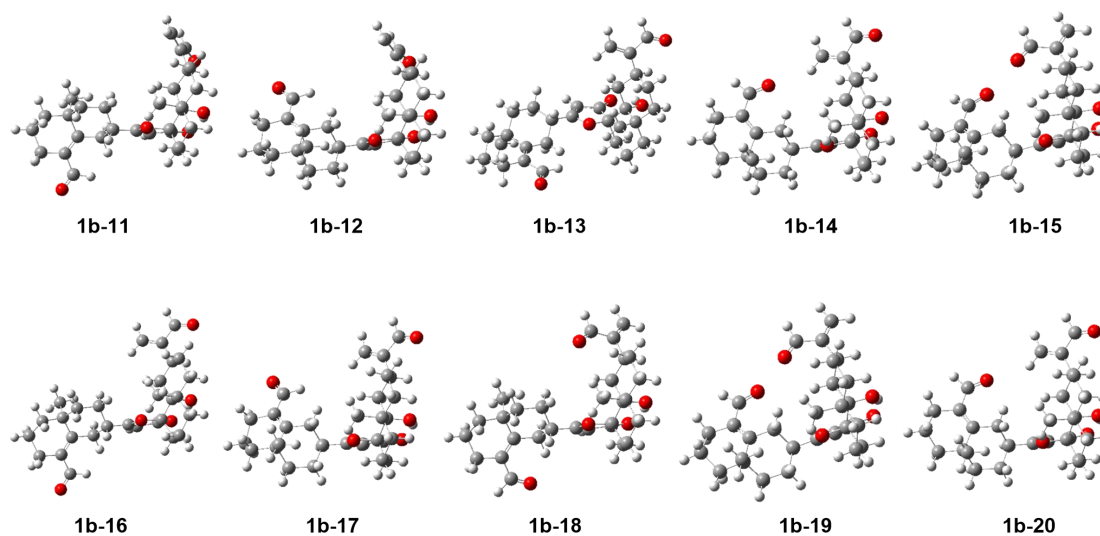


Figure S7. Optimized geometries of predominant conformers for **1b** at the B3LYP/6-31G (d,p) level

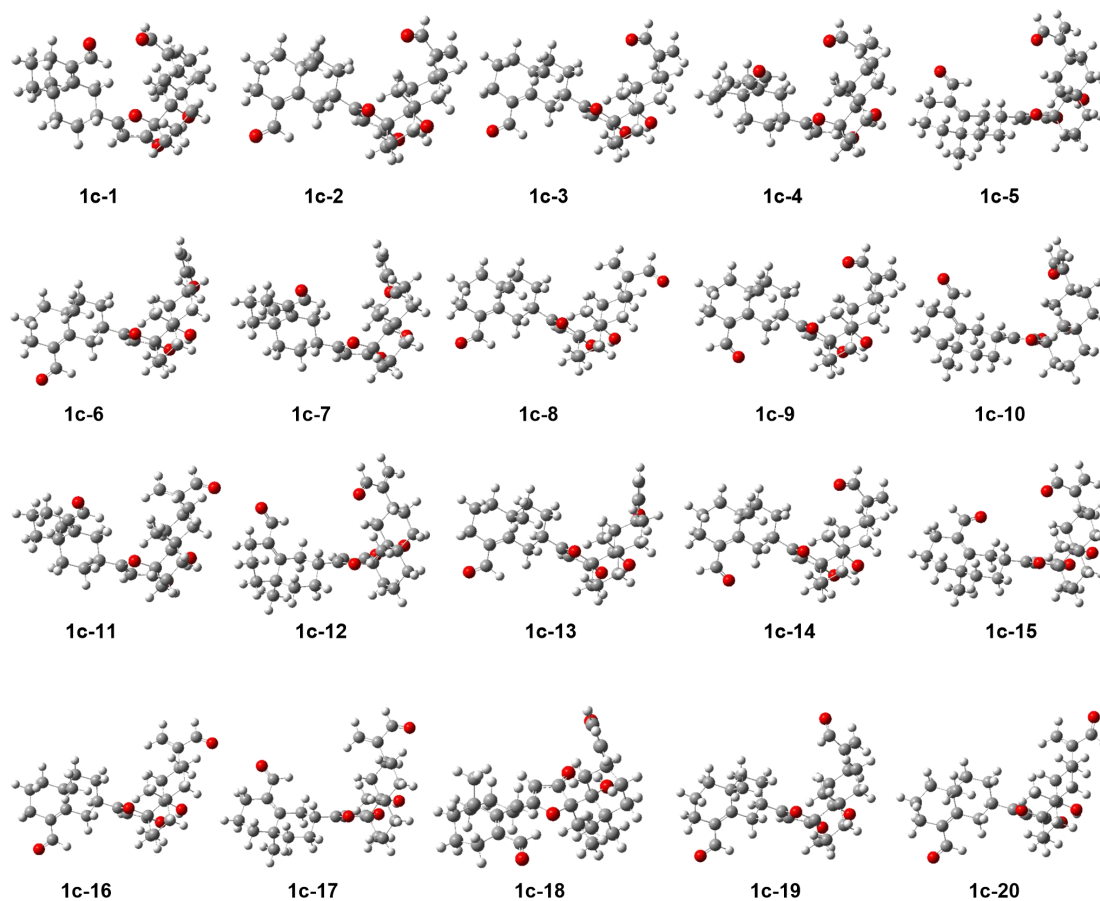


Figure S8. Optimized geometries of predominant conformers for **1c** at the B3LYP/6-31G (d,p) level

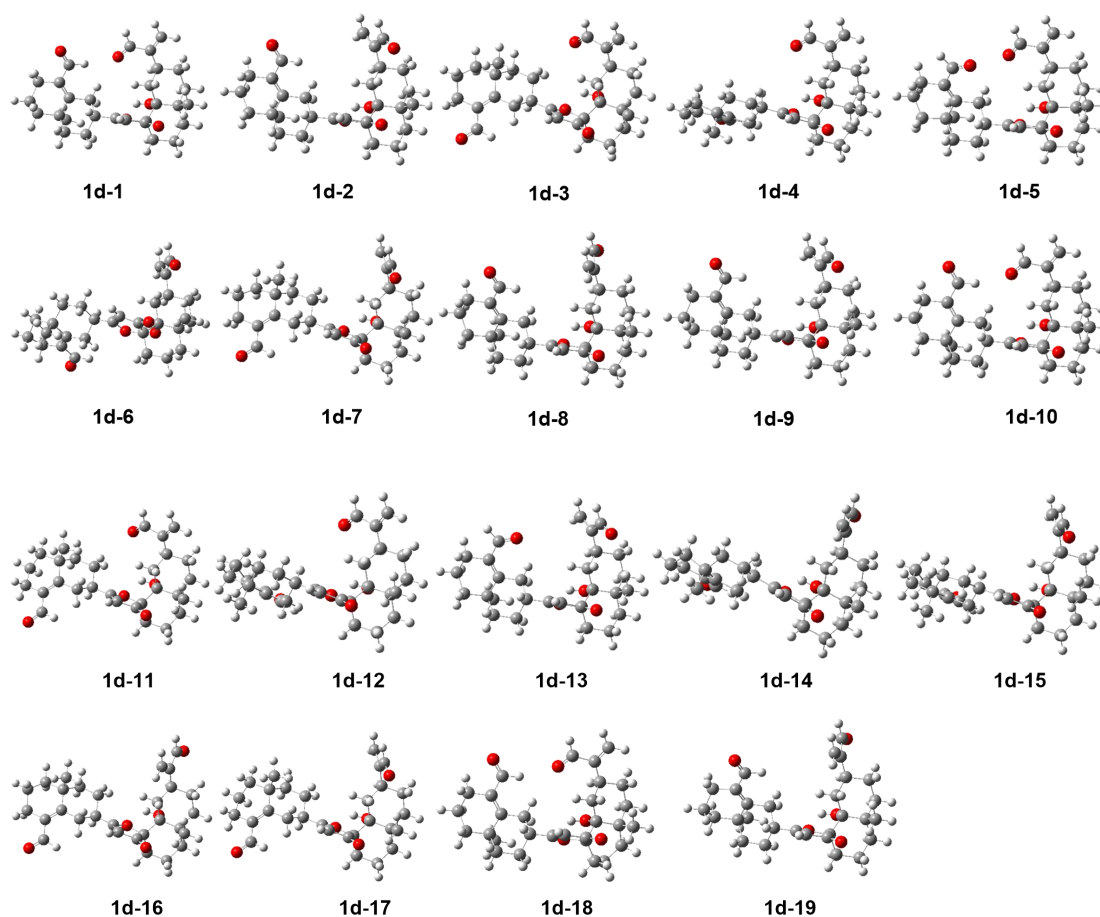


Figure S9. Optimized geometries of predominant conformers for **1d** at the B3LYP/6-31G (d,p) level

Table S2. Conformational analysis of the optimized **1a-1d** at the B3LYP/6-31G(d,p) level in the gas phase

	<i>Conformers</i>	G (Hartree)	ΔG (Kcal/mol)	Population
1a	1a-1	-1503.56085	0.439257	10.87%
	1a-2	-1503.56155	0	22.92%
	1a-3	-1503.55994	1.0102911	4.13%
	1a-4	-1503.55956	1.2487449	2.78%
	1a-5	-1503.55916	1.4997489	1.82%
	1a-6	-1503.55987	1.0542168	3.83%
	1a-7	-1503.55944	1.3240461	2.45%
	1a-8	-1503.55998	0.9851907	4.34%
	1a-9	-1503.5608	0.4706325	10.30%
	1a-10	-1503.55861	1.8448794	1.02%
	1a-11	-1503.55934	1.3867971	2.20%

	1a-12	-1503.55915	1.506024	1.79%
	1a-13	-1503.559	1.6001505	1.54%
	1a-14	-1503.55856	1.8762549	0.96%
	1a-15	-1503.56067	0.5522088	8.96%
	1a-16	-1503.55892	1.6503513	1.41%
	1a-17	-1503.56111	0.2761044	14.26%
	1a-18	-1503.55933	1.3930722	2.16%
	1a-19	-1503.55832	2.0268573	0.75%
	1a-20	-1503.559	1.6001505	1.53%
	<i>Conformers</i>	G (Hartree)	ΔG (Kcal/mol)	Population
1b	1b-1	-1503.56912	0	19.86%
	1b-2	-1503.5672	1.2048192	2.61%
	1b-3	-1503.56866	0.2886546	12.17%
	1b-4	-1503.5682	0.5773092	7.52%
	1b-5	-1503.5685	0.3890562	10.26%
	1b-6	-1503.56655	1.6127007	1.30%
	1b-7	-1503.5681	0.6400602	6.75%
	1b-8	-1503.56808	0.6526104	6.58%
	1b-9	-1503.56696	1.3554216	2.02%
	1b-10	-1503.56752	1.004016	3.66%
	1b-11	-1503.56795	0.7341867	5.76%
	1b-12	-1503.56686	1.4181726	1.82%
	1b-13	-1503.568	0.7028112	6.04%
	1b-14	-1503.56623	1.8135039	0.93%
	1b-15	-1503.56504	2.5602408	0.26%
	1b-16	-1503.56812	0.62751	6.90%
	1b-17	-1503.56698	1.3428714	2.06%
	1b-18	-1503.56652	1.631526	1.26%
	1b-19	-1503.56655	1.6127007	1.30%
	1b-20	-1503.56624	1.8072288	0.94%
	<i>Conformers</i>	G (Hartree)	ΔG (Kcal/mol)	Population
1c	1c-1	-1503.56819	0.7781124	6.56%
	1c-2	-1503.56943	0	24.54%

	1c-3	-1503.56812	0.8220381	6.10%
	1c-4	-1503.56736	1.2989457	2.72%
	1c-5	-1503.5683	0.7090863	7.38%
	1c-6	-1503.56855	0.5522088	9.61%
	1c-7	-1503.56796	0.9224397	5.16%
	1c-8	-1503.56847	0.6024096	8.84%
	1c-9	-1503.56733	1.317771	2.65%
	1c-10	-1503.56817	0.7906626	6.47%
	1c-11	-1503.56747	1.2299196	3.09%
	1c-12	-1503.56671	1.7068272	1.37%
	1c-13	-1503.56696	1.5499497	1.78%
	1c-14	-1503.56733	1.317771	2.65%
	1c-15	-1503.56626	1.9892067	0.85%
	1c-16	-1503.56739	1.2801204	2.83%
	1c-17	-1503.56802	0.8847891	5.50%
	1c-18	-1503.56679	1.6566264	1.49%
	1c-19	-1503.56452	3.0810741	0.14%
	1c-20	-1503.56524	2.6292669	0.29%
	<i>Conformers</i>	G (Hartree)	ΔG (Kcal/mol)	Population
1d	1d-1	-1503.56122	0	17.14%
	1d-2	-1503.55989	0.8345883	4.18%
	1d-3	-1503.56013	0.6839859	5.36%
	1d-4	-1503.5607	0.3263052	9.90%
	1d-5	-1503.56117	0.0313755	16.14%
	1d-6	-1503.55817	1.9139055	0.68%
	1d-7	-1503.55967	0.9726405	3.31%
	1d-8	-1503.55927	1.2236445	2.16%
	1d-9	-1503.5608	0.2635542	10.90%
	1d-10	-1503.55849	1.7131023	0.94%
	1d-11	-1503.55968	0.9663654	3.33%
	1d-12	-1503.56012	0.690261	5.33%
	1d-13	-1503.55815	1.9264557	0.66%
	1d-14	-1503.56052	0.439257	8.16%

1d-15	-1503.5584	1.7695782	0.86%
1d-16	-1503.56037	0.5333835	6.96%
1d-17	-1503.5584	1.7695782	0.86%
1d-18	-1503.55564	3.5015058	0.05%
1d-19	-1503.5596	1.0165662	3.08%

Functional mPW1PW91		Solvent? PCM		Basis Set 6-311+G(d, p)			Type of Data Unscaled Shifts	
		DP4+	0.00%	100.00%	0.00%	0.00%	-	
Nuclei	sp2?	xperimenta	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	
C		17.7	21.28654	22.07557	22.09116	21.24867		
C		30.7	33.77724	35.71667	35.81054	33.68527		
C		92.1	102.37902	99.03029	97.15884	102.34893		
C		75.4	82.53878	82.19809	82.66175	82.48983		
C		36.9	45.10501	42.65638	43.86121	45.11795		
C		33.4	37.07678	36.55575	36.78029	37.04621		
C		31.9	34.7799	34.77982	35.03675	35.00251		
C		33.3	37.25832	39.86039	39.95167	37.23545		
C		25.9	28.51119	28.69531	28.6684	28.14869		
C		36	39.47818	38.79995	38.76548	39.40745		
C		20.4	20.50002	21.19903	21.23672	20.4994		
C	x	154.3	163.99703	163.78546	163.75601	163.90096		
C		17.8	21.2895	21.2645	21.39114	21.28616		
C		24.1	27.87727	27.88899	27.89726	27.55845		
C	x	134.2	142.01403	141.98554	142.04333	142.46944		
C	x	160	176.39492	176.46826	176.6065	176.49577		
C		36.6	43.02031	43.05416	43.13074	43.0569		
C		39.3	41.64778	41.64833	41.6262	41.68942		
C		26.7	30.98049	30.50904	30.35582	30.26555		
C		41.5	46.86069	47.21002	47.43459	46.64085		
C		25.5	28.7168	28.75836	28.91051	29.04269		
C		40.6	43.84776	43.95201	43.83556	43.76821		
C		25.1	26.63376	26.60792	26.62651	26.56878		
C	x	190.4	198.61497	198.2718	198.22167	198.48681		
C	x	195.3	201.74511	206.47181	206.4798	201.74668		
C	x	209.9	212.00301	219.25186	219.22757	212.03273		
C	x	134.1	145.39787	146.67394	146.7036	145.51192		
C	x	101.9	110.10522	107.9646	108.10886	110.01432		
C	x	194.7	205.15187	205.28332	205.33814	205.34177		
H		1.85	2.28218	1.98007	1.5607	2.27434		
H		1.6	1.5479	1.58346	1.97799	1.55381		
H		2.29	2.41156	2.30955	2.3093	2.4218		
H		1.39	1.62133	1.37005	1.38555	1.63799		
H		1.96	2.00099	2.13966	2.13305	1.99955		
H		1.07	1.11285	1.10386	1.09295	1.11724		
H		1	1.3546	0.89333	0.93574	1.45645		
H		1.81	1.41625	1.9711	1.97614	1.30881		
H		3.06	3.21786	3.1437	3.14639	3.19176		
H		1.47	1.49063	1.40784	1.4098	1.41934		
H		1.66	1.73036	1.91263	1.9811	1.8095		
H		1.05	1.104	1.07498	1.074	1.12053		
H		1.99	2.21462	2.13592	2.14339	2.21918		
H		1.23	1.22907	1.92244	1.9283	1.22401		
H		1.23	2.92265	0.40342	0.41759	2.90188		
H		1.23	0.23191	1.65921	1.69075	0.2352		
H		1.6	1.63284	1.63767	1.65598	1.64985		
H		1.69	1.65436	1.66737	1.63868	1.62674		
H		2.37	2.5748	2.5684	2.16664	2.16217		
H		2.13	2.10861	2.13336	2.53257	2.50863		
H		1.6	1.61928	1.62611	1.41536	1.42041		
H		1.4	1.39152	1.40722	1.63557	1.61022		
H		3.59	3.84629	3.85282	2.66768	2.41117		
H		2.37	2.37944	2.48714	3.68219	3.85583		
H		2.68	2.60142	2.72833	2.7531	2.6185		
H		1.89	1.79729	1.85899	2.15631	1.99111		
H		1.95	2.06969	2.07991	1.80134	1.81598		
H		1.58	1.54878	1.6008	1.85998	1.81727		
H		1.78	1.87995	1.8648	1.61331	1.6001		
H		1.25	0.79483	0.80274	1.91053	1.83154		
H		1.25	1.86074	1.8793	0.82408	0.79158		
H		1.25	1.28646	1.3074	1.29032	1.24902		
H	x	10.18	10.62448	10.51367	10.51453	10.62154		
H		4.16	1.88632	4.66387	4.69454	1.87999		
H	x	5.9	6.39039	6.33558	6.32785	6.40405		
H	x	6.17	6.7306	6.75967	6.74802	6.74249		
H	x	5.44	5.46949	5.56341	5.54858	5.44336		
H	x	9.48	9.78494	9.79064	9.78958	9.80753		

Functional mPW1PW91	Solvent? PCM		Basis Set 6-311+G(d,p)		Type of Data Unscaled Shifts	
	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	0.00%	100.00%	0.00%	0.00%	-	-
sDP4+ (C data)	0.00%	91.39%	8.61%	0.00%	-	-
sDP4+ (all data)	0.00%	100.00%	0.00%	0.00%	-	-
uDP4+ (H data)	0.00%	100.00%	0.00%	0.00%	-	-
uDP4+ (C data)	0.81%	53.05%	45.65%	0.49%	-	-
uDP4+ (all data)	0.00%	100.00%	0.00%	0.00%	-	-
DP4+ (H data)	0.00%	100.00%	0.00%	0.00%	-	-
DP4+ (C data)	0.00%	92.50%	7.50%	0.00%	-	-
DP4+ (all data)	0.00%	100.00%	0.00%	0.00%	-	-

Figure S10. DP4+ analysis of experimental NMR data of **1** and unscaled shifts of **1a-1d** (Isomer 1-4)

Table S3. The Cartesian coordinates of the lowest energy conformers for **1a-1d** in the gas phase at the B3LYP/6-31G(d,p) level

1a-1	X axis(Å)	Y axis(Å)	Z axis(Å)	1a-2	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-4.316	-2.335	1.4723	C	2.9752	-3.4615	-1.059
C	-2.7933	-2.4488	1.4915	C	1.581	-2.8637	-0.8882
C	-2.0895	-1.5539	0.4625	C	1.5491	-1.5827	-0.0428
C	-2.6375	-0.0995	0.4738	C	2.6486	-0.5685	-0.4653
C	-4.1967	0.0046	0.408	C	4.081	-1.1871	-0.59
C	-4.8086	-0.884	1.5229	C	4.0152	-2.4315	-1.5138
C	-1.9705	0.8399	-0.5552	C	2.6695	0.7319	0.369
C	-2.3895	2.3165	-0.3564	C	3.642	1.7862	-0.214
C	-3.9275	2.4513	-0.3373	C	5.0482	1.187	-0.4284
C	-4.5979	1.4892	0.6536	C	5.0197	-0.1219	-1.2288
C	-4.8177	-0.4188	-0.9456	C	4.7227	-1.6137	0.7532
O	-0.6769	-1.4821	0.8716	O	0.2475	-0.9483	-0.3114
C	-1.682	3.2165	-1.3589	C	3.6145	3.0572	0.6214
C	6.368	0.45	0.0573	C	-6.4994	1.4234	-0.7517
C	5.5096	1.0691	1.1526	C	-6.6071	0.0614	-0.0788
C	4.0252	0.854	0.9673	C	-5.292	-0.6759	0.0286
C	3.496	-0.0613	0.1177	C	-4.0825	-0.0884	-0.1479
C	4.3984	-0.9614	-0.7495	C	-3.9631	1.4204	-0.457
C	5.876	-0.9502	-0.2695	C	-5.2969	2.1798	-0.2129
C	2.0038	-0.2911	-0.0856	C	-2.7406	-0.8084	-0.0784
C	1.5941	-1.7769	0.0015	C	-1.7487	-0.1174	0.8748
C	2.4325	-2.6229	-0.9654	C	-1.5599	1.3558	0.4946
C	3.9231	-2.4373	-0.6899	C	-2.9019	2.083	0.4622
C	4.3496	-0.4545	-2.2109	C	-3.5585	1.6013	-1.9395
C	3.1982	1.7852	1.8015	C	-5.4673	-2.1328	0.3253
O	3.6865	2.469	2.6963	O	-6.5563	-2.6247	0.602
C	0.1014	-1.9101	-0.1988	C	-0.4214	-0.8296	0.8986
C	-1.9486	-2.2194	-0.8919	C	1.4193	-1.8648	1.4425
O	-2.2535	0.4374	1.7779	O	2.2734	-0.1454	-1.813

C	-2.2382	3.8679	-2.3939	C	4.5745	3.5039	1.4482
O	-2.8407	-2.606	-1.6303	O	2.2045	-2.4633	2.1605
C	-0.5482	-2.3836	-1.2576	C	0.1698	-1.3384	1.9738
C	-0.2175	3.4444	-1.157	C	2.4102	3.9323	0.4855
O	0.4367	2.8763	-0.2899	O	1.4454	3.6393	-0.2107
H	-4.7102	-2.8414	0.5852	H	3.2886	-3.9341	-0.1224
H	-4.7247	-2.8789	2.3325	H	2.9282	-4.2695	-1.7992
H	-2.4359	-2.1941	2.4986	H	1.1677	-2.6511	-1.8836
H	-2.5084	-3.4984	1.3434	H	0.9142	-3.622	-0.4577
H	-4.566	-0.4698	2.5102	H	3.7754	-2.1261	-2.5407
H	-5.9038	-0.8756	1.4535	H	4.9988	-2.9156	-1.5653
H	-0.8838	0.7754	-0.4432	H	1.6631	1.1654	0.3809
H	-2.1909	0.5196	-1.5799	H	2.9246	0.5218	1.414
H	-2.0477	2.641	0.637	H	3.2836	2.0675	-1.2147
H	-4.203	3.4792	-0.0691	H	5.6784	1.9109	-0.9605
H	-4.3422	2.2717	-1.3358	H	5.5397	0.9997	0.5329
H	-5.687	1.6048	0.5815	H	6.0417	-0.5144	-1.3069
H	-4.336	1.7948	1.6747	H	4.7089	0.0987	-2.2579
H	-4.312	0.0279	-1.805	H	4.6326	-0.8503	1.5299
H	-4.8231	-1.498	-1.0938	H	4.3049	-2.5373	1.1521
H	-5.8696	-0.1111	-0.9979	H	5.7938	-1.8113	0.6213
H	6.3494	1.0827	-0.8373	H	-6.422	1.3015	-1.8381
H	7.4123	0.4115	0.3884	H	-7.4154	1.9966	-0.5671
H	5.7402	2.141	1.1905	H	-7.3349	-0.5328	-0.645
H	5.8004	0.644	2.1219	H	-7.0142	0.1891	0.9326
H	6.528	-1.4002	-1.0287	H	-5.2576	3.1782	-0.6664
H	5.9854	-1.5688	0.6321	H	-5.4501	2.3402	0.8633
H	1.406	0.2548	0.6474	H	-2.8373	-1.8467	0.2451
H	1.7213	0.1172	-1.0649	H	-2.3249	-0.8571	-1.0932
H	1.8135	-2.1335	1.0186	H	-2.1786	-0.1508	1.8867
H	2.1799	-3.6844	-0.8485	H	-0.9051	1.8497	1.224
H	2.2142	-2.3632	-2.0077	H	-1.0608	1.4488	-0.4776
H	4.1349	-2.8535	0.3049	H	-3.2826	2.1251	1.4922
H	4.4949	-3.0447	-1.4033	H	-2.7357	3.1237	0.1552
H	5.0049	-1.0519	-2.8552	H	-3.5071	2.6635	-2.2052
H	3.3437	-0.506	-2.6392	H	-2.5784	1.1685	-2.163
H	4.6712	0.5897	-2.2892	H	-4.2766	1.1252	-2.6161
H	2.1244	1.8388	1.5816	H	-4.5715	-2.7645	0.2861
H	-1.2967	0.2657	1.884	H	1.3474	0.1654	-1.7624
H	-1.6646	4.5086	-3.0581	H	4.4834	4.4351	2.0006
H	-3.2958	3.7873	-2.6227	H	5.4953	2.9535	1.6107
H	-0.1934	-2.7778	-2.1904	H	-0.1426	-1.3702	3.0001
H	0.2585	4.1571	-1.8518	H	2.4307	4.8725	1.0624
1a-3	X axis(Å)	Y axis(Å)	Z axis(Å)	1a-4	X axis(Å)	Y axis(Å)	Z axis(Å)
C	2.7488	-3.5198	-1.0029	C	4.3404	-2.8163	-0.5932
C	1.3764	-2.8677	-0.8579	C	2.8311	-2.8157	-0.8238
C	1.3987	-1.537	-0.0918	C	2.1006	-1.6362	-0.1693

C	2.5151	-0.5827	-0.6043	C	2.8065	-0.2767	-0.4399
C	3.9284	-1.2513	-0.7036	C	4.3441	-0.2814	-0.1552
C	3.8135	-2.5555	-1.5364	C	4.9946	-1.4678	-0.9143
C	2.5812	0.7756	0.1296	C	2.1207	0.9404	0.2214
C	3.6083	1.7361	-0.5168	C	2.7285	2.2848	-0.2477
C	4.9882	1.0887	-0.7256	C	4.2622	2.2869	-0.0649
C	4.8941	-0.27	-1.4291	C	4.9414	1.0565	-0.6819
C	4.5738	-1.5977	0.6604	C	4.7248	-0.3959	1.3413
O	0.1089	-0.8805	-0.3734	O	0.7746	-1.5672	-0.8058
C	3.7021	3.0622	0.213	C	2.0105	3.4612	0.4002
C	-6.6415	1.5149	-0.7586	C	-6.6223	0.1886	-0.2284
C	-6.7342	0.2192	0.0364	C	-5.7205	1.4027	-0.4144
C	-5.4222	-0.5219	0.1587	C	-4.2766	1.1642	-0.0356
C	-4.2156	0.0319	-0.1184	C	-3.7531	-0.0651	0.196
C	-4.0957	1.5049	-0.5667	C	-4.5975	-1.3446	0.0165
C	-5.411	2.3003	-0.3378	C	-5.9287	-1.0654	-0.7347
C	-2.8789	-0.6963	-0.0382	C	-2.3306	-0.3365	0.6663
C	-1.8419	0.0647	0.808	C	-1.6001	-1.3438	-0.2408
C	-1.655	1.4948	0.2886	C	-2.3898	-2.6527	-0.348
C	-2.9907	2.2335	0.2451	C	-3.8175	-2.3898	-0.8282
C	-3.7516	1.5469	-2.0747	C	-4.9313	-1.9379	1.4057
C	-5.5997	-1.9432	0.5952	C	-3.4848	2.4322	0.07
O	-6.6843	-2.3958	0.9462	O	-4.0051	3.5424	0.019
C	-0.524	-0.6641	0.8437	C	-0.1812	-1.6042	0.2015
C	1.2908	-1.7342	1.4088	C	1.6995	-1.9131	1.2663
O	2.1245	-0.2409	-1.973	O	2.6624	-0.0566	-1.8773
C	3.3785	4.2359	-0.3555	C	2.5122	4.3159	1.3073
O	2.0467	-2.357	2.1369	O	2.4285	-2.1945	2.2043
C	0.0832	-1.1151	1.9359	C	0.2565	-1.8147	1.4391
C	4.1738	3.1128	1.6246	C	0.6088	3.7361	-0.0432
O	4.4622	2.1155	2.2732	O	-0.0071	3.0018	-0.8072
H	3.0603	-3.9382	-0.0402	H	4.5534	-3.1082	0.4404
H	2.6676	-4.3733	-1.6868	H	4.7964	-3.5909	-1.2216
H	0.9582	-2.7029	-1.8602	H	2.6431	-2.8027	-1.906
H	0.6902	-3.5753	-0.3748	H	2.412	-3.7671	-0.4716
H	3.5709	-2.3147	-2.5797	H	4.9327	-1.3011	-1.9976
H	4.7815	-3.0721	-1.5635	H	6.065	-1.5248	-0.6789
H	1.6022	1.2702	0.0856	H	2.1636	0.8694	1.3143
H	2.7999	0.6176	1.1895	H	1.0583	0.9336	-0.0431
H	3.2291	1.9563	-1.526	H	2.5541	2.3812	-1.3291
H	5.6177	1.7544	-1.3301	H	4.6855	3.1886	-0.5255
H	5.5133	0.9661	0.2279	H	4.5222	2.3336	0.9988
H	5.899	-0.7061	-1.4982	H	6.0177	1.1003	-0.4707
H	4.5707	-0.1098	-2.4657	H	4.8527	1.1145	-1.7743
H	4.5078	-0.779	1.3812	H	4.1689	0.2976	1.977
H	4.1398	-2.4814	1.1263	H	4.5772	-1.3971	1.7441
H	5.6389	-1.8289	0.5343	H	5.7902	-0.1762	1.4836

H	-6.6101	1.2964	-1.8321	H	-6.8911	0.0789	0.8284
H	-7.5438	2.1139	-0.5892	H	-7.5609	0.3431	-0.7732
H	-7.4889	-0.4138	-0.4464	H	-6.1432	2.224	0.1769
H	-7.1002	0.441	1.0473	H	-5.7519	1.7154	-1.4662
H	-5.3809	3.2541	-0.8796	H	-6.6071	-1.9229	-0.6435
H	-5.5183	2.5574	0.7251	H	-5.7389	-0.94	-1.8096
H	-2.972	-1.7003	0.3807	H	-1.7245	0.5695	0.7304
H	-2.5055	-0.8411	-1.0602	H	-2.3815	-0.7161	1.6948
H	-2.2308	0.129	1.8349	H	-1.5526	-0.8946	-1.244
H	-0.9657	2.0435	0.9431	H	-1.8965	-3.3319	-1.0549
H	-1.1961	1.4931	-0.7076	H	-2.4098	-3.1736	0.6169
H	-3.3278	2.373	1.2817	H	-3.7583	-2.0473	-1.8708
H	-2.8279	3.2401	-0.1612	H	-4.3665	-3.34	-0.85
H	-3.702	2.5802	-2.4371	H	-5.5815	-2.8154	1.3113
H	-2.7855	1.0835	-2.2979	H	-4.0386	-2.2608	1.9502
H	-4.5013	1.0209	-2.6759	H	-5.4462	-1.2111	2.0435
H	-4.7102	-2.5849	0.5912	H	-2.4002	2.3349	0.196
H	1.1702	-0.0322	-1.9463	H	1.7115	-0.1584	-2.0835
H	3.4499	5.1838	0.1695	H	1.9364	5.1446	1.7107
H	3.0307	4.2809	-1.384	H	3.524	4.2234	1.688
H	-0.2043	-1.078	2.9695	H	-0.2679	-1.8852	2.3727
H	4.2459	4.1195	2.0704	H	0.1403	4.6443	0.3734
1a-5	X axis(Å)	Y axis(Å)	Z axis(Å)	1a-6	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-4.1872	-2.4654	1.4837	C	-3.0549	-3.4276	1.0576
C	-2.6608	-2.5123	1.4822	C	-1.6439	-2.859	0.9311
C	-2.0113	-1.5777	0.4527	C	-1.556	-1.5891	0.073
C	-2.6217	-0.1488	0.4881	C	-2.65	-0.5488	0.4433
C	-4.1846	-0.1118	0.4432	C	-4.0979	-1.1382	0.5224
C	-4.7425	-1.0381	1.5559	C	-4.0903	-2.3723	1.4622
C	-2.0091	0.8306	-0.5373	C	-2.615	0.7415	-0.406
C	-2.4886	2.2849	-0.314	C	-3.587	1.8213	0.1291
C	-4.0306	2.3528	-0.2768	C	-5.0116	1.2521	0.2985
C	-4.6466	1.3514	0.7106	C	-5.0381	-0.0474	1.1141
C	-4.8046	-0.5471	-0.9069	C	-4.6984	-1.5686	-0.8385
O	-0.5974	-1.4477	0.8415	O	-0.2529	-0.9767	0.3819
C	-1.8307	3.2271	-1.3113	C	-3.5037	3.0816	-0.7188
C	6.2477	-0.3095	0.737	C	6.2313	1.6551	-0.2515
C	5.515	0.9117	1.28	C	6.529	0.1668	-0.1154
C	4.0387	0.8869	0.9678	C	5.2769	-0.6699	-0.0094
C	3.5039	0.1106	-0.0055	C	4.0722	-0.1569	0.3396
C	4.3877	-0.6944	-0.9795	C	3.9131	1.3151	0.7801
C	5.9102	-0.4989	-0.7317	C	5.2616	2.0864	0.8347
C	2.0142	-0.1303	-0.1976	C	2.7463	-0.8995	0.2533
C	1.6699	-1.6323	-0.0653	C	1.7986	-0.1943	-0.7394
C	2.5391	-2.4916	-0.9995	C	1.621	1.2959	-0.403
C	4.0323	-2.1951	-0.8188	C	2.9659	2.0104	-0.2322
C	4.1351	-0.2446	-2.4401	C	3.3178	1.4041	2.2072

C	3.2211	1.773	1.8562	C	5.4857	-2.1075	-0.3664
O	3.6952	2.3417	2.8347	O	6.5527	-2.5386	-0.7901
C	0.1826	-1.8328	-0.2438	C	0.4607	-0.8832	-0.8045
C	-1.862	-2.2243	-0.91	C	-1.3777	-1.8915	-1.4033
O	-2.2446	0.3892	1.7938	O	-2.3158	-0.1167	1.7989
C	-2.4242	3.8634	-2.3348	C	-4.4236	3.5368	-1.5856
O	-2.7475	-2.6409	-1.64	O	-2.1473	-2.4848	-2.1424
C	-0.4613	-2.3266	-1.2966	C	-0.1006	-1.3937	-1.8948
C	-0.3765	3.5192	-1.1169	C	-2.2882	3.9347	-0.5481
O	0.3091	2.9738	-0.2595	O	-1.3559	3.6317	0.1871
H	-4.5706	-2.9797	0.5964	H	-3.0509	-4.2273	1.8082
H	-4.5602	-3.0354	2.3433	H	-3.3433	-3.9054	0.1156
H	-2.3012	-2.2516	2.4869	H	-1.263	-2.6423	1.9385
H	-2.3321	-3.5469	1.3199	H	-0.977	-3.6351	0.534
H	-4.506	-0.6237	2.5446	H	-3.8821	-2.0592	2.4936
H	-5.8379	-1.0773	1.5	H	-5.0845	-2.8367	1.4831
H	-0.9192	0.812	-0.44	H	-1.6006	1.1555	-0.3863
H	-2.229	0.5134	-1.5631	H	-2.8363	0.5238	-1.4572
H	-2.1503	2.6111	0.6801	H	-3.2599	2.1074	1.1391
H	-4.3473	3.3647	0.0061	H	-5.6465	1.9944	0.7988
H	-4.4483	2.1661	-1.2727	H	-5.4713	1.0627	-0.6781
H	-5.7406	1.4205	0.6526	H	-6.0699	-0.4193	1.159
H	-4.3857	1.6568	1.732	H	-4.7609	0.1795	2.1514
H	-4.3287	-0.0709	-1.7677	H	-4.5653	-0.8164	-1.62
H	-4.7671	-1.624	-1.0664	H	-4.2844	-2.5047	-1.2114
H	-5.8689	-0.2831	-0.9433	H	-5.7773	-1.7443	-0.7437
H	7.3285	-0.1733	0.8577	H	7.1637	2.2251	-0.1681
H	5.9736	-1.2032	1.3103	H	5.8156	1.8699	-1.2431
H	5.9502	1.8274	0.8608	H	7.149	-0.0114	0.772
H	5.6835	0.9396	2.3631	H	7.1221	-0.1293	-0.9889
H	6.2712	0.3859	-1.2746	H	5.7509	1.9225	1.8052
H	6.4764	-1.3487	-1.1332	H	5.0876	3.1675	0.7644
H	1.4115	0.4126	0.5337	H	2.8606	-1.9352	-0.0743
H	1.7024	0.2554	-1.1757	H	2.2992	-0.9646	1.2521
H	1.9116	-1.944	0.9619	H	2.2645	-0.2502	-1.7347
H	2.3619	-3.5551	-0.7946	H	1.0562	1.7911	-1.2035
H	2.263	-2.3316	-2.048	H	1.0219	1.4186	0.5075
H	4.3357	-2.5458	0.1766	H	3.4499	2.0688	-1.216
H	4.5979	-2.7964	-1.5422	H	2.7753	3.0458	0.078
H	4.7818	-0.7954	-3.1334	H	3.2485	2.4485	2.5343
H	3.105	-0.4025	-2.7711	H	2.3129	0.9805	2.2861
H	4.3491	0.824	-2.5637	H	3.9484	0.8709	2.9287
H	2.1667	1.9171	1.5846	H	4.6376	-2.7872	-0.2152
H	-1.2797	0.2599	1.8855	H	-1.3827	0.1756	1.7786
H	-1.8859	4.5368	-2.996	H	-4.2939	4.4593	-2.1446
H	-3.4788	3.7365	-2.5566	H	-5.3484	3.0022	-1.776
H	-0.1043	-2.6966	-2.2385	H	0.2479	-1.4425	-2.9087

H	0.0617	4.259	-1.8083	H	-2.2686	4.868	-1.1362
1a-7	X axis(Å)	Y axis(Å)	Z axis(Å)	1a-8	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-3.9279	-2.7173	1.4759	C	3.8128	-3.2715	-0.0136
C	-2.4025	-2.6909	1.4179	C	2.3283	-3.0591	-0.2994
C	-1.8372	-1.6376	0.454	C	1.8253	-1.6505	0.047
C	-2.4981	-0.2442	0.6564	C	2.7557	-0.5393	-0.5183
C	-4.0643	-0.2771	0.6654	C	4.2706	-0.7429	-0.1752
C	-4.5412	-1.3309	1.6999	C	4.6987	-2.1706	-0.6069
C	-1.9589	0.8607	-0.2798	C	2.2918	0.9014	-0.206
C	-2.5434	2.2513	0.0663	C	3.1711	1.9617	-0.9116
C	-4.0777	2.2454	0.1778	C	4.6764	1.7429	-0.6812
C	-4.5903	1.1249	1.0899	C	5.1065	0.3004	-0.9719
C	-4.7091	-0.6079	-0.7027	C	4.6223	-0.5584	1.3212
O	-0.4105	-1.4888	0.7938	O	0.5212	-1.5012	-0.6224
C	-2.0396	3.3407	-0.8605	C	2.7423	3.38	-0.5882
C	6.5358	0.7297	0.0023	C	-6.9214	0.2752	-0.5002
C	5.7241	1.1098	1.2336	C	-6.1023	1.5483	-0.3332
C	4.2382	0.8656	1.0937	C	-4.7113	1.3157	0.2112
C	3.6883	0.1097	0.1106	C	-4.1134	0.0991	0.2535
C	4.5701	-0.5966	-0.9411	C	-4.8199	-1.1597	-0.2949
C	6.0707	-0.6117	-0.5386	C	-6.0746	-0.8104	-1.1428
C	2.1945	-0.1221	-0.0848	C	-2.7286	-0.1781	0.826
C	1.8279	-1.6151	-0.2023	C	-1.8175	-0.9253	-0.1685
C	2.6408	-2.2743	-1.326	C	-2.4847	-2.2283	-0.6267
C	4.139	-2.0792	-1.1008	C	-3.8643	-1.956	-1.2235
C	4.4311	0.1402	-2.2946	C	-5.2609	-2.0504	0.8908
C	3.437	1.5663	2.1475	C	-4.0714	2.5709	0.7181
O	3.955	2.2091	3.0548	O	-4.575	3.6786	0.5644
C	0.3314	-1.7746	-0.3491	C	-0.428	-1.2099	0.353
C	-1.7319	-2.1569	-0.9659	C	1.4065	-1.5284	1.4983
O	-2.0889	0.1814	1.996	O	2.6448	-0.6526	-1.9732
C	-1.3048	4.3822	-0.4352	C	2.2889	4.2382	-1.5174
O	-2.6313	-2.569	-1.6804	O	2.0879	-1.7195	2.4927
C	-0.3487	-2.1732	-1.4196	C	-0.0044	-1.1877	1.613
C	-2.3543	3.2968	-2.3152	C	2.8129	3.888	0.8098
O	-2.9715	2.3803	-2.8419	O	3.163	3.198	1.7585
H	-4.3224	-3.1653	0.558	H	3.9714	-3.348	1.067
H	-4.2422	-3.3809	2.2906	H	4.1211	-4.2384	-0.4294
H	-2.0154	-2.504	2.4288	H	2.143	-3.2598	-1.3634
H	-2.0345	-3.69	1.1511	H	1.7451	-3.8166	0.2401
H	-4.2882	-1.0008	2.7159	H	4.6711	-2.2562	-1.701
H	-5.6351	-1.416	1.6743	H	5.7408	-2.3557	-0.3163
H	-0.8683	0.9339	-0.1798	H	1.2624	1.0459	-0.5598
H	-2.1566	0.5961	-1.3224	H	2.2718	1.0607	0.8758
H	-2.1744	2.4975	1.0732	H	3.0135	1.8215	-1.9916
H	-4.42	3.2085	0.5782	H	5.2485	2.4177	-1.331
H	-4.543	2.1499	-0.8093	H	4.9591	2.005	0.3441

H	-5.6879	1.1367	1.087	H	6.1735	0.1925	-0.7377
H	-4.296	1.348	2.1235	H	5.0217	0.1168	-2.0507
H	-4.2676	-0.0429	-1.5274	H	4.1722	0.3378	1.7554
H	-4.6492	-1.6649	-0.9586	H	4.3262	-1.4063	1.9374
H	-5.7807	-0.3726	-0.69	H	5.7077	-0.4683	1.4531
H	6.4427	1.5072	-0.7644	H	-7.3016	-0.0584	0.4721
H	7.5987	0.6788	0.2657	H	-7.7989	0.4833	-1.1233
H	5.9208	2.1677	1.4472	H	-6.6642	2.2216	0.3258
H	6.0871	0.5354	2.0957	H	-6.0129	2.0507	-1.3051
H	6.6939	-0.8985	-1.395	H	-6.6875	-1.7057	-1.307
H	6.2482	-1.3713	0.2352	H	-5.7734	-0.4611	-2.1401
H	1.6009	0.3082	0.7236	H	-2.2114	0.7348	1.1275
H	1.8758	0.4118	-0.9899	H	-2.8515	-0.764	1.7457
H	2.1092	-2.1121	0.7378	H	-1.6976	-0.2737	-1.0469
H	2.426	-3.3499	-1.3616	H	-1.8667	-2.7245	-1.3859
H	2.3596	-1.8671	-2.3043	H	-2.5678	-2.9326	0.2102
H	4.4174	-2.643	-0.1995	H	-3.7157	-1.4005	-2.16
H	4.6869	-2.5417	-1.9319	H	-4.325	-2.9115	-1.5057
H	5.0777	-0.3121	-3.0554	H	-5.8108	-2.9302	0.5372
H	3.4093	0.1117	-2.6856	H	-4.4133	-2.4189	1.477
H	4.7074	1.1969	-2.2108	H	-5.9139	-1.508	1.5834
H	2.3452	1.488	2.085	H	-3.114	2.4699	1.2436
H	-1.1411	-0.0382	2.0835	H	1.6933	-0.7515	-2.1737
H	-0.9485	5.1627	-1.1009	H	1.984	5.2538	-1.2824
H	-1.0391	4.4876	0.6135	H	2.2117	3.9429	-2.5604
H	-0.025	-2.4667	-2.4	H	-0.5191	-0.9983	2.5355
H	-1.9868	4.1494	-2.9114	H	2.5191	4.9419	0.9527
1a-9	X axis(Å)	Y axis(Å)	Z axis(Å)	1a-10	X axis(Å)	Y axis(Å)	Z axis(Å)
C	2.5552	-3.5709	-1.192	C	2.8268	-3.4976	-0.9908
C	1.2249	-2.8522	-0.9855	C	1.4369	-2.8751	-0.8885
C	1.3126	-1.6237	-0.0683	C	1.4057	-1.5484	-0.1158
C	2.5066	-0.6971	-0.4318	C	2.5183	-0.5683	-0.586
C	3.8732	-1.4457	-0.5937	C	3.9479	-1.2068	-0.6413
C	3.69	-2.6208	-1.5896	C	3.8881	-2.5085	-1.4839
C	2.6537	0.5382	0.4855	C	2.5316	0.7869	0.1566
C	3.7423	1.5202	-0.0201	C	3.5592	1.7722	-0.4505
C	5.0779	0.8049	-0.295	C	4.9585	1.1548	-0.6165
C	4.9165	-0.4451	-1.1682	C	4.9163	-0.2016	-1.3294
C	4.4662	-2.0122	0.72	C	4.5546	-1.5473	0.7418
O	0.0795	-0.8512	-0.3059	O	0.1126	-0.9175	-0.4376
C	3.9664	2.7203	0.8866	C	3.6008	3.0958	0.2887
C	-6.5836	1.7748	-0.7168	C	-6.3268	1.8362	0.1975
C	-6.7513	0.382	-0.1238	C	-6.6442	0.346	0.2188
C	-5.4656	-0.4087	-0.0412	C	-5.4053	-0.5139	0.1449
C	-4.2327	0.1422	-0.1676	C	-4.2114	-0.0535	-0.3016
C	-4.054	1.6602	-0.3893	C	-4.0576	1.3658	-0.8901
C	-5.3625	2.4541	-0.1202	C	-5.3995	2.147	-0.9641

C	-2.9198	-0.6306	-0.1195	C	-2.8905	-0.8025	-0.1977
C	-1.9192	-0.0311	0.8854	C	-1.8945	-0.0169	0.681
C	-1.6692	1.4522	0.5898	C	-1.7166	1.4304	0.1932
C	-2.9829	2.2303	0.5798	C	-3.061	2.1432	0.009
C	-3.6205	1.9082	-1.8537	C	-3.5229	1.3072	-2.3426
C	-5.6992	-1.8724	0.1693	C	-5.6141	-1.9065	0.6505
O	-6.8086	-2.3365	0.4104	O	-6.6714	-2.281	1.1461
C	-0.6222	-0.7976	0.8898	C	-0.5643	-0.7193	0.7587
C	1.1424	-1.9754	1.3983	C	1.2518	-1.7559	1.3794
O	2.1784	-0.1552	-1.7473	O	2.1664	-0.2268	-1.9653
C	3.7668	2.7771	2.2141	C	3.2714	4.2657	-0.2843
O	1.8834	-2.6471	2.0977	O	1.9952	-2.3675	2.1293
C	-0.0902	-1.4179	1.9369	C	0.0152	-1.1635	1.8687
C	4.4375	3.9818	0.2398	C	4.0245	3.1481	1.7153
O	4.6373	4.0819	-0.9641	O	4.3127	2.1534	2.3679
H	2.8182	-4.1236	-0.2843	H	3.1149	-3.9147	-0.0203
H	2.4337	-4.3272	-1.9769	H	2.7863	-4.3489	-1.6811
H	0.8384	-2.5444	-1.9667	H	1.049	-2.7137	-1.9035
H	0.4864	-3.5662	-0.5984	H	0.7501	-3.5996	-0.432
H	3.4825	-2.2332	-2.5955	H	3.6753	-2.2669	-2.5334
H	4.6224	-3.1935	-1.6735	H	4.8671	-3.0046	-1.4812
H	1.706	1.0913	0.5206	H	1.5445	1.2614	0.0826
H	2.866	0.2118	1.508	H	2.7184	0.6274	1.2223
H	3.3737	1.9085	-0.9799	H	3.2092	1.9903	-1.4707
H	5.7718	1.4897	-0.7987	H	5.5936	1.8369	-1.1966
H	5.5607	0.5332	0.652	H	5.4543	1.0379	0.3532
H	5.8937	-0.9337	-1.2746	H	5.932	-0.6163	-1.367
H	4.6318	-0.1332	-2.1813	H	4.6243	-0.0423	-2.3754
H	4.4591	-1.2877	1.538	H	4.448	-0.734	1.4638
H	3.9532	-2.9074	1.0696	H	4.1234	-2.442	1.1889
H	5.5103	-2.3146	0.5705	H	5.6278	-1.7562	0.6502
H	-6.4942	1.7113	-1.8073	H	-7.2564	2.4082	0.0972
H	-7.4807	2.3705	-0.512	H	-5.8678	2.1401	1.1458
H	-7.4915	-0.1518	-0.7323	H	-7.3017	0.091	-0.6217
H	-7.1688	0.4678	0.8878	H	-7.2037	0.144	1.1399
H	-5.2797	3.4742	-0.5158	H	-5.9307	1.8972	-1.8932
H	-5.5263	2.5595	0.9612	H	-5.2119	3.2273	-1.0062
H	-3.0604	-1.6808	0.1443	H	-3.0011	-1.7998	0.2338
H	-2.489	-0.6389	-1.1291	H	-2.4864	-0.9707	-1.2029
H	-2.3677	-0.1028	1.8872	H	-2.3189	0.0316	1.695
H	-1.0075	1.8797	1.3541	H	-1.1135	1.9932	0.9175
H	-1.1523	1.5791	-0.3691	H	-1.1557	1.4556	-0.749
H	-3.3778	2.2299	1.6053	H	-3.502	2.3038	1.0017
H	-2.7737	3.2793	0.3335	H	-2.874	3.1408	-0.4087
H	-3.526	2.981	-2.0584	H	-3.4575	2.3136	-2.773
H	-2.6537	1.452	-2.0883	H	-2.5264	0.864	-2.4212
H	-4.3451	1.4979	-2.5655	H	-4.1888	0.7149	-2.9816

H	-4.828	-2.5352	0.099	H	-4.7764	-2.6073	0.5438
H	1.255	0.1606	-1.7039	H	1.2076	-0.0382	-1.9693
H	3.9445	3.6799	2.7921	H	3.3054	5.2119	0.2476
H	3.4324	1.9162	2.783	H	2.9569	4.3094	-1.3235
H	-0.4374	-1.5169	2.9477	H	-0.3073	-1.1371	2.8922
H	4.5984	4.8384	0.9162	H	4.0602	4.1534	2.1685
1a-11	X axis(Å)	Y axis(Å)	Z axis(Å)	1a-12	X axis(Å)	Y axis(Å)	Z axis(Å)
C	4.2662	-2.8471	-0.6763	C	4.4549	-2.6512	-0.5739
C	2.7513	-2.8261	-0.8656	C	2.9557	-2.7732	-0.8425
C	2.054	-1.643	-0.1826	C	2.1185	-1.6651	-0.1916
C	2.7697	-0.2898	-0.4605	C	2.7127	-0.2504	-0.4566
C	4.314	-0.3162	-0.2185	C	4.235	-0.1252	-0.1199
C	4.9282	-1.5041	-1.0048	C	5.0072	-1.2494	-0.8605
C	2.1188	0.9297	0.2313	C	1.9015	0.91	0.1614
C	2.7278	2.2713	-0.2439	C	2.4233	2.2983	-0.276
C	4.2664	2.2528	-0.1065	C	3.9384	2.4267	-0.0185
C	4.9132	1.0186	-0.7506	C	4.7371	1.2617	-0.6203
C	4.7334	-0.4485	1.2661	C	4.5708	-0.2147	1.3889
O	0.7128	-1.5513	-0.7828	O	0.7941	-1.7027	-0.8306
C	2.0441	3.4509	0.4355	C	1.5673	3.3876	0.3502
C	-6.1344	0.1284	-1.2686	C	-6.4562	0.423	-0.3953
C	-5.6141	1.3863	-0.5839	C	-5.4545	1.5515	-0.6149
C	-4.2561	1.1799	0.0415	C	-4.072	1.2181	-0.1282
C	-3.7762	-0.0433	0.3734	C	-3.6412	-0.034	0.1478
C	-4.6229	-1.3241	0.2057	C	-4.5605	-1.2569	-0.0084
C	-6.0638	-1.0452	-0.3073	C	-5.8507	-0.9132	-0.8067
C	-2.3632	-0.3289	0.8557	C	-2.2329	-0.3517	0.6218
C	-1.6336	-1.2409	-0.1533	C	-1.5725	-1.4429	-0.2418
C	-2.4243	-2.5289	-0.4312	C	-2.43	-2.7113	-0.2642
C	-3.8842	-2.2398	-0.8071	C	-3.8365	-2.396	-0.7781
C	-4.793	-2.0638	1.5558	C	-4.9672	-1.7575	1.3973
C	-3.4807	2.4504	0.2035	C	-3.2085	2.4207	0.0603
O	-3.9942	3.5565	0.0668	O	-2.6035	2.6607	1.0989
C	-0.2153	-1.5587	0.2514	C	-0.1558	-1.7287	0.1853
C	1.6857	-1.9253	1.2604	C	1.7335	-1.9863	1.24
O	2.5885	-0.0542	-1.8912	O	2.6006	-0.0556	-1.9006
C	2.5891	4.3012	1.3216	C	1.9034	4.1927	1.3715
O	2.4329	-2.2378	2.1741	O	2.4746	-2.2784	2.1654
C	0.2516	-1.7851	1.4755	C	0.2905	-1.9203	1.423
C	0.6262	3.7365	0.0537	C	0.2102	3.6081	-0.2401
O	-0.0303	3.0057	-0.6793	O	-0.2029	2.9946	-1.2187
H	4.5036	-3.1498	0.3488	H	4.6657	-2.9381	0.4616
H	4.6953	-3.6222	-1.3229	H	4.9887	-3.3777	-1.1985
H	2.5342	-2.8021	-1.9422	H	2.791	-2.7628	-1.9284
H	2.33	-3.775	-0.5094	H	2.6082	-3.7598	-0.5096
H	4.8383	-1.3278	-2.0846	H	4.9719	-1.0786	-1.9443
H	6.0039	-1.5763	-0.7997	H	6.0693	-1.2209	-0.5858

H	1.0496	0.9373	-0.0022	H	0.8578	0.833	-0.1636
H	2.1926	0.8486	1.3217	H	1.8919	0.8391	1.2552
H	2.5217	2.3799	-1.3185	H	2.2988	2.3879	-1.3646
H	4.6874	3.1524	-0.5732	H	4.3055	3.3666	-0.4499
H	4.5576	2.2888	0.9496	H	4.1473	2.4793	1.0558
H	5.9952	1.0476	-0.5682	H	5.7987	1.3922	-0.3738
H	4.7959	1.0864	-1.8397	H	4.6784	1.3202	-1.7147
H	4.2089	0.2509	1.9217	H	3.9158	0.4035	2.0077
H	4.577	-1.4494	1.6665	H	4.5243	-1.2314	1.7771
H	5.8064	-0.2502	1.3802	H	5.5987	0.1211	1.5744
H	-7.1704	0.2865	-1.5894	H	-6.7651	0.3945	0.656
H	-5.5501	-0.0821	-2.1723	H	-7.3616	0.6184	-0.9814
H	-6.3175	1.7119	0.1924	H	-5.8291	2.4507	-0.1105
H	-5.5759	2.1797	-1.3401	H	-5.3988	1.7857	-1.6855
H	-6.7284	-0.8232	0.5396	H	-6.5979	-1.7075	-0.6852
H	-6.479	-1.9399	-0.7881	H	-5.6279	-0.8665	-1.8816
H	-1.7693	0.5765	0.9973	H	-1.5835	0.5285	0.5982
H	-2.4081	-0.7903	1.8487	H	-2.2834	-0.6637	1.6724
H	-1.579	-0.6781	-1.0978	H	-1.5269	-1.0523	-1.2697
H	-1.9526	-3.0854	-1.2514	H	-1.9724	-3.4638	-0.9188
H	-2.3924	-3.192	0.442	H	-2.4855	-3.1609	0.7345
H	-3.8944	-1.7752	-1.8021	H	-3.7472	-2.1221	-1.8386
H	-4.4148	-3.1951	-0.9094	H	-4.4408	-3.3118	-0.7502
H	-5.4426	-2.9397	1.4392	H	-5.6585	-2.6052	1.327
H	-3.8504	-2.425	1.9757	H	-4.1072	-2.0929	1.9858
H	-5.2504	-1.4083	2.3067	H	-5.464	-0.9731	1.9788
H	-2.4218	2.3605	0.4738	H	-3.196	3.1159	-0.7963
H	1.6312	-0.1443	-2.0718	H	1.6643	-0.2162	-2.1332
H	2.0361	5.1326	1.7505	H	1.2304	4.9528	1.759
H	3.6158	4.2026	1.6585	H	2.8642	4.1192	1.8696
H	-0.2449	-1.8385	2.4252	H	-0.2267	-1.9679	2.362
H	0.1846	4.6498	0.488	H	-0.4114	4.3723	0.257
1a-13	X axis(Å)	Y axis(Å)	Z axis(Å)	1a-14	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-2.943	-3.3791	1.1927	C	-3.751	-2.927	1.3252
C	-1.5465	-2.7865	1.0231	C	-2.231	-2.8162	1.2357
C	-1.5001	-1.5399	0.1283	C	-1.7448	-1.6688	0.3383
C	-2.6084	-0.5118	0.4898	C	-2.4706	-0.3299	0.6548
C	-4.0424	-1.1271	0.6135	C	-4.0324	-0.4462	0.6957
C	-3.9919	-2.3334	1.5876	C	-4.4281	-1.5941	1.6621
C	-2.6143	0.7545	-0.3957	C	-2.0129	0.865	-0.2115
C	-3.6006	1.8286	0.1245	C	-2.6593	2.195	0.2452
C	-5.0095	1.2358	0.3376	C	-4.1878	2.0999	0.3905
C	-4.9934	-0.0386	1.1919	C	-4.6183	0.8925	1.2313
C	-4.6601	-1.6084	-0.7225	C	-4.6944	-0.7132	-0.6781
O	-0.2066	-0.8913	0.3972	O	-0.3193	-1.4701	0.6569
C	-3.5595	3.0628	-0.7637	C	-2.2372	3.3718	-0.6131
C	6.6176	1.2727	0.8053	C	6.5015	-0.1801	0.4286

C	6.6778	-0.0612	0.069	C	5.7822	0.7699	1.378
C	5.3389	-0.7373	-0.0561	C	4.2843	0.7582	1.1865
C	4.1557	-0.1355	0.2044	C	3.6882	0.3099	0.0546
C	4.0736	1.359	0.5612	C	4.5107	-0.1175	-1.1798
C	5.4264	2.0889	0.3221	C	6.0423	0.0749	-0.9959
C	2.8084	-0.8427	0.1734	C	2.1932	0.0798	-0.1156
C	1.8282	-0.1411	-0.7789	C	1.8975	-1.4116	-0.3924
C	1.6637	1.3369	-0.3899	C	2.7165	-1.9254	-1.5917
C	3.0152	2.0524	-0.34	C	4.2112	-1.6159	-1.4447
C	3.6872	1.518	2.0498	C	4.1266	0.7275	-2.4198
C	5.4379	-2.1576	-0.5029	C	3.5287	1.2454	2.3828
O	4.7235	-2.6465	-1.3688	O	4.0824	1.6055	3.4161
C	0.493	-0.8372	-0.8004	C	0.4073	-1.6351	-0.5192
C	-1.3432	-1.8805	-1.3422	C	-1.6493	-2.0792	-1.1173
O	-2.2583	-0.0336	1.8264	O	-2.0495	0.0214	2.012
C	-4.4967	3.4615	-1.6396	C	-1.5475	4.4196	-0.1314
O	-2.1248	-2.492	-2.0535	O	-2.5446	-2.4858	-1.8403
C	-0.076	-1.3911	-1.8653	C	-0.2791	-1.9905	-1.6009
C	-2.3688	3.9561	-0.6283	C	-2.5864	3.4121	-2.06
O	-1.4289	3.7105	0.1184	O	-3.1689	2.5027	-2.6364
H	-3.239	-3.8891	0.2703	H	-4.1457	-3.329	0.3864
H	-2.9086	-4.1568	1.9653	H	-4.01	-3.6622	2.0968
H	-1.1512	-2.5339	2.0166	H	-1.828	-2.6815	2.2487
H	-0.8716	-3.5604	0.6351	H	-1.8195	-3.7731	0.8893
H	-3.7706	-1.9867	2.6054	H	-4.166	-1.3238	2.6933
H	-4.9758	-2.8167	1.641	H	-5.5165	-1.7347	1.6547
H	-1.6087	1.1908	-0.4043	H	-0.9252	0.9888	-0.1301
H	-2.8476	0.5021	-1.4364	H	-2.223	0.6641	-1.2658
H	-3.2622	2.1521	1.1194	H	-2.2772	2.3898	1.2586
H	-5.6505	1.9798	0.8275	H	-4.5685	3.0129	0.8664
H	-5.4834	1.0075	-0.6237	H	-4.6733	2.0495	-0.5902
H	-6.0161	-0.4297	1.2685	H	-5.7148	0.8464	1.2538
H	-4.7008	0.2248	2.2164	H	-4.3091	1.0577	2.2714
H	-4.5532	-0.8784	-1.5285	H	-4.3036	-0.069	-1.4696
H	-4.2379	-2.549	-1.0743	H	-4.5872	-1.7449	-1.0105
H	-5.7341	-1.7981	-0.6026	H	-5.7759	-0.5361	-0.625
H	6.5517	1.1026	1.8861	H	7.584	-0.0266	0.5056
H	7.5465	1.8284	0.6325	H	6.3071	-1.2211	0.7131
H	7.3877	-0.7126	0.5928	H	6.1493	1.7938	1.2344
H	7.0782	0.1011	-0.94	H	6.046	0.472	2.3999
H	5.426	3.068	0.8171	H	6.3281	1.1026	-1.2607
H	5.5649	2.2902	-0.7491	H	6.5957	-0.5772	-1.6833
H	2.8893	-1.8969	-0.1041	H	1.622	0.3852	0.7631
H	2.4028	-0.8569	1.1935	H	1.8123	0.7078	-0.9299
H	2.2559	-0.1765	-1.7915	H	2.2272	-1.988	0.485
H	1.0189	1.8448	-1.1187	H	2.5896	-3.0113	-1.6884
H	1.1615	1.4306	0.5809	H	2.3489	-1.4888	-2.5277

H	3.3941	2.1142	-1.3697	H	4.609	-2.2269	-0.6236
H	2.8596	3.0872	-0.0091	H	4.7282	-1.9491	-2.3538
H	3.6741	2.5748	2.3403	H	4.7408	0.4491	-3.2845
H	2.694	1.1156	2.272	H	3.0826	0.6082	-2.7215
H	4.395	1.0021	2.7079	H	4.2848	1.796	-2.2298
H	6.2462	-2.7368	-0.0255	H	2.4359	1.292	2.3003
H	-1.3267	0.2618	1.7813	H	-1.09	-0.1548	2.0631
H	-4.3973	4.3685	-2.2294	H	-1.25	5.2626	-0.7481
H	-5.4052	2.8927	-1.8079	H	-1.2611	4.4661	0.916
H	0.2675	-1.4774	-2.8784	H	0.0332	-2.1976	-2.6067
H	-2.376	4.8654	-1.253	H	-2.2789	4.3223	-2.6025
1a-15	X axis(Å)	Y axis(Å)	Z axis(Å)	1a-16	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-3.7402	-2.8519	1.626	C	3.7463	-3.2895	-0.2177
C	-2.2229	-2.7096	1.5427	C	2.2557	-3.0536	-0.4482
C	-1.7444	-1.7287	0.4625	C	1.7745	-1.6608	-0.0175
C	-2.5261	-0.3855	0.4949	C	2.6964	-0.5291	-0.5554
C	-4.0836	-0.5507	0.5311	C	4.2191	-0.7588	-0.268
C	-4.4626	-1.5022	1.6962	C	4.6232	-2.1662	-0.7818
C	-2.0978	0.6241	-0.5942	C	2.2531	0.8976	-0.1597
C	-2.7765	2.0071	-0.4152	C	3.1193	1.9854	-0.8388
C	-4.3044	1.881	-0.2703	C	4.6289	1.7464	-0.6635
C	-4.7202	0.8462	0.7821	C	5.0393	0.3173	-1.037
C	-4.7118	-1.1056	-0.7711	C	4.6159	-0.6505	1.2246
O	-0.3396	-1.419	0.7862	O	0.4521	-1.4696	-0.6384
C	-2.4322	3.0143	-1.5016	C	2.7103	3.3888	-0.435
C	6.5568	0.9058	-2.00E-04	C	-6.3082	0.4201	-1.4322
C	5.7061	1.347	1.1833	C	-5.9244	1.5906	-0.5352
C	4.2324	1.0432	1.0304	C	-4.6414	1.3471	0.2227
C	3.7311	0.194	0.0988	C	-4.1201	0.111	0.4153
C	4.6613	-0.564	-0.8718	C	-4.8677	-1.1646	-0.0291
C	6.1528	-0.4902	-0.4422	C	-6.2687	-0.8724	-0.636
C	2.2506	-0.106	-0.1071	C	-2.7348	-0.177	0.9752
C	1.9375	-1.6164	-0.1056	C	-1.8639	-0.8881	-0.0851
C	2.8024	-2.3388	-1.1494	C	-2.5553	-2.1554	-0.617
C	4.2867	-2.0694	-0.9117	C	-3.9884	-1.8792	-1.0877
C	4.5263	0.0503	-2.2855	C	-5.1174	-2.109	1.1726
C	3.3859	1.7981	2.0089	C	-3.9801	2.6025	0.6975
O	3.8668	2.4915	2.899	O	-4.3965	3.721	0.4159
C	0.4518	-1.8479	-0.2742	C	-0.4635	-1.2153	0.3785
C	-1.5766	-2.3874	-0.8923	C	1.4006	-1.6084	1.4502
O	-2.1521	0.2417	1.759	O	2.5418	-0.5704	-2.0102
C	-2.0707	2.7456	-2.7674	C	2.2355	4.2933	-1.3079
O	-2.444	-2.8641	-1.6064	O	2.109	-1.8564	2.4126
C	-0.1773	-2.426	-1.2925	C	-0.0023	-1.2596	1.6246
C	-2.4753	4.4594	-1.125	C	2.8254	3.8284	0.983
O	-2.7656	4.8486	-0.001	O	3.1979	3.0914	1.8869
H	-4.1009	-3.4358	0.773	H	3.936	-3.4205	0.8526

H	-3.9948	-3.4379	2.5174	H	4.0346	-4.2365	-0.6898
H	-1.8489	-2.3803	2.5218	H	2.0374	-3.1999	-1.5148
H	-1.7768	-3.7	1.3844	H	1.6827	-3.8333	0.0703
H	-4.2264	-1.0311	2.6592	H	4.563	-2.1974	-1.8776
H	-5.5461	-1.6769	1.7037	H	5.6718	-2.3722	-0.5317
H	-1.0127	0.7842	-0.5477	H	1.2149	1.0658	-0.4751
H	-2.3133	0.2087	-1.5834	H	2.2664	1.0039	0.9287
H	-2.3885	2.4122	0.53	H	2.9294	1.8987	-1.9192
H	-4.7349	2.8502	0.0116	H	5.1871	2.4487	-1.296
H	-4.7537	1.6245	-1.2378	H	4.943	1.956	0.3647
H	-5.8151	0.769	0.7924	H	6.1118	0.1913	-0.8399
H	-4.4424	1.222	1.7753	H	4.9217	0.1873	-2.1205
H	-4.3441	-0.6032	-1.6692	H	4.1856	0.2258	1.7155
H	-4.5494	-2.1747	-0.9025	H	4.3317	-1.5261	1.8068
H	-5.8014	-0.9767	-0.7568	H	5.7055	-0.5737	1.3284
H	7.6151	0.9166	0.2852	H	-7.3151	0.5806	-1.8345
H	6.4501	1.6176	-0.8267	H	-5.629	0.3617	-2.2911
H	5.8633	2.4238	1.322	H	-6.7276	1.7893	0.1853
H	6.0677	0.8498	2.0927	H	-5.837	2.4772	-1.1744
H	6.8042	-0.8191	-1.2618	H	-7.0178	-0.796	0.1646
H	6.3418	-1.1797	0.3922	H	-6.5918	-1.7062	-1.2719
H	1.6254	0.3694	0.6508	H	-2.2101	0.7279	1.2886
H	1.9345	0.3385	-1.0601	H	-2.8303	-0.7836	1.8829
H	2.2099	-2.0203	0.8806	H	-1.7585	-0.1882	-0.928
H	2.6282	-3.421	-1.0955	H	-1.9856	-2.5674	-1.46
H	2.5299	-2.0287	-2.1651	H	-2.5612	-2.9359	0.1538
H	4.5635	-2.5434	0.0403	H	-3.9354	-1.2699	-1.9996
H	4.8698	-2.5807	-1.6885	H	-4.4498	-2.8307	-1.3817
H	5.204	-0.4414	-2.993	H	-5.6948	-2.988	0.8621
H	3.5148	-0.0473	-2.6915	H	-4.197	-2.4816	1.6305
H	4.7653	1.1194	-2.2867	H	-5.6854	-1.5994	1.9602
H	2.2975	1.7114	1.9053	H	-3.0964	2.4893	1.338
H	-1.1827	0.1611	1.8451	H	1.584	-0.6517	-2.1869
H	-1.8328	3.5275	-3.4836	H	1.9443	5.2979	-1.0155
H	-2.0139	1.7313	-3.1471	H	2.1251	4.049	-2.3611
H	0.1914	-2.8483	-2.2078	H	-0.4863	-1.1094	2.5706
H	-2.2256	5.1739	-1.9277	H	2.5436	4.8759	1.185
1a-17	X axis(Å)	Y axis(Å)	Z axis(Å)	1a-18	X axis(Å)	Y axis(Å)	Z axis(Å)
C	3.4596	-3.5133	-0.1466	C	2.6238	-3.5588	-1.1869
C	2.0229	-3.0886	-0.437	C	1.2764	-2.8608	-1.0245
C	1.6723	-1.6803	0.0655	C	1.3131	-1.6359	-0.0992
C	2.7536	-0.6306	-0.3137	C	2.5053	-0.69	-0.4156
C	4.2185	-1.0633	0.0351	C	3.8878	-1.4176	-0.5321
C	4.4898	-2.4631	-0.5759	C	3.7577	-2.5901	-1.5393
C	2.4578	0.7976	0.1978	C	2.6014	0.5426	0.5121
C	3.4658	1.8399	-0.3527	C	3.6925	1.5431	0.0501
C	4.9245	1.4029	-0.1233	C	5.0475	0.849	-0.1803

C	5.1983	-0.031	-0.5928	C	4.9359	-0.3988	-1.0645
C	4.5381	-1.126	1.5491	C	4.442	-1.982	0.7992
O	0.4329	-1.2956	-0.6329	O	0.0779	-0.8805	-0.3772
C	3.2507	3.2511	0.1718	C	3.8662	2.7418	0.9696
C	-7.014	0.4915	-0.6614	C	-6.3203	1.9536	0.2986
C	-6.2333	1.7001	-0.162	C	-6.6736	0.4874	0.0808
C	-4.8761	1.3613	0.4122	C	-5.4535	-0.3914	-0.0542
C	-4.2594	0.1666	0.2326	C	-4.2247	0.091	-0.3605
C	-4.9055	-0.9463	-0.6208	C	-4.0024	1.5761	-0.7207
C	-6.104	-0.4249	-1.4615	C	-5.319	2.4021	-0.7514
C	-2.9129	-0.225	0.8289	C	-2.9306	-0.7075	-0.2958
C	-1.9211	-0.7447	-0.2317	C	-1.9717	-0.0928	0.7455
C	-2.5372	-1.9184	-1.0048	C	-1.7299	1.404	0.4894
C	-3.8748	-1.5231	-1.6275	C	-3.0434	2.1797	0.3385
C	-5.4126	-2.0713	0.3126	C	-3.3835	1.7156	-2.1336
C	-4.2945	2.4809	1.2189	C	-5.7235	-1.8365	0.2231
O	-4.8285	3.5815	1.3068	O	-6.8098	-2.2452	0.6187
C	-0.5695	-1.1411	0.3186	C	-0.6656	-0.8415	0.7935
C	1.1901	-1.6762	1.5026	C	1.096	-1.9975	1.3587
O	2.6922	-0.5325	-1.769	O	2.2161	-0.1461	-1.7394
C	2.6969	3.601	1.3448	C	3.6188	2.7888	2.2894
O	1.8293	-1.9378	2.5089	O	1.8211	-2.6629	2.0807
C	-0.2216	-1.3285	1.5875	C	-0.1623	-1.4595	1.856
C	3.6753	4.3766	-0.7143	C	4.3408	4.0134	0.3457
O	4.1789	4.2057	-1.8173	O	4.5816	4.1227	-0.8499
H	3.566	-3.7416	0.919	H	2.8625	-4.1123	-0.2729
H	3.6677	-4.4517	-0.6747	H	2.5415	-4.3128	-1.9791
H	1.8569	-3.1373	-1.522	H	0.9205	-2.5538	-2.0175
H	1.3353	-3.8296	-0.0091	H	0.5354	-3.5876	-0.6673
H	4.4883	-2.4024	-1.672	H	3.5803	-2.2004	-2.5502
H	5.4922	-2.8101	-0.2945	H	4.701	-3.1485	-1.5926
H	1.4555	1.1085	-0.125	H	1.6449	1.0815	0.5161
H	2.4514	0.8008	1.2921	H	2.7821	0.2141	1.54
H	3.2996	1.8743	-1.4386	H	3.3524	1.9308	-0.9205
H	5.6055	2.0762	-0.6591	H	5.7486	1.5466	-0.6559
H	5.183	1.4991	0.9386	H	5.5003	0.5796	0.782
H	6.2356	-0.2938	-0.3484	H	5.9234	-0.8724	-1.1381
H	5.1375	-0.0611	-1.6883	H	4.6829	-0.0859	-2.0856
H	4.2026	-0.2393	2.0925	H	4.3952	-1.2618	1.6198
H	4.1062	-1.9965	2.0416	H	3.9302	-2.8863	1.1263
H	5.6204	-1.2081	1.7097	H	5.4951	-2.2685	0.6857
H	-7.4554	-0.0474	0.1847	H	-7.2285	2.5637	0.2336
H	-7.8495	0.8279	-1.2863	H	-5.9109	2.1	1.3052
H	-6.8514	2.2081	0.5884	H	-7.2875	0.3803	-0.8221
H	-6.0902	2.4052	-0.9911	H	-7.29	0.1699	0.9303
H	-6.6867	-1.265	-1.8599	H	-5.8001	2.3085	-1.7351
H	-5.7402	0.1342	-2.3346	H	-5.1039	3.4703	-0.6222

H	-2.4331	0.603	1.354	H	-3.0907	-1.7533	-0.0243
H	-3.0899	-0.9933	1.5923	H	-2.4704	-0.7384	-1.2903
H	-1.7444	0.0781	-0.9403	H	-2.4559	-0.1803	1.7297
H	-1.8612	-2.2417	-1.8067	H	-1.1581	1.834	1.322
H	-2.6687	-2.7856	-0.346	H	-1.1128	1.5493	-0.4056
H	-3.669	-0.7785	-2.4091	H	-3.5392	2.2065	1.3178
H	-4.2996	-2.3951	-2.1413	H	-2.8077	3.2213	0.0851
H	-5.922	-2.8555	-0.2592	H	-3.2688	2.7719	-2.4046
H	-4.6016	-2.5557	0.8653	H	-2.3948	1.257	-2.222
H	-6.1207	-1.6912	1.0571	H	-4.0238	1.246	-2.89
H	-3.3516	2.2852	1.7432	H	-4.903	-2.5415	0.0384
H	1.75	-0.4384	-2.01	H	1.2871	0.1558	-1.7273
H	2.571	4.6383	1.6433	H	3.7623	3.6912	2.8775
H	2.36	2.8635	2.0651	H	3.2774	1.9202	2.8421
H	-0.7875	-1.2677	2.4974	H	-0.5435	-1.5679	2.8536
H	3.5083	5.3919	-0.3164	H	4.4649	4.8689	1.0313
1a-19	X axis(Å)	Y axis(Å)	Z axis(Å)	1a-20	X axis(Å)	Y axis(Å)	Z axis(Å)
C	4.0233	-2.7213	-1.2544	C	2.8694	-3.4584	-1.0039
C	2.497	-2.7601	-1.276	C	1.4863	-2.8387	-0.8226
C	1.8388	-1.6953	-0.3871	C	1.4848	-1.5405	-0.0033
C	2.4501	-0.2833	-0.6158	C	2.5916	-0.5501	-0.4616
C	4.0143	-0.2452	-0.5466	C	4.0131	-1.1911	-0.5972
C	4.589	-1.3197	-1.5077	C	3.9151	-2.4516	-1.4959
C	1.8203	0.8338	0.2456	C	2.6428	0.7648	0.3486
C	2.3521	2.2328	-0.141	C	3.6228	1.7943	-0.2656
C	3.8888	2.2978	-0.1796	C	5.0162	1.1706	-0.4943
C	4.4993	1.1607	-1.0084	C	4.9555	-0.1512	-1.271
C	4.601	-0.4876	0.8653	C	4.6709	-1.6016	0.7432
O	0.4269	-1.6253	-0.7985	O	0.1905	-0.8917	-0.2677
C	1.739	3.328	0.7088	C	3.6303	3.0771	0.5524
C	-6.4972	0.7587	-0.2972	C	-6.6044	1.3562	-0.6824
C	-5.603	1.1664	-1.4619	C	-6.6822	0.0351	0.0725
C	-4.1398	0.9089	-1.2173	C	-5.3593	-0.6776	0.1757
C	-3.6607	0.0987	-0.2439	C	-4.16	-0.0903	-0.0486
C	-4.6033	-0.6171	0.7377	C	-4.0568	1.3934	-0.4481
C	-6.0777	-0.6008	0.2448	C	-5.3936	2.155	-0.2223
C	-2.1792	-0.166	-0.0172	C	-2.8222	-0.8131	0.0514
C	-1.8429	-1.6644	0.1222	C	-1.8022	-0.0546	0.9199
C	-2.7132	-2.3135	1.2067	C	-1.6335	1.3936	0.4439
C	-4.1966	-2.1049	0.9034	C	-2.9797	2.113	0.4054
C	-4.5309	0.0998	2.1069	C	-3.6854	1.484	-1.9472
C	-3.2567	1.6843	-2.1415	C	-5.5173	-2.125	0.5151
O	-2.2313	2.2546	-1.7914	O	-4.8548	-3.0263	0.0195
C	-0.3565	-1.8362	0.3324	C	-0.472	-0.7616	0.9447
C	1.6825	-2.1617	1.0469	C	1.3725	-1.7891	1.4895
O	2.0947	0.0631	-1.9925	O	2.202	-0.1445	-1.8107
C	0.9179	4.2668	0.209	C	4.6082	3.5151	1.3628

O	2.5575	-2.5392	1.8099	O	2.1706	-2.3633	2.2135
C	0.2828	-2.1692	1.4493	C	0.127	-1.2557	2.0224
C	2.0157	3.3941	2.1696	C	2.4429	3.9751	0.4185
O	2.6946	2.5673	2.7651	O	1.4654	3.6962	-0.2654
H	4.3874	-3.112	-0.2985	H	3.1917	-3.9167	-0.0633
H	4.4081	-3.4039	-2.0218	H	2.7997	-4.2801	-1.7271
H	2.1561	-2.6306	-2.3121	H	1.0596	-2.6406	-1.8154
H	2.1575	-3.763	-0.9864	H	0.8168	-3.5792	-0.3661
H	4.3765	-1.0441	-2.5489	H	3.662	-2.1624	-2.5242
H	5.6826	-1.3552	-1.4227	H	4.8912	-2.95	-1.5546
H	0.7336	0.851	0.0971	H	1.643	1.2137	0.3659
H	1.9838	0.6285	1.3077	H	2.9091	0.5694	1.3937
H	2.0234	2.414	-1.1754	H	3.2523	2.0668	-1.2643
H	4.2042	3.2566	-0.6111	H	5.6473	1.8762	-1.0494
H	4.3102	2.2718	0.8308	H	5.5221	0.9922	0.4611
H	5.5935	1.2241	-0.949	H	5.9705	-0.5599	-1.3592
H	4.2519	1.3228	-2.0654	H	4.6306	0.0557	-2.2986
H	4.1035	0.1025	1.6388	H	4.6033	-0.823	1.507
H	4.559	-1.532	1.1712	H	4.2478	-2.5122	1.1658
H	5.6642	-0.2184	0.891	H	5.7371	-1.8158	0.5979
H	-6.4523	1.5166	0.4932	H	-6.554	1.1704	-1.7613
H	-7.5402	0.721	-0.6324	H	-7.5204	1.9324	-0.5076
H	-5.7723	2.2298	-1.6713	H	-7.4204	-0.6041	-0.4274
H	-5.9046	0.6131	-2.3605	H	-7.0558	0.2189	1.088
H	-6.7546	-0.8964	1.0563	H	-5.3743	3.1225	-0.7396
H	-6.2163	-1.3425	-0.5539	H	-5.523	2.3828	0.8448
H	-1.5724	0.2264	-0.8379	H	-2.9261	-1.8134	0.4802
H	-1.8623	0.3763	0.8833	H	-2.4311	-0.9576	-0.9638
H	-2.0896	-2.1602	-0.8284	H	-2.1973	-0.0233	1.9461
H	-2.5093	-3.3907	1.2541	H	-0.9608	1.9336	1.1227
H	-2.4768	-1.9071	2.1969	H	-1.1626	1.4292	-0.5459
H	-4.432	-2.6568	-0.0171	H	-3.3355	2.2124	1.4403
H	-4.7919	-2.5703	1.6995	H	-2.8273	3.1349	0.035
H	-5.2104	-0.3662	2.8298	H	-3.6319	2.5285	-2.2753
H	-3.527	0.0703	2.5423	H	-2.7147	1.0283	-2.1669
H	-4.8076	1.1568	2.027	H	-4.4228	0.9762	-2.5785
H	-3.6248	1.7472	-3.1797	H	-6.3257	-2.3381	1.2352
H	1.1314	-0.0817	-2.076	H	1.2703	0.1491	-1.7564
H	0.4703	5.0455	0.8186	H	4.5421	4.4552	1.9034
H	0.6522	4.2712	-0.8455	H	5.519	2.9479	1.5234
H	-0.0768	-2.3948	2.4348	H	-0.181	-1.2772	3.05
H	1.5584	4.243	2.7056	H	2.4887	4.9207	0.985
1b-1	X axis(Å)	Y axis(Å)	Z axis(Å)	1b-2	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-3.0422	-2.9659	-1.4355	C	-3.0111	-3.0569	-1.2765
C	-2.8087	-2.9308	0.0756	C	-2.7279	-2.9622	0.2236
C	-2.1089	-1.6462	0.5395	C	-2.0468	-1.6449	0.6177
C	-2.8469	-0.3724	0.0253	C	-2.8355	-0.4092	0.0854

C	-2.9733	-0.3915	-1.5434	C	-3.013	-0.4869	-1.4765
C	-3.7077	-1.6925	-1.9695	C	-3.7268	-1.8202	-1.8318
C	-2.2071	0.9515	0.5013	C	-2.2167	0.9468	0.494
C	-2.9628	2.1961	-0.015	C	-3.0222	2.1525	-0.0388
C	-3.2084	2.1647	-1.5322	C	-3.3139	2.0618	-1.5452
C	-3.8126	0.8352	-1.9962	C	-3.8982	0.7021	-1.9429
C	-1.6172	-0.3289	-2.2967	C	-1.6849	-0.4172	-2.2774
O	-0.7237	-1.6707	0.1304	O	-0.6762	-1.6496	0.1613
C	-2.31	3.4943	0.4222	C	-2.3924	3.4819	0.3339
C	6.0877	0.2148	-0.9502	C	6.1633	-0.1188	0.0048
C	5.475	1.3283	-0.1101	C	5.5189	1.263	-0.0136
C	3.9964	1.158	0.1441	C	4.0138	1.1986	0.0548
C	3.328	-0.007	-0.0404	C	3.3087	0.0789	-0.2341
C	4.0456	-1.2708	-0.5567	C	3.9817	-1.182	-0.8144
C	5.5919	-1.141	-0.4731	C	5.51	-1.0064	-1.0414
C	1.8394	-0.1979	0.2139	C	1.8273	-0.1062	0.0524
C	1.5344	-1.4329	1.0859	C	1.6024	-1.288	1.0232
C	2.1505	-2.6955	0.4784	C	2.263	-2.5766	0.5145
C	3.6554	-2.515	0.2867	C	3.7411	-2.3554	0.1713
C	3.6474	-1.4994	-2.0346	C	3.3826	-1.5294	-2.1998
C	3.3289	2.4231	0.5862	C	3.3686	2.4726	0.5011
O	3.9616	3.3983	0.9792	O	4.0065	3.4105	0.9682
C	0.0493	-1.5906	1.2831	C	0.1326	-1.4929	1.281
C	-1.9831	-1.6392	2.047	C	-1.8693	-1.5787	2.1186
O	-4.1991	-0.3842	0.5529	O	-4.1688	-0.4373	0.6586
C	-2.9411	4.4119	1.1738	C	-3.0276	4.409	1.0704
O	-2.9089	-1.5977	2.8456	O	-2.7678	-1.5395	2.9478
C	-0.5863	-1.6078	2.4522	C	-0.4614	-1.4821	2.4719
C	-0.9082	3.81	0.0254	C	-1.0105	3.8199	-0.1115
O	-0.1926	3.0369	-0.6002	O	-0.2907	3.0455	-0.7306
H	-2.0888	-3.1353	-1.948	H	-2.0712	-3.221	-1.8152
H	-3.672	-3.8294	-1.6812	H	-3.6262	-3.9439	-1.4701
H	-3.7753	-3.0377	0.5844	H	-3.6736	-3.075	0.769
H	-2.2125	-3.8093	0.3537	H	-2.0998	-3.815	0.5114
H	-4.7464	-1.6698	-1.6149	H	-4.7535	-1.8108	-1.4433
H	-3.7648	-1.7524	-3.0638	H	-3.8183	-1.9206	-2.9209
H	-2.2216	0.997	1.5983	H	-2.1962	1.0305	1.5885
H	-1.1556	0.9785	0.2061	H	-1.177	0.9907	0.162
H	-3.9594	2.1628	0.4503	H	-4.0024	2.1086	0.4593
H	-3.8927	2.9769	-1.8098	H	-4.0272	2.8466	-1.8286
H	-2.2809	2.3565	-2.0831	H	-2.409	2.2569	-2.1314
H	-3.9062	0.849	-3.0897	H	-4.0275	0.6751	-3.0325
H	-4.8376	0.7595	-1.6109	H	-4.9077	0.6145	-1.5212
H	-1.0234	-1.2392	-2.1948	H	-1.0647	-1.3085	-2.165
H	-1.7834	-0.1963	-3.3728	H	-1.8902	-0.3265	-3.3511
H	-0.9885	0.5014	-1.9653	H	-1.0673	0.4395	-1.9962
H	5.8413	0.3631	-2.0078	H	7.2359	-0.0263	-0.2006

H	7.1805	0.2599	-0.8766	H	6.0678	-0.5688	1.0003
H	5.6693	2.2791	-0.6214	H	5.8092	1.7993	-0.9255
H	5.9884	1.3744	0.8589	H	5.9233	1.8261	0.8358
H	6.0743	-1.9344	-1.0578	H	5.6963	-0.5554	-2.0262
H	5.927	-1.2798	0.5641	H	6.0095	-1.9832	-1.0592
H	1.3901	0.665	0.7113	H	1.3727	0.7786	0.5043
H	1.3357	-0.2788	-0.7577	H	1.2933	-0.2577	-0.8926
H	1.9991	-1.2707	2.0696	H	2.0857	-1.0266	1.9764
H	1.9756	-3.5534	1.1399	H	2.1905	-3.3583	1.2815
H	1.6754	-2.9424	-0.4786	H	1.7313	-2.9639	-0.3631
H	4.1121	-2.441	1.2835	H	4.2869	-2.1727	1.1064
H	4.0676	-3.4234	-0.1711	H	4.1469	-3.2868	-0.2441
H	4.1693	-2.3685	-2.4516	H	3.8856	-2.4023	-2.6326
H	2.5746	-1.6806	-2.1558	H	2.3147	-1.7626	-2.1641
H	3.8939	-0.6342	-2.6598	H	3.5044	-0.6945	-2.9004
H	2.2325	2.451	0.5425	H	2.28	2.5479	0.3746
H	-4.1581	-0.537	1.5199	H	-4.092	-0.5557	1.6282
H	-2.4731	5.3407	1.4867	H	-2.5767	5.3601	1.3378
H	-3.9653	4.256	1.5024	H	-4.0381	4.2383	1.4325
H	-0.2166	-1.5382	3.457	H	-0.06	-1.3558	3.4589
H	-0.5319	4.7978	0.3423	H	-0.6529	4.8274	0.1618
1b-3	X axis(Å)	Y axis(Å)	Z axis(Å)	1b-4	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-1.6326	-3.4687	0.2686	C	-2.6369	-3.2335	-1.6522
C	-1.4387	-2.6017	1.5127	C	-2.0249	-3.2024	-0.2513
C	-1.5227	-1.0976	1.2076	C	-1.7294	-1.7761	0.2362
C	-2.8319	-0.7425	0.4429	C	-2.9851	-0.861	0.1223
C	-2.9608	-1.5831	-0.8811	C	-3.5354	-0.8365	-1.3518
C	-2.8865	-3.0942	-0.528	C	-3.8376	-2.2932	-1.7996
C	-2.9939	0.7653	0.1449	C	-2.7598	0.578	0.6398
C	-4.3256	1.0756	-0.5773	C	-4.0389	1.4407	0.5415
C	-4.5515	0.2013	-1.8222	C	-4.678	1.4101	-0.8568
C	-4.3402	-1.2884	-1.5339	C	-4.8557	-0.0172	-1.3843
C	-1.8676	-1.2759	-1.939	C	-2.566	-0.2004	-2.3833
O	-0.3343	-0.6825	0.4985	O	-0.5927	-1.246	-0.4796
C	-4.4892	2.5524	-0.8809	C	-3.8209	2.8576	1.0364
C	6.716	0.6887	-0.8068	C	6.4887	1.6644	-0.6367
C	5.8866	-0.1714	-1.7514	C	6.612	0.1573	-0.4545
C	4.5532	-0.6031	-1.1835	C	5.3771	-0.4965	0.1236
C	3.9976	-0.0597	-0.0716	C	4.167	0.112	0.1952
C	4.683	1.1015	0.6788	C	3.955	1.5378	-0.3587
C	5.8373	1.7366	-0.1451	C	5.1404	2.0086	-1.2463
C	2.686	-0.5081	0.5621	C	2.913	-0.4949	0.8134
C	1.6993	0.6569	0.7745	C	1.6994	-0.4548	-0.137
C	2.3611	1.764	1.6087	C	1.4398	0.9841	-0.607
C	3.6613	2.2361	0.9595	C	2.6865	1.5865	-1.2506
C	5.2638	0.574	2.0122	C	3.8039	2.525	0.8231
C	3.9185	-1.7057	-1.9748	C	5.6393	-1.8826	0.6262

O	4.4401	-2.1847	-2.9767	O	6.7277	-2.4355	0.5069
C	0.3969	0.1458	1.3492	C	0.4304	-1.0375	0.4439
C	-1.3987	-0.3127	2.4928	C	-1.2037	-1.8192	1.652
O	-3.9574	-1.117	1.2818	O	-4.0358	-1.4317	0.9472
C	-5.4751	3.3018	-0.3598	C	-4.4765	3.3733	2.0898
O	-2.2345	-0.2529	3.3843	O	-1.839	-2.1397	2.6473
C	-0.1425	0.418	2.5361	C	0.1785	-1.3705	1.7085
C	-3.5377	3.2442	-1.7945	C	-2.8469	3.7543	0.3537
O	-2.5736	2.6912	-2.3082	O	-2.1522	3.4019	-0.5911
H	-0.7449	-3.3967	-0.3695	H	-1.8689	-2.9828	-2.3922
H	-1.7009	-4.5205	0.5711	H	-2.9533	-4.2578	-1.8829
H	-2.1957	-2.8776	2.258	H	-2.7094	-3.7042	0.4447
H	-0.4645	-2.8471	1.955	H	-1.1034	-3.7986	-0.264
H	-3.7681	-3.3859	0.0576	H	-4.6703	-2.7008	-1.2118
H	-2.9206	-3.698	-1.4438	H	-4.1731	-2.3047	-2.8445
H	-2.9958	1.3307	1.0861	H	-2.4687	0.5495	1.6981
H	-2.1361	1.128	-0.4289	H	-1.9264	1.0416	0.1046
H	-5.1265	0.8036	0.1265	H	-4.7744	0.976	1.2153
H	-5.5753	0.346	-2.1909	H	-5.6615	1.8965	-0.8212
H	-3.8942	0.5073	-2.6431	H	-4.0857	1.9899	-1.5729
H	-4.445	-1.8508	-2.4707	H	-5.2497	0.0279	-2.4078
H	-5.152	-1.6396	-0.8841	H	-5.6301	-0.5185	-0.7896
H	-0.8723	-1.6101	-1.64	H	-1.674	-0.8029	-2.5654
H	-2.0909	-1.7926	-2.8805	H	-3.061	-0.0906	-3.356
H	-1.791	-0.2103	-2.1697	H	-2.2243	0.7938	-2.0844
H	7.1994	0.0589	-0.0513	H	6.6165	2.1717	0.3263
H	7.5221	1.1758	-1.3676	H	7.2957	2.022	-1.2867
H	6.4908	-1.0466	-2.0202	H	7.4814	-0.0293	0.1879
H	5.701	0.3876	-2.6777	H	6.8249	-0.3073	-1.4259
H	6.4529	2.3829	0.4931	H	5.0817	3.0902	-1.4217
H	5.4293	2.3857	-0.9322	H	5.0839	1.5363	-2.2367
H	2.1858	-1.2805	-0.0243	H	3.06	-1.5315	1.1217
H	2.9099	-0.9854	1.5252	H	2.6898	0.0554	1.7364
H	1.4612	1.0868	-0.2097	H	1.9543	-1.0633	-1.0172
H	1.6819	2.6212	1.6997	H	0.6254	1.003	-1.3426
H	2.5635	1.4159	2.6286	H	1.1082	1.6082	0.2321
H	3.3997	2.7372	0.0171	H	2.8737	1.0401	-2.1856
H	4.1189	3.0038	1.5968	H	2.4713	2.623	-1.5409
H	5.7982	1.3671	2.548	H	3.7012	3.5552	0.4628
H	4.4899	0.1982	2.6886	H	2.9234	2.3132	1.4376
H	5.9685	-0.2487	1.8495	H	4.6717	2.4927	1.4909
H	2.9478	-2.0803	-1.6286	H	4.809	-2.4053	1.1157
H	-3.8339	-0.7139	2.1668	H	-3.6741	-1.5999	1.8424
H	-5.591	4.3589	-0.5797	H	-4.3201	4.3884	2.4422
H	-6.2094	2.8678	0.3137	H	-5.2045	2.7812	2.6383
H	0.1961	1.0321	3.3481	H	0.7771	-1.3062	2.5964
H	-3.747	4.3104	-1.9857	H	-2.7753	4.7787	0.7573

1b-5	X axis(Å)	Y axis(Å)	Z axis(Å)	1b-6	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-2.5495	-3.424	-1.0085	C	-3.0448	-2.9845	-1.4003
C	-2.338	-3.0643	0.462	C	-2.7845	-2.9353	0.1058
C	-1.8401	-1.6241	0.6617	C	-2.0565	-1.6572	0.5435
C	-2.7451	-0.5948	-0.0769	C	-2.7779	-0.3758	0.0218
C	-2.8659	-0.9396	-1.6068	C	-2.9391	-0.414	-1.5429
C	-3.3973	-2.3912	-1.7576	C	-3.7031	-1.7082	-1.9356
C	-2.3037	0.8759	0.1078	C	-2.0995	0.9413	0.4596
C	-3.2686	1.8722	-0.5801	C	-2.8434	2.1935	-0.0524
C	-3.49	1.5073	-2.0625	C	-3.137	2.1481	-1.5609
C	-3.8826	0.0391	-2.258	C	-3.7698	0.8206	-1.9933
C	-1.5327	-0.8272	-2.3945	C	-1.5988	-0.3841	-2.3253
O	-0.458	-1.5248	0.2469	O	-0.6767	-1.7115	0.1209
C	-2.8093	3.3048	-0.3501	C	-2.1389	3.4717	0.362
C	6.3182	0.3937	-1.0123	C	6.0199	0.4654	-1.0393
C	5.7087	1.575	-0.2686	C	5.3882	1.523	-0.1393
C	4.2342	1.4215	0.0276	C	3.9451	1.2512	0.1822
C	3.5666	0.2445	-0.0635	C	3.3158	0.0801	-0.0624
C	4.2925	-1.0591	-0.4622	C	4.0589	-1.1309	-0.6458
C	5.8383	-0.9133	-0.404	C	5.6006	-0.9326	-0.5998
C	2.0751	0.0615	0.188	C	1.8356	-0.15	0.1833
C	1.7771	-1.0733	1.1856	C	1.5844	-1.3954	1.0513
C	2.4166	-2.3874	0.725	C	2.234	-2.6328	0.4188
C	3.9184	-2.2109	0.51	C	3.7298	-2.4043	0.1816
C	3.8878	-1.4407	-1.9063	C	3.6305	-1.3368	-2.1175
C	3.5818	2.7144	0.4083	C	3.2376	2.4163	0.7866
O	4.2118	3.7566	0.5543	O	2.6258	2.3555	1.8464
C	0.293	-1.2392	1.3825	C	0.1067	-1.5914	1.2644
C	-1.7412	-1.3286	2.1427	C	-1.9159	-1.6333	2.05
O	-4.0825	-0.701	0.4721	O	-4.1196	-0.3509	0.5767
C	-2.2237	4.1226	-1.2407	C	-2.703	4.3875	1.1673
O	-2.674	-1.2452	2.9284	O	-2.8348	-1.5873	2.8566
C	-0.3576	-1.116	2.5368	C	-0.516	-1.5875	2.4406
C	-3.0689	3.8902	0.9998	C	-0.7522	3.7601	-0.1051
O	-3.5662	3.2505	1.9181	O	-0.1282	3.0354	-0.8708
H	-1.5774	-3.5426	-1.4995	H	-2.1031	-3.1726	-1.9277
H	-3.039	-4.4033	-1.0717	H	-3.6906	-3.8419	-1.6247
H	-3.2834	-3.2125	0.9998	H	-3.7442	-3.0205	0.6316
H	-1.622	-3.7768	0.8914	H	-2.1978	-3.82	0.3845
H	-4.4285	-2.4541	-1.3862	H	-4.733	-1.6649	-1.5583
H	-3.4423	-2.6685	-2.8185	H	-3.7855	-1.7811	-3.0276
H	-2.2807	1.1097	1.179	H	-2.0812	1.0011	1.5558
H	-1.2819	1.0268	-0.2594	H	-1.0569	0.9495	0.1326
H	-4.254	1.7773	-0.1017	H	-3.8262	2.1898	0.4424
H	-4.2802	2.1426	-2.4825	H	-3.8199	2.966	-1.8251
H	-2.5895	1.71	-2.6524	H	-2.2275	2.3219	-2.1456
H	-3.9707	-0.1659	-3.3327	H	-3.8873	0.8213	-3.0846

H	-4.8861	-0.1169	-1.8418	H	-4.787	0.7653	-1.5849
H	-0.8047	-1.5938	-2.122	H	-1.01	-1.2959	-2.2088
H	-1.7132	-0.9485	-3.4696	H	-1.7867	-0.2802	-3.401
H	-1.0407	0.1395	-2.2603	H	-0.9567	0.4498	-2.0314
H	6.0559	0.4425	-2.0752	H	5.7304	0.6402	-2.0819
H	7.4116	0.4521	-0.9588	H	7.1116	0.5571	-1.0003
H	5.8879	2.4746	-0.8703	H	5.4948	2.5006	-0.6246
H	6.2381	1.7144	0.6828	H	5.9471	1.5729	0.804
H	6.3218	-1.7555	-0.9149	H	6.1009	-1.6804	-1.2277
H	6.1835	-0.9508	0.6385	H	5.9723	-1.0939	0.4215
H	1.5977	0.9672	0.5674	H	1.3499	0.7112	0.6503
H	1.5886	-0.1391	-0.7755	H	1.342	-0.258	-0.7913
H	2.228	-0.7989	2.1505	H	2.0588	-1.2277	2.0292
H	2.2536	-3.1674	1.4796	H	1.7422	-2.8905	-0.527
H	1.947	-2.7496	-0.1975	H	2.1058	-3.5001	1.0788
H	4.3759	-2.0259	1.4919	H	4.2152	-2.3379	1.1653
H	4.3403	-3.1581	0.1501	H	4.153	-3.2904	-0.3087
H	4.4212	-2.3388	-2.2386	H	4.1861	-2.1637	-2.5748
H	2.8179	-1.6514	-2.0008	H	2.5666	-1.5743	-2.2158
H	4.116	-0.6383	-2.6163	H	3.8126	-0.4412	-2.7215
H	2.4953	2.7047	0.5559	H	3.3498	3.3628	0.2316
H	-4.0406	-0.5327	1.4375	H	-4.0612	-0.4893	1.545
H	-1.9398	5.143	-0.9977	H	-2.1952	5.2985	1.4696
H	-2.0007	3.8059	-2.254	H	-3.7085	4.2463	1.5548
H	-0.0077	-0.8914	3.526	H	-0.1348	-1.4762	3.4373
H	-2.7767	4.9456	1.1327	H	-0.303	4.6908	0.2817
1b-7	X axis(Å)	Y axis(Å)	Z axis(Å)	1b-8	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-2.254	-3.4913	-1.1462	C	-1.4895	3.1862	-1.5248
C	-2.0014	-3.2554	0.3431	C	-1.3575	1.8758	-2.3004
C	-1.6201	-1.8008	0.6603	C	-1.4619	0.6329	-1.4009
C	-2.6529	-0.7966	0.0701	C	-2.741	0.6711	-0.5152
C	-2.8181	-1.0005	-1.4813	C	-2.8016	1.99	0.3397
C	-3.2254	-2.4745	-1.7543	C	-2.7189	3.2148	-0.6119
C	-2.3356	0.6846	0.3813	C	-2.9133	-0.5672	0.3946
C	-3.4221	1.6473	-0.1625	C	-4.2341	-0.5249	1.2016
C	-3.6891	1.4112	-1.6601	C	-4.3745	0.7991	1.9804
C	-3.9464	-0.0625	-1.9912	C	-4.1591	2.0312	1.0954
C	-1.5426	-0.6882	-2.3094	C	-1.6703	2.1192	1.3947
O	-0.2755	-1.5386	0.1973	O	-0.2552	0.5001	-0.6143
C	-3.1359	3.1187	0.0966	C	-4.3767	-1.7735	2.0595
C	6.3492	0.83	-1.1185	C	6.7975	-0.4904	0.9722
C	5.7311	1.8827	-0.2078	C	6.0206	0.704	1.5102
C	4.2791	1.6289	0.1279	C	4.6841	0.9225	0.8377
C	3.6546	0.4428	-0.0781	C	4.0757	-0.0027	0.0543
C	4.4118	-0.7694	-0.6636	C	4.7049	-1.3929	-0.1769
C	5.9518	-0.5617	-0.656	C	5.8724	-1.6841	0.8064
C	2.1856	0.1636	0.2145	C	2.751	0.1992	-0.6723

C	1.9835	-1.0939	1.0802	C	1.7312	-0.917	-0.371
C	2.651	-2.3134	0.4356	C	2.3359	-2.2889	-0.7051
C	4.1321	-2.0448	0.1771	C	3.6472	-2.5066	0.048
C	3.9524	-0.9937	-2.1241	C	5.2501	-1.4691	-1.6228
C	3.5944	2.8359	0.6892	C	4.1126	2.2788	1.1167
O	4.192	3.8725	0.9582	O	4.6414	3.0721	1.8889
C	0.5193	-1.3511	1.3233	C	0.4186	-0.6342	-1.0671
C	-1.4671	-1.6319	2.1562	C	-1.405	-0.6092	-2.2607
O	-3.9432	-1.0817	0.6646	O	-3.8919	0.7041	-1.3968
C	-1.9349	3.6862	0.2991	C	-4.2174	-1.8661	3.3903
O	-2.3694	-1.6492	2.9814	O	-2.2599	-0.9845	-3.0498
C	-0.0772	-1.3952	2.5121	C	-0.1751	-1.3475	-2.0222
C	-4.3133	4.0364	0.1651	C	-4.7767	-3.0323	1.3617
O	-5.467	3.6562	0.0107	O	-4.9332	-3.1016	0.149
H	-1.3008	-3.4718	-1.6861	H	-0.5795	3.3581	-0.9394
H	-2.6579	-4.5012	-1.2862	H	-1.5511	4.0192	-2.2354
H	-2.9018	-3.5385	0.9033	H	-2.1353	1.8452	-3.0744
H	-1.2059	-3.9376	0.6698	H	-0.3952	1.8838	-2.8283
H	-4.2275	-2.6681	-1.3499	H	-3.6171	3.2628	-1.2413
H	-3.2978	-2.6524	-2.8349	H	-2.7095	4.1453	-0.0299
H	-2.2849	0.8323	1.4678	H	-2.9242	-1.4697	-0.2285
H	-1.3491	0.9421	-0.0172	H	-2.0593	-0.6755	1.0733
H	-4.3449	1.4013	0.3817	H	-5.07	-0.5377	0.4873
H	-4.5618	1.9927	-1.983	H	-5.375	0.8572	2.428
H	-2.8464	1.7831	-2.2558	H	-3.6645	0.8384	2.8137
H	-4.0651	-0.1677	-3.0774	H	-4.2183	2.9325	1.719
H	-4.911	-0.3561	-1.5573	H	-4.9919	2.1056	0.3845
H	-0.7334	-1.4015	-2.1414	H	-0.6829	2.2649	0.9523
H	-1.7649	-0.7298	-3.3828	H	-1.8462	2.9896	2.0386
H	-1.1384	0.3068	-2.1064	H	-1.5994	1.2469	2.0494
H	6.0327	0.996	-2.1545	H	7.2692	-0.2333	0.0169
H	7.4407	0.9307	-1.1065	H	7.6106	-0.7401	1.6637
H	5.8468	2.8567	-0.6989	H	6.6558	1.5913	1.3985
H	6.2989	1.9269	0.7306	H	5.8469	0.5666	2.5854
H	6.4425	-1.3128	-1.2878	H	6.4506	-2.5531	0.4679
H	6.3492	-0.71	0.3576	H	5.4772	-1.9487	1.7969
H	1.6921	0.995	0.722	H	2.2894	1.1575	-0.429
H	1.6602	0.0569	-0.7435	H	2.9477	0.243	-1.7516
H	2.4712	-0.9158	2.0498	H	1.5221	-0.9058	0.7089
H	2.5566	-3.1845	1.0965	H	1.6343	-3.0855	-0.4268
H	2.151	-2.5838	-0.5023	H	2.5088	-2.3869	-1.7834
H	4.6299	-1.9581	1.1529	H	3.4083	-2.5763	1.1184
H	4.5727	-2.9223	-0.3136	H	4.0631	-3.4819	-0.2362
H	4.5039	-1.8208	-2.586	H	5.7432	-2.4308	-1.8057
H	2.8883	-1.2394	-2.1966	H	4.4619	-1.3666	-2.3752
H	4.1141	-0.1028	-2.7407	H	5.982	-0.6786	-1.8216
H	2.513	2.7669	0.857	H	3.1836	2.55	0.6012

H	-3.8552	-1.063	1.6405	H	-3.869	-0.0905	-1.9716
H	-1.8184	4.7499	0.4896	H	-4.3543	-2.7984	3.9313
H	-1.0153	3.1129	0.2721	H	-3.9395	-1.0111	3.9975
H	0.3126	-1.2694	3.5039	H	0.1134	-2.2528	-2.5207
H	-4.086	5.0972	0.3654	H	-4.9201	-3.9164	2.0059
1b-9	X axis(Å)	Y axis(Å)	Z axis(Å)	1b-10	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-2.5139	-3.2829	-1.6079	C	1.7125	-3.3215	1.0669
C	-1.9509	-3.2189	-0.1877	C	1.499	-3.004	-0.4132
C	-1.6829	-1.7808	0.2806	C	1.5268	-1.4957	-0.7071
C	-2.9406	-0.8782	0.1051	C	2.8159	-0.8281	-0.1437
C	-3.4397	-0.8876	-1.3873	C	2.9626	-1.0928	1.4006
C	-3.7156	-2.3552	-1.8157	C	2.9451	-2.6256	1.653
C	-2.744	0.5725	0.601	C	2.922	0.6837	-0.4464
C	-4.0252	1.4228	0.4411	C	4.2355	1.2945	0.0949
C	-4.6149	1.3594	-0.9776	C	4.4808	0.9721	1.5785
C	-4.7639	-0.0795	-1.482	C	4.3248	-0.5211	1.8836
C	-2.4397	-0.2646	-2.3974	C	1.8499	-0.4438	2.2661
O	-0.5264	-1.2558	-0.4062	O	0.3183	-0.8844	-0.2041
C	-3.835	2.851	0.9147	C	4.3445	2.7798	-0.1909
C	5.9809	1.2962	-1.5698	C	-6.0129	1.8077	0.6598
C	6.452	0.1544	-0.6778	C	-5.67	0.7874	1.738
C	5.3309	-0.452	0.132	C	-4.4608	-0.0454	1.3848
C	4.1609	0.1896	0.37	C	-4.0097	-0.1891	0.1145
C	3.9302	1.6492	-0.0783	C	-4.7674	0.4118	-1.0885
C	5.1775	2.2897	-0.7494	C	-6.0937	1.1182	-0.6905
C	2.9257	-0.4404	0.9971	C	-2.6955	-0.8481	-0.279
C	1.745	-0.4347	-2.00E-04	C	-1.7584	0.1748	-0.9591
C	1.4803	0.9824	-0.5431	C	-2.4569	0.8565	-2.1511
C	2.751	1.6473	-1.084	C	-3.8228	1.4387	-1.766
C	3.5911	2.5557	1.131	C	-5.166	-0.6902	-2.1012
C	5.6222	-1.842	0.6031	C	-3.7879	-0.6483	2.5785
O	6.6653	-2.4291	0.3359	O	-4.2194	-0.5145	3.719
C	0.4621	-1.0188	0.5476	C	-0.4343	-0.4704	-1.3026
C	-1.2062	-1.7911	1.7142	C	1.3862	-1.2667	-2.194
O	-4.0152	-1.4408	0.9047	O	3.9613	-1.4544	-0.7814
C	-4.5312	3.3823	1.9337	C	5.3085	3.3075	-0.964
O	-1.8726	-2.0975	2.6934	O	2.2267	-1.5228	-3.0454
C	0.1694	-1.3283	1.8093	C	0.1056	-0.653	-2.5063
C	-2.844	3.7417	0.2489	C	3.361	3.734	0.3926
O	-2.1134	3.3761	-0.6633	O	2.4119	3.3855	1.0832
H	-1.7227	-3.041	-2.326	H	0.817	-3.0431	1.6335
H	-2.8147	-4.3141	-1.8285	H	1.8207	-4.4058	1.1895
H	-2.6553	-3.7121	0.4943	H	2.2721	-3.5164	-1.0003
H	-1.0252	-3.8078	-0.1566	H	0.5382	-3.435	-0.7228
H	-4.5652	-2.7576	-1.2488	H	3.8417	-3.0871	1.2191
H	-4.0146	-2.3904	-2.8711	H	2.9921	-2.8313	2.73
H	-2.4896	0.5675	1.669	H	2.9123	0.8456	-1.5323

H	-1.8959	1.032	0.0855	H	2.0469	1.2073	-0.0506
H	-4.7802	0.9656	1.0982	H	5.0517	0.8027	-0.4553
H	-5.6024	1.8387	-0.9861	H	5.4955	1.2837	1.8585
H	-4.002	1.9295	-1.6842	H	3.8056	1.5451	2.223
H	-5.1225	-0.058	-2.5192	H	4.4411	-0.678	2.9637
H	-5.5548	-0.5749	-0.9043	H	5.1544	-1.0647	1.4133
H	-1.5378	-0.8636	-2.5367	H	0.8697	-0.9029	2.1234
H	-2.9016	-0.1778	-3.3885	H	2.0831	-0.5522	3.3324
H	-2.1155	0.738	-2.1069	H	1.7333	0.6253	2.0716
H	6.8484	1.7953	-2.0165	H	-6.9724	2.2825	0.895
H	5.3772	0.9068	-2.3982	H	-5.2606	2.6052	0.6381
H	7.2306	0.5109	0.008	H	-6.5231	0.1188	1.908
H	6.9136	-0.5987	-1.3277	H	-5.5022	1.3412	2.6695
H	5.8448	2.7083	0.0171	H	-6.9117	0.3857	-0.6436
H	4.88	3.1346	-1.3831	H	-6.3856	1.8458	-1.4583
H	3.0937	-1.4717	1.3136	H	-2.1747	-1.2831	0.5758
H	2.6705	0.1026	1.9144	H	-2.891	-1.6963	-0.946
H	2.0412	-1.0673	-0.8504	H	-1.5378	0.9658	-0.2265
H	0.7401	0.9421	-1.3529	H	-1.8256	1.6675	-2.5361
H	1.0359	1.6108	0.2388	H	-2.5865	0.1489	-2.9786
H	3.0458	1.1226	-2.0024	H	-3.6546	2.2906	-1.0938
H	2.5078	2.675	-1.3829	H	-4.2953	1.8481	-2.668
H	3.4784	3.5995	0.814	H	-5.7429	-0.2643	-2.9309
H	2.6623	2.2774	1.6361	H	-4.3093	-1.2052	-2.544
H	4.3889	2.5209	1.8826	H	-5.7881	-1.4558	-1.6222
H	4.863	-2.3278	1.2281	H	-2.8846	-1.2439	2.3989
H	-3.6833	-1.5887	1.8149	H	3.8315	-1.4248	-1.7526
H	-4.3947	4.4055	2.2709	H	5.3852	4.3717	-1.1662
H	-5.2739	2.7955	2.468	H	6.0638	2.6754	-1.4236
H	0.7359	-1.2401	2.7159	H	-0.2463	-0.4078	-3.4896
H	-2.7945	4.7746	0.6338	H	3.5312	4.7991	0.1603
1b-11	X axis(Å)	Y axis(Å)	Z axis(Å)	1b-12	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-2.4629	-3.4812	-1.2784	C	-2.4975	-3.4996	-0.7378
C	-1.898	-3.1745	0.1083	C	-2.2382	-3.0345	0.6949
C	-1.659	-1.6739	0.3406	C	-1.7765	-1.5708	0.7759
C	-2.9287	-0.8329	0.0176	C	-2.742	-0.6201	0.0094
C	-3.4311	-1.1014	-1.4483	C	-2.9139	-1.0716	-1.4875
C	-3.6834	-2.6236	-1.6261	C	-3.406	-2.5445	-1.5181
C	-2.7552	0.6853	0.2557	C	-2.3396	0.8717	0.0766
C	-4.0614	1.4751	-0.0041	C	-3.3629	1.7906	-0.6344
C	-4.6384	1.1623	-1.4	C	-3.6317	1.32	-2.0786
C	-4.7698	-0.3415	-1.6625	C	-3.986	-0.1686	-2.1591
C	-2.4449	-0.6409	-2.5551	C	-1.6178	-0.9758	-2.3369
O	-0.5086	-1.2405	-0.421	O	-0.4163	-1.4625	0.2962
C	-3.8534	2.9577	0.2688	C	-2.9415	3.2484	-0.5194
C	6.5959	1.5925	-0.8278	C	6.4231	0.0743	-0.0787
C	6.6951	0.1317	-0.4088	C	5.8014	1.4615	-0.1848

C	5.4375	-0.4119	0.2313	C	4.2963	1.4339	-0.0693
C	4.2335	0.2099	0.1718	C	3.5603	0.3141	-0.271
C	4.0542	1.5322	-0.6047	C	4.2024	-1.003	-0.7591
C	5.2686	1.8483	-1.5213	C	5.7264	-0.8751	-1.0376
C	2.9562	-0.2833	0.8414	C	2.0762	0.1747	0.0333
C	1.7701	-0.3833	-0.139	C	1.8439	-0.9083	1.1086
C	1.5396	0.9655	-0.8351	C	2.4968	-2.2462	0.7258
C	2.8105	1.4505	-1.5291	C	3.9699	-2.0752	0.3374
C	3.8837	2.694	0.4028	C	3.5669	-1.4663	-2.0937
C	5.6701	-1.702	0.9555	C	3.7035	2.7487	0.3284
O	6.7495	-2.2843	0.9388	O	4.3854	3.737	0.5775
C	0.4795	-0.8615	0.4873	C	0.3733	-1.0884	1.3787
C	-1.186	-1.4575	1.7598	C	-1.6255	-1.1723	2.2281
O	-3.9922	-1.2738	0.8994	O	-4.052	-0.7265	0.6208
C	-3.7428	3.9423	-0.6386	C	-2.419	4.0212	-1.4862
O	-1.8404	-1.6336	2.7774	O	-2.5277	-1.0568	3.0449
C	0.1841	-0.9702	1.7812	C	-0.2327	-0.9031	2.5488
C	-3.8059	3.3827	1.7003	C	-3.1661	3.9156	0.7984
O	-3.8652	2.5914	2.6331	O	-3.6067	3.3254	1.7767
H	-1.6786	-3.3453	-2.0312	H	-1.5427	-3.6243	-1.2603
H	-2.7437	-4.5402	-1.3254	H	-2.9589	-4.4942	-0.7144
H	-2.5909	-3.5657	0.8646	H	-3.1562	-3.1714	1.281
H	-0.9602	-3.732	0.2295	H	-1.4842	-3.696	1.1407
H	-4.5222	-2.9418	-0.9934	H	-4.419	-2.6108	-1.1002
H	-3.9874	-2.8379	-2.6587	H	-3.485	-2.8947	-2.5552
H	-2.4589	0.8516	1.2983	H	-1.3388	1.0264	-0.3432
H	-1.9426	1.0877	-0.3602	H	-2.2803	1.1784	1.1278
H	-4.8181	1.1272	0.7138	H	-4.3248	1.6993	-0.1096
H	-5.6285	1.6254	-1.5	H	-4.4575	1.9026	-2.5066
H	-4.0151	1.6015	-2.1866	H	-2.7621	1.5077	-2.7179
H	-5.132	-0.4939	-2.6874	H	-4.1107	-0.4486	-3.213
H	-5.5509	-0.7477	-1.0072	H	-4.9666	-0.3244	-1.6914
H	-1.5301	-1.2354	-2.5915	H	-0.8563	-1.7017	-2.0453
H	-2.9093	-0.7365	-3.5442	H	-1.838	-1.1746	-3.393
H	-2.1408	0.4031	-2.4447	H	-1.1507	0.0111	-2.2884
H	6.7047	2.2434	0.0472	H	7.4909	0.1311	-0.3189
H	7.4242	1.837	-1.5029	H	6.3483	-0.2977	0.95
H	7.5455	0.0403	0.2781	H	6.0741	1.9223	-1.1424
H	6.926	-0.4815	-1.2894	H	6.2408	2.0785	0.608
H	5.2283	2.8895	-1.8652	H	5.8935	-0.5028	-2.0581
H	5.2324	1.2272	-2.4269	H	6.2077	-1.8603	-0.9946
H	3.0823	-1.2605	1.311	H	1.6271	1.1031	0.3929
H	2.7147	0.4062	1.6604	H	1.5362	-0.0607	-0.8915
H	2.0437	-1.1232	-0.9056	H	2.3268	-0.5621	2.0345
H	0.7453	0.8743	-1.5872	H	2.4317	-2.9441	1.5705
H	1.1931	1.7158	-0.1137	H	1.9524	-2.7211	-0.0994
H	3.0162	0.7631	-2.3615	H	4.5341	-1.8113	1.2418

H	2.6158	2.4304	-1.9838	H	4.3591	-3.0461	0.0052
H	3.8029	3.6555	-0.1174	H	4.0553	-2.377	-2.4606
H	2.9846	2.5881	1.0178	H	2.4997	-1.6904	-2.0125
H	4.733	2.7604	1.0915	H	3.675	-0.6964	-2.8671
H	4.8266	-2.124	1.5148	H	2.609	2.8106	0.3719
H	-3.6976	-1.1605	1.828	H	-3.9761	-0.4908	1.5699
H	-3.6116	4.9835	-0.3572	H	-2.1593	5.0638	-1.3236
H	-3.7769	3.7483	-1.7053	H	-2.2268	3.6433	-2.4847
H	0.7493	-0.7475	2.6655	H	0.1518	-0.6077	3.5061
H	-3.7047	4.4667	1.8786	H	-2.9023	4.9857	0.849
1b-13	X axis(Å)	Y axis(Å)	Z axis(Å)	1b-14	X axis(Å)	Y axis(Å)	Z axis(Å)
C	1.3458	3.2956	1.1189	C	-2.3385	-3.4667	-1.31
C	1.1709	2.1267	2.0885	C	-2.0909	-3.3177	0.1913
C	1.3225	0.7573	1.4062	C	-1.6144	-1.9109	0.5821
C	2.6519	0.6636	0.6022	C	-2.5604	-0.8062	0.0236
C	2.7597	1.8254	-0.4533	C	-2.7148	-0.9293	-1.5374
C	2.6237	3.1874	0.281	C	-3.2253	-2.3554	-1.8811
C	2.8744	-0.7032	-0.0854	C	-2.1341	0.631	0.4025
C	4.2409	-0.7804	-0.8135	C	-3.125	1.7024	-0.1169
C	4.4317	0.3979	-1.7855	C	-3.3966	1.547	-1.6239
C	4.155	1.7561	-1.1325	C	-3.7622	0.1122	-2.0183
C	1.6905	1.7717	-1.5774	C	-1.4066	-0.6772	-2.3347
O	0.1607	0.4918	0.5868	O	-0.248	-1.7208	0.1517
C	4.4921	-2.0993	-1.5286	C	-2.7088	3.1313	0.1966
C	-6.8606	-0.5965	-1.0817	C	6.225	1.1066	-0.9802
C	-6.0314	0.469	-1.7865	C	5.5455	2.0629	-0.0077
C	-4.713	0.7705	-1.1102	C	4.1128	1.7041	0.2898
C	-4.1587	-0.0186	-0.1562	C	3.563	0.4954	0.0247
C	-4.836	-1.3327	0.2867	C	4.3781	-0.6305	-0.6375
C	-5.9766	-1.7637	-0.6766	C	5.9044	-0.3357	-0.6148
C	-2.8546	0.2764	0.5756	C	2.1159	0.1336	0.3241
C	-1.8581	-0.8984	0.5133	C	1.9758	-1.2019	1.0792
C	-2.5143	-2.1771	1.055	C	2.6993	-2.3337	0.3431
C	-3.8041	-2.4923	0.2993	C	4.166	-1.9737	0.1109
C	-5.433	-1.1441	1.7015	C	3.9245	-0.7752	-2.1097
C	-4.0938	2.0451	-1.5962	C	3.3474	2.8488	0.8748
O	-4.5737	2.7049	-2.5124	O	2.1809	3.1085	0.6095
C	-0.5635	-0.5289	1.2027	C	0.5213	-1.5283	1.2942
C	1.2161	-0.3365	2.4439	C	-1.479	-1.8208	2.0868
O	3.7483	0.8475	1.5321	O	-3.8784	-1.0173	0.588
C	3.5674	-2.9619	-1.9824	C	-1.4598	3.5829	0.3998
O	2.05	-0.6094	3.2958	O	-2.3919	-1.8712	2.8993
C	-0.0257	-1.0773	2.2906	C	-0.0941	-1.6013	2.4717
C	5.917	-2.5027	-1.7269	C	-3.7972	4.146	0.3185
O	6.8635	-1.8219	-1.3527	O	-4.9828	3.8785	0.1671
H	0.4697	3.3619	0.4644	H	-1.3788	-3.4923	-1.8379
H	1.3679	4.2332	1.6872	H	-2.8121	-4.4371	-1.501

H	1.9055	2.2263	2.8981	H	-3.0172	-3.5627	0.7268
H	0.1814	2.2126	2.5559	H	-1.3493	-4.0678	0.4948
H	3.4858	3.3453	0.942	H	-4.2442	-2.4925	-1.4961
H	2.6457	4.0113	-0.4438	H	-3.2958	-2.4793	-2.9693
H	2.8608	-1.503	0.6663	H	-2.0931	0.7295	1.495
H	2.0498	-0.9071	-0.7759	H	-1.1228	0.8235	0.0313
H	5.007	-0.6916	-0.0303	H	-4.0717	1.519	0.4108
H	5.4593	0.4053	-2.1705	H	-4.2196	2.207	-1.9263
H	3.7858	0.2704	-2.663	H	-2.5235	1.8773	-2.2001
H	4.2458	2.5418	-1.8935	H	-3.8747	0.0609	-3.1089
H	4.9459	1.9599	-0.3992	H	-4.7517	-0.1239	-1.6061
H	0.6783	1.9698	-1.2196	H	-0.6539	-1.4539	-2.1863
H	1.898	2.5342	-2.3382	H	-1.614	-0.658	-3.4117
H	1.6647	0.8077	-2.0919	H	-0.9344	0.2763	-2.0847
H	-7.6559	-0.9439	-1.7513	H	5.9039	1.3227	-2.0055
H	-7.3576	-0.1673	-0.2043	H	7.3091	1.2664	-0.9533
H	-6.6442	1.3764	-1.8538	H	5.6051	3.0764	-0.4233
H	-5.8248	0.1439	-2.8144	H	6.102	2.0734	0.9383
H	-6.591	-2.5477	-0.2163	H	6.4344	-1.0131	-1.2962
H	-5.555	-2.2048	-1.5904	H	6.3116	-0.5309	0.3869
H	-2.3566	1.1666	0.1878	H	1.6189	0.8948	0.9313
H	-3.0872	0.5126	1.6223	H	1.5673	0.0985	-0.626
H	-1.6102	-1.08	-0.543	H	2.4551	-1.0823	2.062
H	-1.8271	-3.0258	0.9467	H	2.6473	-3.2567	0.9345
H	-2.7279	-2.0823	2.1263	H	2.2121	-2.5544	-0.6142
H	-3.5299	-2.7522	-0.7327	H	4.6592	-1.9303	1.0919
H	-4.2581	-3.3938	0.7308	H	4.6507	-2.7907	-0.439
H	-5.9599	-2.048	2.0284	H	4.5061	-1.5485	-2.6248
H	-4.6689	-0.9301	2.4551	H	2.8697	-1.0543	-2.1977
H	-6.1482	-0.3148	1.7317	H	4.0508	0.1596	-2.6667
H	-3.175	2.3802	-1.1003	H	3.9349	3.4888	1.5553
H	3.6613	0.195	2.2582	H	-3.8047	-1.0482	1.5643
H	3.8321	-3.8931	-2.4759	H	-1.2415	4.6223	0.6287
H	2.5045	-2.7677	-1.8895	H	-0.5891	2.9372	0.3329
H	-0.3586	-1.8753	2.926	H	0.2746	-1.4684	3.4703
H	6.0774	-3.4663	-2.2395	H	-3.4727	5.1733	0.5561
1b-15	X axis(Å)	Y axis(Å)	Z axis(Å)	1b-16	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-2.8156	-3.2342	-1.0664	C	2.212	-3.4827	1.4084
C	-2.4761	-3.0279	0.41	C	1.6484	-3.2422	0.0076
C	-1.8816	-1.6413	0.6956	C	1.4878	-1.75	-0.3231
C	-2.7842	-0.5024	0.1325	C	2.8077	-0.9629	-0.0732
C	-3.0364	-0.6897	-1.4095	C	3.3097	-1.1528	1.4056
C	-3.6562	-2.0937	-1.6501	C	3.4807	-2.6706	1.6879
C	-2.2488	0.9179	0.4222	C	2.7143	0.5423	-0.4145
C	-3.1837	2.0208	-0.1229	C	4.0656	1.2764	-0.2198
C	-3.5592	1.8183	-1.6004	C	4.6451	1.0325	1.1853
C	-4.0423	0.3934	-1.8902	C	4.6878	-0.4526	1.5597

C	-1.7607	-0.564	-2.2849	C	2.3634	-0.5619	2.485
O	-0.5354	-1.5747	0.1786	O	0.3726	-1.2042	0.4175
C	-2.64	3.4108	0.1463	C	4.0117	2.7674	-0.5164
C	6.2871	0.0745	-0.2494	C	-6.6503	1.8364	0.7226
C	5.654	1.4409	-0.0106	C	-6.7939	0.3515	0.4162
C	4.1722	1.3364	0.2107	C	-5.5617	-0.272	-0.2003
C	3.4204	0.3053	-0.2345	C	-4.3415	0.3205	-0.2072
C	4.0239	-0.8595	-1.0366	C	-4.1155	1.6922	0.4642
C	5.5355	-0.6616	-1.3496	C	-5.3049	2.108	1.3737
C	1.9493	0.1205	0.0904	C	-3.0894	-0.2551	-0.8579
C	1.7665	-1.1475	0.9465	C	-1.8886	-0.3122	0.108
C	2.381	-2.3818	0.2603	C	-1.612	1.0787	0.6962
C	3.8334	-2.1413	-0.1806	C	-2.8577	1.6476	1.3719
C	3.3221	-1.0289	-2.4055	C	-3.9341	2.7701	-0.6308
C	3.6196	2.4314	1.0578	C	-5.8395	-1.6069	-0.8199
O	2.9248	2.2376	2.0474	O	-6.9346	-2.1546	-0.748
C	0.3106	-1.3632	1.2621	C	-0.6216	-0.8695	-0.5011
C	-1.6515	-1.4793	2.1823	C	1.0087	-1.597	-1.7484
O	-4.0821	-0.5917	0.7786	O	3.8318	-1.5234	-0.9321
C	-3.272	4.3047	0.9254	C	2.9296	3.5626	-0.4705
O	-2.5208	-1.4297	3.0421	O	1.6571	-1.8295	-2.7588
C	-0.2363	-1.3234	2.4747	C	-0.3507	-1.0818	-1.7874
C	-1.3462	3.845	-0.4523	C	5.2883	3.4224	-0.9337
O	-0.6664	3.1354	-1.1833	O	6.3493	2.819	-1.0307
H	-1.8904	-3.3529	-1.6411	H	1.4446	-3.2523	2.1556
H	-3.363	-4.1775	-1.1804	H	2.4358	-4.5496	1.5268
H	-3.3859	-3.1776	1.0055	H	2.3104	-3.7204	-0.7258
H	-1.7725	-3.813	0.7155	H	0.681	-3.7551	-0.0674
H	-4.6595	-2.1415	-1.207	H	4.2946	-3.0774	1.0737
H	-3.7935	-2.2664	-2.7252	H	3.7831	-2.8292	2.7309
H	-2.1684	1.0685	1.5069	H	2.4256	0.6667	-1.4662
H	-1.2369	1.0262	0.0214	H	1.9257	1.0079	0.1852
H	-4.1257	1.9291	0.4384	H	4.7598	0.8315	-0.9467
H	-4.3553	2.5223	-1.8755	H	5.6658	1.4309	1.2457
H	-2.7157	2.0535	-2.258	H	4.0646	1.5865	1.9333
H	-4.2238	0.2913	-2.9679	H	5.0489	-0.5492	2.5917
H	-5.0182	0.2477	-1.4095	H	5.4399	-0.9504	0.934
H	-1.058	-1.3877	-2.1451	H	1.4151	-1.0964	2.5662
H	-2.0257	-0.5693	-3.3493	H	2.8306	-0.6209	3.4757
H	-1.2092	0.3609	-2.0977	H	2.1232	0.4896	2.3085
H	7.3372	0.2013	-0.5363	H	-6.7583	2.4227	-0.197
H	6.2789	-0.5143	0.6757	H	-7.4601	2.1525	1.3904
H	5.8416	2.0999	-0.8672	H	-7.6581	0.2317	-0.2488
H	6.1408	1.8975	0.8597	H	-7.0252	-0.1877	1.3439
H	5.6528	-0.0821	-2.2762	H	-5.2322	3.1706	1.6376
H	6.0161	-1.6299	-1.5376	H	-5.2681	1.5556	2.3228
H	1.5184	0.9806	0.6109	H	-3.2482	-1.2611	-1.2506

H	1.3753	0.0539	-0.8416	H	-2.8455	0.3644	-1.7304
H	2.308	-0.9941	1.8916	H	-2.1667	-0.985	0.9326
H	2.356	-3.2367	0.9482	H	-0.8067	1.0235	1.4401
H	1.782	-2.6772	-0.6098	H	-1.26	1.7632	-0.0854
H	4.4571	-2.0811	0.7213	H	-3.0654	1.0304	2.2572
H	4.1819	-3.0213	-0.7361	H	-2.6304	2.6535	1.748
H	3.7982	-1.8257	-2.9893	H	-3.8203	3.7656	-0.1862
H	2.2634	-1.2893	-2.3216	H	-3.0491	2.5949	-1.2503
H	3.3815	-0.105	-2.9933	H	-4.7937	2.8067	-1.309
H	3.9323	3.4454	0.7563	H	-5.0151	-2.0954	-1.3528
H	-3.9453	-0.6322	1.7484	H	3.5097	-1.5171	-1.8576
H	-2.8792	5.2981	1.1202	H	2.975	4.6217	-0.7092
H	-4.2187	4.0604	1.3999	H	1.9533	3.1898	-0.181
H	0.2032	-1.15	3.438	H	-0.9253	-0.9097	-2.677
H	-1.0212	4.8679	-0.1969	H	5.2258	4.5015	-1.1542
1b-17	X axis(Å)	Y axis(Å)	Z axis(Å)	1b-18	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-2.2046	-3.5552	-0.9265	C	-2.71	-3.0876	-1.831
C	-1.9107	-3.2259	0.5373	C	-2.0591	-3.1554	-0.4492
C	-1.5619	-1.7454	0.757	C	-1.7141	-1.7686	0.1141
C	-2.6427	-0.8062	0.1462	C	-2.9485	-0.8181	0.0904
C	-2.8523	-1.1045	-1.3845	C	-3.5394	-0.6929	-1.3627
C	-3.2246	-2.6026	-1.5586	C	-3.8906	-2.1127	-1.8867
C	-2.3598	0.6988	0.3613	C	-2.6713	0.5821	0.6835
C	-3.492	1.5974	-0.1988	C	-3.9303	1.479	0.6752
C	-3.7996	1.2678	-1.6707	C	-4.6116	1.5461	-0.7019
C	-4.0238	-0.2293	-1.9084	C	-4.8394	0.1573	-1.3074
C	-1.6142	-0.8059	-2.2723	C	-2.5838	-0.0192	-2.3831
O	-0.2418	-1.4742	0.2329	O	-0.5846	-1.2229	-0.6003
C	-3.2427	3.0889	-0.0328	C	-3.6598	2.8579	1.2457
C	6.5136	0.3797	-0.2311	C	6.5556	1.5537	-0.7455
C	5.8391	1.7424	-0.1302	C	6.6614	0.0476	-0.5402
C	4.3425	1.6391	0.0394	C	5.4198	-0.5675	0.0497
C	3.638	0.5249	-0.2748	C	4.2104	0.0403	0.0816
C	4.3036	-0.6923	-0.9534	C	4.0121	1.4581	-0.4818
C	5.8075	-0.4668	-1.2758	C	5.2109	1.9096	-1.3633
C	2.1756	0.2871	0.0709	C	2.9563	-0.5877	0.6755
C	2.0337	-0.9307	1.0089	C	1.741	-0.5204	-0.2719
C	2.7146	-2.1818	0.4309	C	1.4961	0.9259	-0.7276
C	4.1608	-1.903	0.0057	C	2.747	1.5163	-1.3751
C	3.624	-1.0094	-2.3088	C	3.866	2.449	0.6973
C	3.7205	2.8669	0.6247	C	5.6744	-1.9155	0.6427
O	4.3771	3.8332	0.9969	O	5.1976	-2.2995	1.7025
C	0.5855	-1.2052	1.3183	C	0.4686	-1.1007	0.3055
C	-1.364	-1.4851	2.2344	C	-1.154	-1.9108	1.5101
O	-3.9038	-1.0921	0.8001	O	-3.9909	-1.4106	0.9111
C	-2.054	3.7008	0.1	C	-4.2631	3.3224	2.3528
O	-2.2377	-1.4762	3.0899	O	-1.7763	-2.2706	2.5004

C	0.0305	-1.1947	2.5277	C	0.2415	-1.5058	1.554
C	-4.4447	3.9752	0.0203	C	-2.6887	3.7722	0.5824
O	-5.5905	3.5543	-0.0769	O	-2.046	3.4675	-0.4143
H	-2.583	-4.5821	-0.9944	H	-1.9568	-2.8103	-2.5767
H	-1.2705	-3.5411	-1.4988	H	-3.058	-4.0885	-2.1133
H	-2.7838	-3.5001	1.1434	H	-2.7368	-3.682	0.2351
H	-1.0856	-3.8659	0.8753	H	-1.1538	-3.7715	-0.5241
H	-4.207	-2.7998	-1.1099	H	-4.7161	-2.5353	-1.2993
H	-3.3266	-2.8451	-2.624	H	-4.2558	-2.0539	-2.92
H	-2.2779	0.9107	1.4352	H	-2.3501	0.4842	1.7289
H	-1.3951	0.9603	-0.0851	H	-1.8425	1.0574	0.151
H	-4.389	1.357	0.3894	H	-4.6572	0.9932	1.3433
H	-4.6989	1.8051	-1.9968	H	-5.5816	2.0513	-0.6067
H	-2.9876	1.6277	-2.3145	H	-4.0276	2.154	-1.4012
H	-4.1744	-0.4004	-2.982	H	-5.2609	0.2726	-2.3143
H	-4.9646	-0.5238	-1.4257	H	-5.6089	-0.3606	-0.7207
H	-0.7795	-1.486	-2.0921	H	-1.7114	-0.6293	-2.6248
H	-1.8702	-0.9153	-3.3334	H	-3.1025	0.1577	-3.3333
H	-1.2328	0.2098	-2.1401	H	-2.2111	0.9483	-2.0376
H	7.5666	0.5106	-0.5056	H	6.6877	2.0734	0.2104
H	6.4996	-0.124	0.7428	H	7.3681	1.8921	-1.3989
H	6.0528	2.3337	-1.0292	H	7.5274	-0.1527	0.1027
H	6.2912	2.2693	0.7186	H	6.8619	-0.4367	-1.5045
H	5.9135	0.04	-2.2453	H	5.1655	2.9908	-1.5452
H	6.325	-1.4286	-1.3811	H	5.1542	1.4318	-2.3511
H	1.7112	1.1436	0.5649	H	3.1085	-1.641	0.9249
H	1.6012	0.1473	-0.8525	H	2.734	-0.075	1.62
H	2.5482	-0.6838	1.9495	H	1.9866	-1.1203	-1.1606
H	2.714	-2.9829	1.1813	H	0.6786	0.9615	-1.4591
H	2.1489	-2.5706	-0.4246	H	1.1764	1.5467	0.1184
H	4.7571	-1.7327	0.9118	H	2.9297	0.9668	-2.309
H	4.568	-2.8074	-0.4642	H	2.5407	2.5541	-1.6672
H	4.1273	-1.8454	-2.809	H	3.7555	3.4772	0.334
H	2.5705	-1.2861	-2.2127	H	2.9921	2.2329	1.3201
H	3.6684	-0.1443	-2.9812	H	4.7391	2.4239	1.3585
H	2.6257	2.8863	0.6949	H	6.3751	-2.5433	0.0662
H	-3.7845	-1.0136	1.7696	H	-3.6062	-1.6439	1.7822
H	-1.964	4.7765	0.2264	H	-4.0682	4.3099	2.7601
H	-1.1187	3.1531	0.0776	H	-4.9842	2.7139	2.8922
H	0.4501	-1.0041	3.4967	H	0.8703	-1.5179	2.4236
H	-4.2436	5.0517	0.1533	H	-2.5699	4.7645	1.0501
1b-19	X axis(Å)	Y axis(Å)	Z axis(Å)	1b-20	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-3.4275	-2.7895	-1.2852	C	-2.2646	-3.4793	-1.3451
C	-3.0509	-2.7719	0.1955	C	-2.0237	-3.3386	0.1588
C	-2.1838	-1.5663	0.5852	C	-1.5772	-1.9258	0.5607
C	-2.806	-0.2189	0.1032	C	-2.5494	-0.8387	0.0108
C	-3.0893	-0.2439	-1.4432	C	-2.6915	-0.9467	-1.552

C	-4.0048	-1.4551	-1.7672	C	-3.1697	-2.38	-1.9128
C	-1.9511	1.0128	0.4677	C	-2.1659	0.6041	0.4121
C	-2.5635	2.3455	-0.0132	C	-3.1818	1.6567	-0.0965
C	-3.0279	2.3239	-1.4802	C	-3.4232	1.517	-1.6108
C	-3.8277	1.0664	-1.8352	C	-3.7559	0.0797	-2.0278
C	-1.8157	-0.3504	-2.3243	C	-1.3846	-0.6588	-2.3393
O	-0.8358	-1.7391	0.0927	O	-0.2153	-1.7053	0.1294
C	-1.6252	3.5017	0.2852	C	-2.8128	3.0902	0.2582
C	6.015	0.2406	-0.9631	C	6.2119	1.2043	-1.0344
C	5.578	1.0674	0.2398	C	5.4007	2.2342	-0.2562
C	4.1159	0.9209	0.5775	C	3.9828	1.8053	0.0224
C	3.332	-0.0789	0.1085	C	3.5303	0.5405	-0.1438
C	3.8854	-1.168	-0.8296	C	4.4676	-0.6048	-0.5713
C	5.4392	-1.165	-0.8734	C	5.9638	-0.1921	-0.482
C	1.8531	-0.2278	0.4271	C	2.0855	0.11	0.0537
C	1.4894	-1.6402	0.9253	C	1.9761	-1.0536	1.0544
C	1.9523	-2.7111	-0.0674	C	2.8166	-2.2441	0.5756
C	3.45	-2.578	-0.3443	C	4.2755	-1.8306	0.3651
C	3.3514	-0.9185	-2.2602	C	4.1548	-1.0078	-2.0316
C	3.63	2.0252	1.4668	C	3.1182	2.9334	0.4897
O	2.5173	2.5326	1.4196	O	2.244	2.828	1.3404
C	0.0095	-1.7166	1.1984	C	0.54	-1.4505	1.269
C	-1.9656	-1.5718	2.0831	C	-1.4442	-1.8338	2.0653
O	-4.0896	-0.0444	0.7573	O	-3.8648	-1.0905	0.565
C	-1.927	4.4902	1.1431	C	-1.5975	3.5563	0.593
O	-2.83	-1.4314	2.9377	O	-2.3525	-1.938	2.8776
C	-0.5529	-1.6884	2.4042	C	-0.0748	-1.5292	2.4467
C	-0.2808	3.5617	-0.3633	C	-3.9222	4.0903	0.285
O	0.0714	2.7925	-1.2495	O	-5.0853	3.8084	0.0255
H	-2.5506	-3.0611	-1.8829	H	-1.3028	-3.483	-1.8697
H	-4.1651	-3.5823	-1.4583	H	-2.7193	-4.4568	-1.5455
H	-3.9741	-2.7757	0.7893	H	-2.9458	-3.6073	0.6901
H	-2.5266	-3.7072	0.43	H	-1.267	-4.0751	0.458
H	-4.9908	-1.3153	-1.3055	H	-4.1884	-2.5417	-1.5371
H	-4.1841	-1.5145	-2.8484	H	-3.2295	-2.4949	-3.0026
H	-1.8479	1.0789	1.5591	H	-2.1333	0.6875	1.5061
H	-0.9396	0.892	0.0723	H	-1.1596	0.8314	0.0467
H	-3.4752	2.4954	0.5844	H	-4.1312	1.4382	0.4129
H	-2.1816	2.4094	-2.1689	H	-4.253	2.1633	-1.9224
H	-3.6522	3.2056	-1.6753	H	-2.5458	1.8712	-2.1657
H	-4.0408	1.0734	-2.912	H	-3.8583	0.0409	-3.1199
H	-4.8054	1.118	-1.3392	H	-4.7437	-0.1823	-1.6272
H	-1.3028	-1.3092	-2.2276	H	-0.6209	-1.427	-2.2043
H	-2.0758	-0.2481	-3.3849	H	-1.5885	-0.6217	-3.4166
H	-1.0797	0.425	-2.1002	H	-0.9282	0.2966	-2.0684
H	5.6946	0.7282	-1.8909	H	5.9514	1.2473	-2.0981
H	7.1097	0.1943	-0.9972	H	7.278	1.4499	-0.9645

H	5.8172	2.119	0.0388	H	5.4129	3.1753	-0.8192
H	6.1664	0.7689	1.117	H	5.8946	2.4312	0.704
H	5.7991	-1.7638	-1.7195	H	6.5931	-0.9156	-1.0151
H	5.8437	-1.6409	0.0305	H	6.2999	-0.2088	0.564
H	1.5242	0.479	1.1926	H	1.4363	0.9251	0.3791
H	1.28	0.0176	-0.4761	H	1.6814	-0.1884	-0.9226
H	2.0247	-1.8099	1.8712	H	2.3875	-0.7128	2.0159
H	1.7501	-3.7098	0.3399	H	2.7792	-3.052	1.3173
H	1.3937	-2.6433	-1.0085	H	2.408	-2.6594	-0.3538
H	3.9842	-2.8285	0.5828	H	4.7005	-1.6062	1.3534
H	3.7447	-3.3361	-1.0813	H	4.8382	-2.6902	-0.0209
H	3.7571	-1.6547	-2.9638	H	4.8502	-1.779	-2.3827
H	2.2605	-0.9868	-2.319	H	3.1452	-1.4137	-2.1483
H	3.6259	0.0765	-2.6273	H	4.2355	-0.1539	-2.7131
H	4.3871	2.3933	2.1806	H	3.3499	3.9093	0.0303
H	-3.9758	-0.1884	1.7196	H	-3.7943	-1.1403	1.5409
H	-1.244	5.3063	1.3593	H	-1.4216	4.5964	0.8534
H	-2.8816	4.508	1.6613	H	-0.7183	2.9199	0.6263
H	-0.117	-1.6337	3.3829	H	0.2859	-1.3567	3.4424
H	0.3888	4.3623	-0.0057	H	-3.635	5.1202	0.5571
1c-1	X axis(Å)	Y axis(Å)	Z axis(Å)	1c-2	X axis(Å)	Y axis(Å)	Z axis(Å)
C	3.275	-2.0522	2.4671	C	1.66	-3.0381	1.9006
C	2.9305	-2.6849	1.1185	C	1.4451	-3.1216	0.3892
C	2.1491	-1.739	0.1961	C	1.4938	-1.7469	-0.2947
C	2.866	-0.3634	0.0403	C	2.7935	-0.9708	0.0722
C	3.1049	0.3063	1.4448	C	2.9387	-0.8167	1.6317
C	3.9239	-0.6705	2.332	C	2.9027	-2.2272	2.2819
C	2.1328	0.6124	-0.9069	C	2.9164	0.4051	-0.6209
C	2.8563	1.9703	-1.0436	C	4.234	1.1272	-0.2568
C	3.2222	2.6031	0.3089	C	4.4788	1.2046	1.2595
C	3.9203	1.6134	1.2465	C	4.3082	-0.1534	1.9474
C	1.8043	0.6813	2.2058	C	1.8353	0.0527	2.2921
O	0.7968	-1.5868	0.6791	O	0.2996	-1.0026	0.031
C	2.0965	2.9426	-1.9268	C	4.3508	2.4852	-0.9218
C	-6.1402	0.7202	0.2225	C	-6.249	1.7582	0.8461
C	-5.1713	1.3309	1.2267	C	-6.4759	0.4243	0.1469
C	-3.7195	1.0151	0.9514	C	-5.2171	-0.3905	-0.0434
C	-3.308	0.0315	0.1132	C	-3.9656	0.1156	0.0857
C	-4.3202	-0.8458	-0.6494	C	-3.7355	1.6052	0.4236
C	-5.757	-0.721	-0.0717	C	-5.0287	2.4525	0.2655
C	-1.8507	-0.3024	-0.1736	C	-2.6771	-0.6844	-0.0673
C	-1.5292	-1.8069	-0.0414	C	-1.6896	-0.032	-1.0518
C	-2.4756	-2.6361	-0.9176	C	-1.3905	1.4168	-0.6484
C	-3.9314	-2.3457	-0.557	C	-2.6811	2.2241	-0.5331
C	-4.3428	-0.4031	-2.1321	C	-3.2473	1.7212	1.8874
C	-2.7796	1.9284	1.6797	C	-5.4986	-1.8254	-0.3642
O	-3.1585	2.6733	2.5787	O	-6.6286	-2.2413	-0.5981

C	-0.0619	-2.0336	-0.3227	C	-0.4114	-0.8231	-1.1505
C	1.9197	-2.4025	-1.1424	C	1.3515	-1.9171	-1.7911
O	4.1751	-0.5918	-0.5425	O	3.93	-1.7571	-0.3746
C	2.6108	3.4587	-3.0557	C	5.3193	2.7874	-1.8027
O	2.7845	-2.7036	-1.9537	O	2.1738	-2.4285	-2.5388
C	0.4986	-2.5813	-1.3992	C	0.1036	-1.3391	-2.2638
C	0.7159	3.3748	-1.5648	C	3.3698	3.5631	-0.6137
O	0.0971	2.9315	-0.6047	O	2.4172	3.4132	0.1412
H	3.9568	-2.7167	3.0114	H	1.7553	-4.0525	2.3062
H	2.3697	-1.985	3.0805	H	0.7698	-2.6084	2.3731
H	3.8615	-3.0008	0.6303	H	2.2081	-3.7833	-0.0405
H	2.3514	-3.5987	1.3035	H	0.4766	-3.6041	0.2047
H	4.9315	-0.7998	1.916	H	3.7925	-2.7986	1.9869
H	4.0642	-0.2435	3.3333	H	2.9499	-2.1401	3.375
H	2.0713	0.176	-1.9127	H	2.9099	0.2725	-1.7108
H	1.1033	0.7484	-0.5685	H	2.0462	1.0233	-0.3821
H	3.8134	1.7564	-1.5427	H	5.0463	0.5027	-0.658
H	3.8884	3.4599	0.144	H	5.4971	1.5687	1.4482
H	2.3339	3.0102	0.8046	H	3.8109	1.9345	1.7295
H	4.0958	2.1023	2.2134	H	4.4255	-0.0211	3.0307
H	4.9154	1.3858	0.8433	H	5.1307	-0.8109	1.6376
H	1.2443	-0.1866	2.5589	H	0.8502	-0.4175	2.28
H	2.0411	1.2717	3.0994	H	2.0717	0.2329	3.348
H	1.1179	1.2784	1.6003	H	1.7278	1.0311	1.8171
H	-7.1589	0.7612	0.6252	H	-7.1346	2.3921	0.7218
H	-6.1474	1.3118	-0.7	H	-6.1265	1.6022	1.924
H	-5.4177	0.9669	2.2325	H	-6.9224	0.6045	-0.8395
H	-5.334	2.4158	1.2297	H	-7.2119	-0.1383	0.7344
H	-5.8395	-1.2929	0.8629	H	-5.2239	2.6513	-0.7974
H	-6.4866	-1.1605	-0.7635	H	-4.9038	3.4339	0.7402
H	-1.6088	0.0441	-1.1871	H	-2.2177	-0.7862	0.9245
H	-1.1738	0.2363	0.4928	H	-2.855	-1.7057	-0.41
H	-1.7055	-2.1059	1.0023	H	-2.1658	-0.0145	-2.0431
H	-2.3094	-2.4313	-1.9815	H	-0.8406	1.4544	0.2999
H	-2.2799	-3.7058	-0.7709	H	-0.7412	1.8876	-1.3977
H	-4.5846	-2.9432	-1.2061	H	-2.4353	3.2446	-0.212
H	-4.1022	-2.7087	0.466	H	-3.1081	2.3153	-1.5416
H	-3.3741	-0.5365	-2.624	H	-2.2872	1.2218	2.0508
H	-5.0768	-0.9831	-2.7034	H	-3.1148	2.7707	2.1746
H	-4.6047	0.6555	-2.2359	H	-3.9603	1.2736	2.5885
H	-1.7252	1.9138	1.3737	H	-4.6439	-2.5125	-0.3836
H	4.0722	-1.1578	-1.3356	H	3.7946	-1.9951	-1.3158
H	2.0671	4.1556	-3.6865	H	5.4017	3.7606	-2.2774
H	3.6124	3.194	-3.3845	H	6.0728	2.0537	-2.0772
H	0.0706	-2.9848	-2.2963	H	-0.2445	-1.3173	-3.2784
H	0.261	4.1275	-2.2312	H	3.5454	4.5285	-1.1182
1c-3	X axis(Å)	Y axis(Å)	Z axis(Å)	1c-4	X axis(Å)	Y axis(Å)	Z axis(Å)

C	1.7676	-3.0382	1.9057	C	3.0813	-2.1824	2.49
C	1.4972	-3.1303	0.4038	C	2.7382	-2.7796	1.125
C	1.4918	-1.7568	-0.2843	C	2.0417	-1.7791	0.1921
C	2.7884	-0.9534	0.0313	C	2.8435	-0.4477	0.0726
C	2.9895	-0.792	1.5839	C	3.0826	0.1921	1.4909
C	3.0071	-2.2011	2.2379	C	3.8159	-0.8414	2.389
C	2.8566	0.4228	-0.6687	C	2.1965	0.5803	-0.8823
C	4.1718	1.1729	-0.3563	C	3.0044	1.8931	-0.9833
C	4.4726	1.2593	1.1494	C	3.3709	2.4887	0.3859
C	4.3562	-0.1001	1.8459	C	3.981	1.449	1.3306
C	1.8944	0.0566	2.284	C	1.786	0.6373	2.22
O	0.2963	-1.0359	0.0858	O	0.6876	-1.5506	0.6383
C	4.2347	2.5313	-1.0276	C	2.3287	2.918	-1.8751
C	-6.0213	2.0077	-0.1306	C	-6.0382	0.0129	0.8968
C	-6.4066	0.5378	-0.0164	C	-5.1901	1.1861	1.3743
C	-5.2075	-0.3792	-0.0044	C	-3.7409	1.0522	0.9752
C	-3.9542	0.0461	0.2867	C	-3.3229	0.2286	-0.0162
C	-3.675	1.4915	0.7538	C	-4.3178	-0.5258	-0.9213
C	-4.9655	2.3443	0.9078	C	-5.8049	-0.2195	-0.5861
C	-2.6864	-0.7763	0.106	C	-1.869	-0.1207	-0.292
C	-1.7499	-0.1051	-0.9206	C	-1.6265	-1.6411	-0.1419
C	-1.4602	1.3621	-0.5612	C	-2.6017	-2.4503	-1.0131
C	-2.7452	2.1537	-0.2959	C	-4.0587	-2.0462	-0.7565
C	-2.9934	1.502	2.1447	C	-4.124	-0.1152	-2.4022
C	-5.5288	-1.7899	-0.3839	C	-2.8091	1.8856	1.8005
O	-6.6433	-2.1405	-0.7567	O	-3.1811	2.4984	2.7963
C	-0.4622	-0.8723	-1.0681	C	-0.1674	-1.944	-0.3886
C	1.2956	-1.9339	-1.7738	C	1.8118	-2.4152	-1.1596
O	3.9229	-1.7176	-0.4569	O	4.1524	-0.7483	-0.4769
C	5.1622	2.8514	-1.9455	C	2.9014	3.4098	-2.9866
O	2.0986	-2.4311	-2.5513	O	2.68	-2.7554	-1.9516
C	0.0195	-1.3814	-2.1993	C	0.3904	-2.5143	-1.4546
C	3.2438	3.5893	-0.684	C	0.9694	3.4328	-1.5416
O	2.3245	3.4217	0.1074	O	0.303	3.0245	-0.5981
H	1.899	-4.0493	2.3094	H	3.706	-2.8923	3.0454
H	0.8874	-2.6254	2.4109	H	2.1646	-2.0666	3.0785
H	2.2567	-3.7775	-0.0534	H	3.6622	-3.1462	0.6593
H	0.5325	-3.6329	0.2572	H	2.1003	-3.6587	1.283
H	3.8965	-2.7551	1.9104	H	4.8253	-1.0274	1.9994
H	3.0939	-2.11	3.3282	H	3.9535	-0.4337	3.3986
H	2.8117	0.2869	-1.7573	H	2.1366	0.1586	-1.8944
H	1.9836	1.0236	-0.3984	H	1.168	0.7751	-0.5704
H	4.9811	0.5644	-0.7871	H	3.9601	1.6266	-1.4592
H	5.4896	1.6445	1.2984	H	4.0926	3.3045	0.2487
H	3.8082	1.9766	1.6432	H	2.4961	2.9448	0.8624
H	4.5119	0.0375	2.9237	H	4.1583	1.9166	2.3077
H	5.1796	-0.7415	1.5062	H	4.9715	1.1654	0.9524

H	0.9194	-0.4336	2.3107	H	1.1647	-0.1987	2.5468
H	2.1672	0.2448	3.3297	H	2.0325	1.2028	3.1271
H	1.7488	1.0313	1.8113	H	1.1543	1.2813	1.6031
H	-5.6497	2.2254	-1.139	H	-5.7931	-0.8905	1.4682
H	-6.9086	2.6327	0.0223	H	-7.0974	0.227	1.0795
H	-7.0654	0.3057	-0.8617	H	-5.2903	1.2398	2.4648
H	-6.9863	0.373	0.9003	H	-5.5846	2.1248	0.966
H	-4.7261	3.4139	0.8557	H	-6.4526	-1.0324	-0.9378
H	-5.4081	2.1827	1.9007	H	-6.1356	0.6813	-1.1218
H	-2.191	-0.8991	1.0763	H	-1.592	0.2201	-1.297
H	-2.8857	-1.7927	-0.2409	H	-1.1852	0.3958	0.385
H	-2.2684	-0.1078	-1.891	H	-1.8357	-1.9156	0.9029
H	-0.8036	1.4244	0.3152	H	-2.3722	-2.324	-2.0774
H	-0.9112	1.8422	-1.3818	H	-2.488	-3.5207	-0.7993
H	-2.472	3.1667	0.0265	H	-4.7043	-2.6149	-1.4379
H	-3.2796	2.2682	-1.2481	H	-4.3299	-2.3622	0.2596
H	-2.015	1.0135	2.1533	H	-3.1307	-0.3536	-2.7923
H	-2.8377	2.5301	2.4928	H	-4.8508	-0.6259	-3.0451
H	-3.6144	0.9894	2.8892	H	-4.2668	0.9645	-2.5316
H	-4.7196	-2.5262	-0.298	H	-1.7652	1.9501	1.4644
H	3.7567	-1.9611	-1.3917	H	4.0379	-1.2986	-1.2795
H	5.2061	3.8249	-2.4247	H	2.4178	4.1443	-3.6236
H	5.9198	2.1329	-2.2474	H	3.8922	3.0853	-3.2941
H	-0.3675	-1.3686	-3.1999	H	-0.0347	-2.8884	-2.3657
H	3.3795	4.5568	-1.1968	H	0.5771	4.2154	-2.2134
1c-5	X axis(Å)	Y axis(Å)	Z axis(Å)	1c-6	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-2.8627	-3.3756	-0.8834	C	1.4748	-3.1888	1.6883
C	-2.2514	-3.0551	0.4806	C	1.3161	-3.0666	0.173
C	-1.8466	-1.5791	0.6187	C	1.4151	-1.6157	-0.325
C	-3.0274	-0.6271	0.2648	C	2.7062	-0.9175	0.1933
C	-3.5756	-0.9172	-1.1813	C	2.7937	-0.9784	1.7627
C	-3.9884	-2.4121	-1.2727	C	2.715	-2.4617	2.2168
C	-2.6912	0.8728	0.4255	C	2.874	0.5393	-0.2975
C	-3.9011	1.7796	0.1018	C	4.2047	1.1713	0.1791
C	-4.5446	1.4607	-1.2582	C	4.3709	1.0448	1.7073
C	-4.8299	-0.0344	-1.432	C	4.1608	-0.388	2.2079
C	-2.5611	-0.6216	-2.3177	C	1.6772	-0.187	2.4959
O	-0.6692	-1.3235	-0.1782	O	0.219	-0.8926	0.0475
C	-3.5739	3.2536	0.2452	C	4.3413	2.5915	-0.3497
C	6.7923	0.2773	-0.8158	C	-6.4048	1.6812	0.9176
C	6.047	1.5682	-0.5027	C	-6.5813	0.4551	0.0315
C	4.7054	1.3603	0.1634	C	-5.3044	-0.3173	-0.2095
C	4.0731	0.1617	0.2234	C	-4.0669	0.1735	0.0496
C	4.6722	-1.0935	-0.4467	C	-3.8726	1.6027	0.6015
C	5.84	-0.7459	-1.4111	C	-5.1671	2.4562	0.4983
C	2.7535	-0.1016	0.9385	C	-2.7627	-0.5901	-0.1492
C	1.7098	-0.7767	0.0269	C	-1.7372	0.1988	-0.9838

C	2.2787	-2.0743	-0.5631	C	-1.476	1.5787	-0.3691
C	3.5931	-1.8152	-1.2975	C	-2.7809	2.3547	-0.2069
C	5.2057	-2.0502	0.6459	C	-3.457	1.517	2.0896
C	4.1563	2.6183	0.7628	C	-5.5531	-1.6944	-0.742
O	4.7499	3.6906	0.7118	O	-6.6681	-2.0827	-1.0745
C	0.3827	-1.0541	0.6964	C	-0.448	-0.5668	-1.129
C	-1.3286	-1.324	2.015	C	1.3296	-1.5984	-1.8359
O	-4.1187	-0.9024	1.1835	O	3.8462	-1.6599	-0.3078
C	-4.1801	4.0547	1.1373	C	4.1968	3.7331	0.3437
O	-1.9943	-1.3188	3.0415	O	2.1604	-2.0451	-2.6135
C	0.0964	-1.0351	1.9968	C	0.1092	-0.9423	-2.2776
C	-2.5406	3.884	-0.6231	C	4.7165	2.7451	-1.7876
O	-1.8853	3.2625	-1.4499	O	4.8572	1.7931	-2.545
H	-3.2559	-4.3992	-0.869	H	1.539	-4.2498	1.9581
H	-2.0774	-3.3664	-1.6473	H	0.5742	-2.8078	2.1822
H	-2.9732	-3.3222	1.2632	H	2.0837	-3.6833	-0.3123
H	-1.3792	-3.7048	0.6287	H	0.3474	-3.4996	-0.1079
H	-4.8493	-2.6038	-0.6191	H	3.6063	-3.0059	1.8783
H	-4.3246	-2.6492	-2.2902	H	2.724	-2.5221	3.3126
H	-2.4011	1.078	1.4644	H	2.8662	0.55	-1.3941
H	-1.825	1.1301	-0.191	H	2.0272	1.1591	0.0197
H	-4.6683	1.5474	0.8557	H	5.0318	0.5928	-0.2571
H	-5.4889	2.0122	-1.3552	H	5.3771	1.375	1.9956
H	-3.913	1.8064	-2.0835	H	3.6711	1.7048	2.2315
H	-5.2201	-0.2072	-2.4433	H	4.2392	-0.398	3.3027
H	-5.6398	-0.3199	-0.7483	H	4.9858	-1.014	1.8444
H	-1.7156	-1.3119	-2.3311	H	0.6868	-0.6319	2.3813
H	-3.0458	-0.7167	-3.2971	H	1.8744	-0.1592	3.5746
H	-2.1478	0.3887	-2.2625	H	1.6006	0.8497	2.1584
H	7.6059	0.4859	-1.5202	H	-7.2915	2.3209	0.8385
H	7.2612	-0.1165	0.0932	H	-6.3318	1.3789	1.9685
H	5.8856	2.1259	-1.4343	H	-6.9843	0.7669	-0.9407
H	6.6989	2.1826	0.1303	H	-7.3361	-0.188	0.5005
H	5.4465	-0.338	-2.3524	H	-5.3139	2.7986	-0.5354
H	6.3963	-1.6522	-1.6816	H	-5.0773	3.3634	1.1091
H	2.9613	-0.7351	1.8104	H	-2.3499	-0.826	0.8402
H	2.308	0.8084	1.3441	H	-2.9112	-1.5551	-0.6381
H	1.5071	-0.0825	-0.8021	H	-2.166	0.3518	-1.985
H	2.4287	-2.8214	0.226	H	-0.973	1.4871	0.6012
H	1.5643	-2.5146	-1.2706	H	-0.7974	2.1527	-1.0131
H	3.9861	-2.7696	-1.671	H	-2.5638	3.3219	0.2644
H	3.3621	-1.2113	-2.1862	H	-3.16	2.5828	-1.2128
H	4.4131	-2.4219	1.3026	H	-2.4995	1.0057	2.2295
H	5.6861	-2.9278	0.1981	H	-3.3522	2.5172	2.5256
H	5.9452	-1.5592	1.2879	H	-4.197	0.9719	2.6857
H	3.1806	2.5546	1.2587	H	-4.6885	-2.3638	-0.8276
H	-3.7717	-0.8661	2.0996	H	3.8043	-1.6759	-1.2876

H	-3.9445	5.11	1.2372	H	4.3283	4.7119	-0.1094
H	-4.946	3.6681	1.8046	H	3.9378	3.7377	1.3971
H	0.7042	-0.8398	2.8589	H	-0.2013	-0.7997	-3.2948
H	-2.3864	4.9666	-0.4755	H	4.8564	3.7804	-2.1419
1c-7	X axis(Å)	Y axis(Å)	Z axis(Å)	1c-8	X axis(Å)	Y axis(Å)	Z axis(Å)
C	2.6305	-2.5483	2.4786	C	1.3285	-3.0982	1.7841
C	2.3774	-2.9333	1.0212	C	1.1311	-3.0862	0.268
C	1.8487	-1.7644	0.1747	C	1.2741	-1.6823	-0.3409
C	2.7522	-0.5033	0.307	C	2.6101	-1.007	0.0859
C	2.9167	-0.0777	1.8123	C	2.7389	-0.9468	1.6529
C	3.4777	-1.28	2.6198	C	2.6119	-2.386	2.2237
C	2.2799	0.7004	-0.5415	C	2.8233	0.3994	-0.5202
C	3.2438	1.9079	-0.4397	C	4.1938	1.0088	-0.1287
C	3.5089	2.2931	1.0304	C	4.4044	0.994	1.3961
C	3.9319	1.0966	1.8887	C	4.1387	-0.381	2.0178
C	1.6013	0.391	2.4909	C	1.6785	-0.0528	2.3505
O	0.4746	-1.4873	0.5305	O	0.1202	-0.883	0.0068
C	2.7541	3.0578	-1.3081	C	4.4342	2.4056	-0.6812
C	-6.3571	1.0304	0.0785	C	-6.4223	1.8872	0.8964
C	-5.4887	1.3015	1.3002	C	-6.6532	0.594	0.1258
C	-4.0243	0.9823	1.0998	C	-5.3998	-0.2224	-0.0925
C	-3.5487	0.2546	0.0586	C	-4.1451	0.2634	0.0777
C	-4.4998	-0.3518	-0.9947	C	-3.9054	1.7305	0.4964
C	-5.9856	-0.3055	-0.5427	C	-5.1881	2.5983	0.3675
C	-2.0773	-0.0409	-0.2042	C	-2.8632	-0.541	-0.1028
C	-1.7959	-1.5455	-0.3878	C	-1.8575	0.1526	-1.04
C	-2.6752	-2.1126	-1.512	C	-1.5488	1.5744	-0.5563
C	-4.1543	-1.8464	-1.235	C	-2.8327	2.388	-0.4134
C	-4.3635	0.4388	-2.3177	C	-3.4346	1.764	1.97
C	-3.153	1.5694	2.1679	C	-5.6921	-1.6354	-0.492
O	-3.6035	2.215	3.1087	O	-6.8233	-2.0251	-0.7621
C	-0.3146	-1.7766	-0.5821	C	-0.5882	-0.6487	-1.167
C	1.7094	-2.2114	-1.2627	C	1.1452	-1.7678	-1.8461
O	4.0776	-0.852	-0.1656	O	3.7004	-1.836	-0.3874
C	2.1813	4.2006	-0.8946	C	3.5027	3.3026	-1.0462
O	2.6214	-2.5061	-2.0216	O	1.9576	-2.2637	-2.6139
C	0.3127	-2.224	-1.6681	C	-0.0826	-1.1334	-2.2985
C	2.965	2.9312	-2.7816	C	5.8559	2.8241	-0.8718
O	3.4445	1.9322	-3.3029	O	6.8077	2.1059	-0.5934
H	3.1387	-3.3772	2.9858	H	1.3571	-4.137	2.1341
H	1.6729	-2.4226	2.9955	H	0.4588	-2.6418	2.2695
H	3.3123	-3.3153	0.5911	H	1.8587	-3.7696	-0.1884
H	1.6646	-3.7678	1.0042	H	0.138	-3.4979	0.0468
H	4.5004	-1.508	2.2924	H	3.4704	-2.9925	1.9071
H	3.5536	-1.0184	3.6829	H	2.6488	-2.362	3.3203
H	2.2261	0.3959	-1.5936	H	2.7957	0.3388	-1.6159
H	1.265	1.0039	-0.2594	H	2.002	1.0582	-0.2209

H	4.2183	1.6007	-0.8457	H	4.9557	0.3542	-0.5752
H	4.2981	3.0545	1.0735	H	5.4344	1.2858	1.6368
H	2.6201	2.7489	1.4801	H	3.763	1.746	1.8719
H	4.0499	1.4281	2.9284	H	4.2448	-0.3052	3.1077
H	4.9274	0.7651	1.567	H	4.9261	-1.072	1.69
H	0.88	-0.4156	2.636	H	0.6662	-0.4571	2.2908
H	1.8098	0.7953	3.4891	H	1.9038	0.0427	3.4198
H	1.09	1.1765	1.9287	H	1.6425	0.96	1.9411
H	-7.4128	1.0254	0.3735	H	-7.3001	2.5358	0.7949
H	-6.2422	1.8396	-0.6517	H	-6.3147	1.6739	1.966
H	-5.8584	0.7048	2.1441	H	-7.0861	0.83	-0.855
H	-5.6178	2.3564	1.5721	H	-7.4015	0.0089	0.6745
H	-6.1814	-1.0923	0.1988	H	-5.3682	2.8544	-0.6857
H	-6.6505	-0.5143	-1.3903	H	-5.0596	3.5521	0.8946
H	-1.7667	0.5081	-1.1031	H	-3.0474	-1.5407	-0.5016
H	-1.4316	0.3348	0.5911	H	-2.4162	-0.7004	0.8871
H	-2.0771	-2.0631	0.541	H	-2.3223	0.2285	-2.0339
H	-2.398	-1.6804	-2.4808	H	-1.0104	1.5555	0.3991
H	-2.5217	-3.1958	-1.5972	H	-0.8855	2.0772	-1.2718
H	-4.749	-2.2393	-2.0698	H	-2.5809	3.3873	-0.0355
H	-4.439	-2.4362	-0.3526	H	-3.2463	2.5372	-1.4206
H	-3.3595	0.3691	-2.7476	H	-2.4816	1.2467	2.1184
H	-5.0616	0.061	-3.0737	H	-3.2955	2.7955	2.3138
H	-4.5736	1.5045	-2.176	H	-4.1607	1.2875	2.6379
H	-2.0728	1.3998	2.0869	H	-4.8446	-2.3303	-0.5364
H	4.0087	-1.1657	-1.0923	H	3.5962	-1.9787	-1.3513
H	1.8741	4.9825	-1.5837	H	3.7604	4.28	-1.4449
H	1.9932	4.4041	0.1543	H	2.4413	3.101	-0.9523
H	-0.0519	-2.5116	-2.6354	H	-0.4307	-1.0723	-3.3117
H	2.653	3.7971	-3.3899	H	6.0087	3.8358	-1.2843
1c-9	X axis(Å)	Y axis(Å)	Z axis(Å)	1c-10	X axis(Å)	Y axis(Å)	Z axis(Å)
C	1.643	-2.8836	2.0867	C	-2.753	-3.5458	-0.5512
C	1.3883	-3.0491	0.5884	C	-2.1806	-2.9984	0.756
C	1.4329	-1.7156	-0.1733	C	-1.7917	-1.5137	0.666
C	2.7487	-0.9343	0.1171	C	-2.9625	-0.645	0.1202
C	2.9371	-0.6961	1.6613	C	-3.4677	-1.1791	-1.27
C	2.9039	-2.0678	2.3898	C	-3.8733	-2.671	-1.1219
C	2.8658	0.4005	-0.6533	C	-2.636	0.8637	0.0293
C	4.2011	1.1245	-0.3658	C	-3.8491	1.7012	-0.4444
C	4.4889	1.2826	1.1367	C	-4.4346	1.1471	-1.7597
C	4.3216	-0.0328	1.9039	C	-4.7171	-0.3575	-1.6941
C	1.8608	0.2213	2.3008	C	-2.4227	-1.0723	-2.4126
O	0.2554	-0.9404	0.1383	O	-0.59	-1.3719	-0.1264
C	4.3142	2.441	-1.1103	C	-3.4921	3.1797	-0.4921
C	-6.3826	1.646	0.8784	C	6.8556	0.2692	-0.8009
C	-6.5649	0.3267	0.136	C	6.0711	1.5732	-0.7389
C	-5.2806	-0.434	-0.0579	C	4.7217	1.4468	-0.0688

C	-4.0497	0.0872	0.1497	C	4.1108	0.2607	0.1753
C	-3.853	1.5696	0.5122	C	4.7549	-1.0747	-0.2559
C	-5.165	2.3881	0.3442	C	5.9455	-0.868	-1.2331
C	-2.7544	-0.7052	0.0498	C	2.7706	0.0928	0.8811
C	-1.7771	-0.0599	-0.9444	C	1.774	-0.7553	0.0657
C	-1.4979	1.4005	-0.5543	C	2.387	-2.1212	-0.2699
C	-2.7961	2.2014	-0.435	C	3.7191	-1.9596	-0.9996
C	-3.3856	1.6885	1.9813	C	5.2729	-1.8165	0.9992
C	-5.4935	-1.8406	-0.5087	C	4.1407	2.7725	0.3149
O	-4.8513	-2.3687	-1.4075	O	4.6562	3.8382	-0.006
C	-0.4929	-0.8416	-1.0302	C	0.4272	-0.9432	0.726
C	1.2532	-1.97	-1.6537	C	-1.3219	-1.0385	2.0219
O	3.8666	-1.7556	-0.3148	O	-4.079	-0.7755	1.0363
C	5.2553	2.677	-2.0398	C	-3.2661	3.9253	-1.5866
O	2.0612	-2.5184	-2.3912	O	-2.0102	-0.9084	3.0238
C	-0.0093	-1.4251	-2.1243	C	0.0965	-0.7184	1.9962
C	3.3598	3.5502	-0.8312	C	-3.4206	3.9016	0.814
O	2.4384	3.4629	-0.0295	O	-3.5773	3.3439	1.893
H	1.7381	-3.8747	2.5463	H	-3.1408	-4.5568	-0.3776
H	0.7701	-2.4172	2.5567	H	-1.9476	-3.6556	-1.2856
H	2.1334	-3.7424	0.1776	H	-2.9215	-3.1444	1.5527
H	0.4107	-3.5304	0.4561	H	-1.3074	-3.6044	1.0301
H	3.7794	-2.6653	2.1038	H	-4.7498	-2.7589	-0.4668
H	2.9812	-1.921	3.4746	H	-4.1825	-3.0765	-2.0938
H	2.8269	0.2087	-1.7337	H	-2.3396	1.2253	1.0213
H	2.0097	1.042	-0.4248	H	-1.7766	1.0389	-0.6284
H	4.995	0.4684	-0.7532	H	-4.6486	1.5955	0.3031
H	5.5163	1.6431	1.277	H	-5.3698	1.6714	-1.9945
H	3.8431	2.0458	1.5837	H	-3.7576	1.3396	-2.5991
H	4.4688	0.1583	2.9747	H	-5.0775	-0.6953	-2.6743
H	5.1286	-0.7165	1.6106	H	-5.5459	-0.5314	-0.996
H	0.8702	-0.236	2.3373	H	-1.5731	-1.7456	-2.2837
H	2.1254	0.4542	3.3395	H	-2.8791	-1.3391	-3.3737
H	1.753	1.1746	1.7771	H	-2.0151	-0.0641	-2.5218
H	-7.2804	2.2626	0.7549	H	7.6855	0.3744	-1.5092
H	-6.2763	1.4606	1.9535	H	7.3046	0.053	0.1753
H	-7.001	0.5251	-0.8515	H	5.9161	1.9504	-1.758
H	-7.2905	-0.2825	0.6884	H	6.692	2.3102	-0.2146
H	-5.3411	2.6093	-0.7176	H	5.5734	-0.6413	-2.2418
H	-5.0771	3.36	0.8458	H	6.5302	-1.7919	-1.3255
H	-2.3025	-0.755	1.0491	H	2.9563	-0.3718	1.8578
H	-2.9165	-1.7495	-0.2295	H	2.2914	1.0492	1.0989
H	-2.2525	-0.0591	-1.9361	H	1.5912	-0.22	-0.8779
H	-0.9457	1.4524	0.3921	H	2.5256	-2.7148	0.6421
H	-0.8561	1.8721	-1.3095	H	1.7055	-2.6962	-0.91
H	-2.558	3.221	-0.1056	H	4.1432	-2.9539	-1.1906
H	-3.2191	2.2971	-1.4448	H	3.5055	-1.5243	-1.9858

H	-2.4112	1.2204	2.1523	H	4.4678	-2.0857	1.69
H	-3.2894	2.7394	2.2778	H	5.7809	-2.7477	0.7228
H	-4.0931	1.2133	2.6696	H	5.9853	-1.206	1.5648
H	-6.3175	-2.3689	-1.00E-04	H	3.2166	2.7643	0.9052
H	3.6995	-2.0479	-1.2356	H	-3.7895	-0.4846	1.9272
H	5.3347	3.6201	-2.572	H	-3.0302	4.9846	-1.533
H	5.9874	1.9163	-2.298	H	-3.3041	3.5064	-2.5865
H	-0.3952	-1.4742	-3.1241	H	0.6707	-0.3763	2.8354
H	3.5264	4.4794	-1.4022	H	-3.2078	4.9826	0.7569
1c-11	X axis(Å)	Y axis(Å)	Z axis(Å)	1c-12	X axis(Å)	Y axis(Å)	Z axis(Å)
C	2.3436	-2.8025	2.3604	C	-2.7479	-3.3475	-1.0651
C	2.0544	-3.1593	0.9021	C	-2.1787	-3.0869	0.3296
C	1.6325	-1.9431	0.0629	C	-1.8013	-1.614	0.5522
C	2.6534	-0.7749	0.1941	C	-2.9868	-0.6624	0.2132
C	2.8559	-0.3661	1.7	C	-3.4913	-0.8879	-1.26
C	3.3033	-1.617	2.505	C	-3.8779	-2.3821	-1.4368
C	2.2948	0.4695	-0.6511	C	-2.6782	0.8321	0.457
C	3.3695	1.5819	-0.5483	C	-3.8928	1.7369	0.145
C	3.6744	1.9413	0.9171	C	-4.4953	1.4766	-1.246
C	3.9727	0.7107	1.7798	C	-4.7523	-0.0119	-1.5011
C	1.591	0.2227	2.3809	C	-2.4514	-0.5213	-2.3519
O	0.2914	-1.543	0.4257	O	-0.6067	-1.3016	-0.1976
C	3.0424	2.8381	-1.3413	C	-3.5914	3.2064	0.3688
C	-6.3721	1.3973	0.1022	C	6.0806	0.5121	-1.6787
C	-5.4779	1.5866	1.3206	C	5.8504	1.6346	-0.6746
C	-4.0395	1.1746	1.1006	C	4.6411	1.3942	0.1973
C	-3.622	0.4369	0.0415	C	4.0951	0.167	0.3794
C	-4.6208	-0.0869	-1.0119	C	4.7395	-1.1046	-0.2142
C	-6.0965	0.0508	-0.5454	C	6.074	-0.826	-0.9614
C	-2.1758	0.0502	-0.2414	C	2.7752	-0.1119	1.0832
C	-1.9952	-1.4665	-0.4522	C	1.7588	-0.738	0.102
C	-2.9225	-1.9568	-1.5741	C	2.3405	-1.9882	-0.5822
C	-4.3778	-1.5971	-1.2778	C	3.7185	-1.7258	-1.2017
C	-4.4433	0.7138	-2.3238	C	5.0859	-2.1253	0.898
C	-3.1235	1.6813	2.1724	C	4.0832	2.6477	0.795
O	-3.524	2.3358	3.1294	O	4.6004	3.7478	0.6316
C	-0.5346	-1.7926	-0.6696	C	0.4173	-1.0645	0.7185
C	1.4452	-2.3618	-1.3773	C	-1.3255	-1.4224	1.9734
O	3.9375	-1.2479	-0.2824	O	-4.0979	-0.9987	1.0868
C	1.8235	3.2708	-1.7053	C	-4.2324	3.9543	1.2826
O	2.3296	-2.6873	-2.1567	O	-2.019	-1.4768	2.9799
C	0.0444	-2.2892	-1.7611	C	0.0955	-1.1157	2.0097
C	4.1958	3.6734	-1.794	C	-2.5456	3.8927	-0.4401
O	5.3621	3.3922	-1.5489	O	-1.8609	3.3214	-1.2791
H	2.774	-3.6758	2.865	H	-3.125	-4.3761	-1.1124
H	1.4018	-2.5904	2.8784	H	-1.9426	-3.2886	-1.8055
H	2.9496	-3.6231	0.4679	H	-2.9171	-3.4033	1.0776

H	1.2688	-3.9255	0.884	H	-1.3007	-3.7306	0.4693
H	4.301	-1.9372	2.1773	H	-4.7528	-2.6187	-0.8173
H	3.4024	-1.366	3.5688	H	-4.183	-2.5729	-2.4736
H	2.2179	0.189	-1.7096	H	-2.4194	0.9895	1.5124
H	1.3111	0.8464	-0.3536	H	-1.7998	1.1319	-0.1217
H	4.2859	1.159	-0.9837	H	-4.6761	1.4574	0.8655
H	4.5402	2.6135	0.9671	H	-5.4453	2.0185	-1.341
H	2.8365	2.5022	1.3493	H	-3.8479	1.872	-2.036
H	4.1165	1.0315	2.8196	H	-5.1126	-0.1398	-2.53
H	4.9344	0.2861	1.4642	H	-5.5755	-0.3427	-0.8548
H	0.795	-0.5111	2.5204	H	-1.5947	-1.1975	-2.3757
H	1.8362	0.5978	3.3821	H	-2.9079	-0.5749	-3.3479
H	1.1603	1.0592	1.8245	H	-2.0561	0.4909	-2.2357
H	-7.4234	1.4582	0.4065	H	5.308	0.5335	-2.4565
H	-6.2082	2.2099	-0.6147	H	7.0426	0.6613	-2.1824
H	-5.8798	0.9998	2.1567	H	5.7397	2.565	-1.2445
H	-5.5342	2.6424	1.6129	H	6.7324	1.7512	-0.0325
H	-6.3388	-0.7342	0.1842	H	6.2862	-1.6289	-1.6786
H	-6.7808	-0.0977	-1.3903	H	6.9118	-0.8286	-0.25
H	-1.4996	0.3704	0.5528	H	2.9559	-0.7725	1.939
H	-1.8383	0.5924	-1.1347	H	2.3258	0.787	1.5095
H	-2.2986	-1.9794	0.4723	H	1.5699	0.012	-0.6809
H	-2.6267	-1.5297	-2.5397	H	2.4075	-2.8157	0.1349
H	-2.8429	-3.0465	-1.6765	H	1.6631	-2.3307	-1.3752
H	-5.0052	-1.9368	-2.112	H	4.1074	-2.6708	-1.6023
H	-4.6927	-2.1803	-0.4012	H	3.5831	-1.0599	-2.0644
H	-3.4499	0.5846	-2.7643	H	4.2097	-2.495	1.4374
H	-5.1714	0.3954	-3.0789	H	5.5907	-3.0027	0.4761
H	-4.5809	1.7888	-2.1636	H	5.758	-1.681	1.642
H	-2.0575	1.4421	2.0791	H	3.1848	2.5501	1.4164
H	3.8286	-1.6087	-1.187	H	-3.7763	-1.0027	2.0127
H	1.6772	4.1792	-2.2836	H	-4.0151	5.0066	1.44
H	0.9184	2.7409	-1.4303	H	-5.0094	3.5251	1.9097
H	-0.3549	-2.5615	-2.719	H	0.6766	-0.9574	2.8974
H	3.9383	4.5764	-2.373	H	-2.4108	4.9685	-0.2356
1c-13	X axis(Å)	Y axis(Å)	Z axis(Å)	1c-14	X axis(Å)	Y axis(Å)	Z axis(Å)
C	1.5791	-3.2105	1.6696	C	1.5314	-3.0214	1.8506
C	1.3663	-3.0821	0.1614	C	1.3322	-3.0763	0.3358
C	1.414	-1.6259	-0.3287	C	1.4223	-1.6928	-0.326
C	2.7052	-0.9007	0.1506	C	2.7356	-0.9541	0.0682
C	2.8473	-0.9698	1.7158	C	2.8669	-0.8283	1.6314
C	2.8191	-2.4575	2.1613	C	2.7893	-2.2475	2.2585
C	2.822	0.5628	-0.3349	C	2.8994	0.4297	-0.6009
C	4.1529	1.223	0.1012	C	4.2319	1.1105	-0.2124
C	4.3736	1.0906	1.622	C	4.461	1.1598	1.3075
C	4.2144	-0.35	2.1188	C	4.2485	-0.2036	1.973
C	1.738	-0.21	2.4922	C	1.7774	0.0573	2.2934

O	0.2149	-0.9341	0.0904	O	0.2436	-0.924	-0.0041
C	4.2381	2.6495	-0.4216	C	4.3941	2.4732	-0.8581
C	-6.1306	2.069	0.0195	C	-6.3651	1.7118	0.7861
C	-6.5035	0.5973	-0.1097	C	-6.5628	0.4215	6.00E-04
C	-5.2953	-0.3056	-0.1771	C	-5.2943	-0.3689	-0.187
C	-4.0632	0.0758	0.2387	C	-4.0509	0.1359	-0.0065
C	-3.8253	1.4339	0.9338	C	-3.8346	1.5978	0.4264
C	-5.1316	2.2485	1.1491	C	-5.1296	2.4474	0.2881
C	-2.7785	-0.7045	2.00E-04	C	-2.7678	-0.665	-0.1904
C	-1.7995	0.1193	-0.8628	C	-1.7429	0.0532	-1.0871
C	-1.5453	1.5154	-0.27	C	-1.4614	1.4744	-0.5835
C	-2.8514	2.2521	0.0463	C	-2.7566	2.2736	-0.4612
C	-3.2147	1.2349	2.3433	C	-3.3859	1.6211	1.9069
C	-5.5819	-1.6428	-0.7839	C	-5.5604	-1.7929	-0.5569
O	-6.6766	-1.9391	-1.2503	O	-4.9307	-2.7482	-0.1235
C	-0.4993	-0.6149	-1.0599	C	-0.4627	-0.7348	-1.1872
C	1.2758	-1.6002	-1.8356	C	1.2948	-1.837	-1.8264
O	3.8446	-1.6127	-0.3942	O	3.859	-1.7595	-0.3792
C	4.0897	3.7828	0.2844	C	5.3783	2.7579	-1.7275
O	2.0894	-2.0221	-2.6446	O	2.1223	-2.3412	-2.5738
C	0.0262	-0.9694	-2.2299	C	0.0562	-1.2429	-2.3024
C	4.5614	2.821	-1.87	C	3.4432	3.5758	-0.5436
O	4.6996	1.8775	-2.6383	O	2.4827	3.4469	0.2047
H	1.6776	-4.2714	1.9292	H	1.5972	-4.0439	2.2413
H	0.687	-2.8544	2.1965	H	0.6467	-2.5771	2.3198
H	2.1313	-3.677	-0.3541	H	2.0841	-3.7496	-0.0957
H	0.3991	-3.5362	-0.0898	H	0.3547	-3.5324	0.133
H	3.711	-2.978	1.789	H	3.6681	-2.8358	1.9639
H	2.8666	-2.5248	3.2557	H	2.8262	-2.1789	3.3532
H	2.7769	0.5805	-1.4305	H	2.9	0.315	-1.6929
H	1.9722	1.1603	0.0152	H	2.0433	1.0666	-0.3599
H	4.9782	0.6671	-0.3668	H	5.0317	0.4697	-0.613
H	5.3809	1.4428	1.8786	H	5.4858	1.4953	1.5131
H	3.6766	1.7303	2.1742	H	3.8059	1.8992	1.7808
H	4.3303	-0.3653	3.2102	H	4.356	-0.0903	3.0594
H	5.0411	-0.9538	1.7231	H	5.0582	-0.8767	1.6629
H	0.7551	-0.6777	2.4084	H	0.781	-0.3876	2.261
H	1.9714	-0.1841	3.5637	H	2.0049	0.2133	3.3551
H	1.6253	0.8267	2.1648	H	1.7006	1.0462	1.8344
H	-5.712	2.4388	-0.9241	H	-7.2501	2.3488	0.6729
H	-7.0317	2.6599	0.22	H	-6.2748	1.4909	1.8558
H	-7.1176	0.4935	-1.0122	H	-6.9718	0.6587	-0.9899
H	-7.1251	0.2924	0.7414	H	-7.3156	-0.1852	0.5189
H	-4.9024	3.3146	1.2716	H	-5.2953	2.7148	-0.7647
H	-5.6212	1.9365	2.0823	H	-5.0241	3.3959	0.8296
H	-2.3305	-0.9717	0.9645	H	-2.34	-0.8635	0.8006
H	-2.9483	-1.657	-0.5066	H	-2.9547	-1.6439	-0.6399

H	-2.2692	0.2632	-1.8472	H	-2.1799	0.1363	-2.093
H	-0.9344	1.4458	0.6384	H	-0.9436	1.4535	0.3831
H	-0.9616	2.1171	-0.9788	H	-0.7882	1.9906	-1.28
H	-2.6069	3.2051	0.5326	H	-2.5232	3.2736	-0.0734
H	-3.3387	2.5083	-0.9038	H	-3.1544	2.4233	-1.4745
H	-2.2324	0.7547	2.3279	H	-2.4368	1.0993	2.0659
H	-3.0887	2.1986	2.8512	H	-3.2498	2.6502	2.259
H	-3.8663	0.6124	2.9682	H	-4.1229	1.1423	2.5609
H	-4.7667	-2.3773	-0.7813	H	-6.4174	-1.9338	-1.2376
H	3.7698	-1.623	-1.3721	H	3.7229	-1.9855	-1.3233
H	4.1828	4.7673	-0.1658	H	5.4934	3.7342	-2.1885
H	3.866	3.7745	1.3458	H	6.1114	2.0053	-2.0059
H	-0.3226	-0.8267	-3.2346	H	-0.2899	-1.2157	-3.3172
H	4.6644	3.8617	-2.2215	H	3.6501	4.5408	-1.0367
1c-15	X axis(Å)	Y axis(Å)	Z axis(Å)	1c-16	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-3.6878	-2.6959	-1.5329	C	1.4184	-3.1241	1.7817
C	-3.0618	-2.9067	-0.1543	C	1.1706	-3.1076	0.2731
C	-2.1596	-1.7442	0.2802	C	1.2669	-1.698	-0.3316
C	-2.8831	-0.3667	0.1523	C	2.6036	-1.0001	0.0545
C	-3.4246	-0.1442	-1.308	C	2.7832	-0.9458	1.6168
C	-4.3596	-1.3266	-1.681	C	2.7021	-2.3901	2.1828
C	-2.0104	0.8322	0.5861	C	2.7705	0.4132	-0.5499
C	-2.7423	2.1856	0.4622	C	4.1417	1.0462	-0.2004
C	-3.417	2.3932	-0.904	C	4.4028	1.0273	1.3166
C	-4.2411	1.1782	-1.3439	C	4.1837	-0.3558	1.9385
C	-2.3178	-0.0402	-2.3914	C	1.7301	-0.0756	2.3545
O	-0.9229	-1.7686	-0.4655	O	0.111	-0.9224	0.0598
C	-1.8315	3.3382	0.8427	C	4.3375	2.4502	-0.7523
C	6.2262	0.5989	-0.7443	C	-6.1741	2.2027	-0.061
C	5.1509	1.6634	-0.9359	C	-6.5802	0.7341	-0.0469
C	3.8323	1.2893	-0.3199	C	-5.3932	-0.1985	-0.0726
C	3.4927	0.0349	0.0548	C	-4.1399	0.1901	0.2661
C	4.4627	-1.1474	-0.1044	C	-3.8509	1.5986	0.8288
C	5.6619	-0.7881	-1.0277	C	-5.1328	2.4581	1.0145
C	2.1435	-0.3218	0.6536	C	-2.8803	-0.6372	0.0543
C	1.4832	-1.499	-0.0889	C	-1.9175	0.0849	-0.912
C	2.4025	-2.7226	-0.0927	C	-1.6145	1.5217	-0.4546
C	3.7462	-2.3727	-0.7377	C	-2.8936	2.313	-0.1605
C	5.0087	-1.5326	1.2905	C	-3.1944	1.5113	2.2289
C	2.9224	2.4543	-0.1138	C	-5.7266	-1.5778	-0.5463
O	2.4182	2.7283	0.9694	O	-6.8381	-1.8865	-0.962
C	0.1147	-1.8045	0.4624	C	-0.6399	-0.6931	-1.0883
C	-1.6669	-1.9785	1.6914	C	1.089	-1.7773	-1.8322
O	-4.0409	-0.3746	1.0274	O	3.6928	-1.806	-0.4596
C	-2.0662	4.1384	1.8962	C	3.378	3.3311	-1.0818
O	-2.3644	-2.0646	2.6928	O	1.8838	-2.2542	-2.6298
C	-0.2134	-1.9943	1.739	C	-0.1644	-1.1621	-2.2392

C	-0.5946	3.6179	0.0558	C	5.7442	2.8966	-0.9865
O	-0.291	3.0143	-0.9671	O	6.7179	2.1953	-0.7431
H	-4.432	-3.4811	-1.7126	H	1.478	-4.1641	2.1243
H	-2.9224	-2.8267	-2.3057	H	0.5569	-2.6869	2.2983
H	-3.8677	-3.0493	0.5771	H	1.8952	-3.7747	-0.2114
H	-2.4899	-3.8432	-0.1733	H	0.1785	-3.5368	0.0823
H	-5.2569	-1.3097	-1.0488	H	3.5608	-2.9787	1.8344
H	-4.7162	-1.2147	-2.7129	H	2.7748	-2.3714	3.2778
H	-1.0795	0.8432	0.0121	H	2.7077	0.358	-1.6444
H	-1.7228	0.7161	1.6395	H	1.9475	1.055	-0.2197
H	-3.561	2.159	1.197	H	4.9004	0.4084	-0.6756
H	-4.0782	3.2681	-0.8546	H	5.4346	1.3372	1.5249
H	-2.6796	2.6257	-1.6792	H	3.7635	1.7645	1.8177
H	-4.6271	1.3581	-2.3556	H	4.3245	-0.2838	3.0247
H	-5.1252	1.0988	-0.6985	H	4.9724	-1.0301	1.5807
H	-1.7882	-0.9799	-2.559	H	0.7242	-0.4988	2.3265
H	-2.7547	0.2393	-3.3579	H	1.9894	0.0188	3.4162
H	-1.5618	0.7119	-2.1531	H	1.6614	0.9384	1.9523
H	7.0672	0.8037	-1.4168	H	-5.7817	2.4786	-1.047
H	6.624	0.6474	0.2759	H	-7.0558	2.8292	0.1162
H	4.9963	1.8354	-2.0086	H	-7.2267	0.5652	-0.9164
H	5.5161	2.6063	-0.5109	H	-7.1784	0.5197	0.8475
H	5.3486	-0.8168	-2.0804	H	-4.8786	3.5254	1.0345
H	6.4587	-1.5357	-0.9266	H	-5.5952	2.2403	1.9875
H	2.2877	-0.5623	1.7144	H	-2.4028	-0.8285	1.0225
H	1.4469	0.5218	0.6256	H	-3.0871	-1.6265	-0.3601
H	1.3468	-1.1831	-1.1344	H	-2.42	0.1523	-1.8884
H	2.5586	-3.0965	0.9262	H	-0.9728	1.5184	0.435
H	1.9382	-3.5408	-0.6573	H	-1.0449	2.0451	-1.2335
H	4.4011	-3.2526	-0.6991	H	-2.6129	3.2993	0.2306
H	3.5607	-2.1776	-1.8031	H	-3.4095	2.4956	-1.1124
H	4.2189	-1.8731	1.9678	H	-2.2229	1.0094	2.2231
H	5.74	-2.3457	1.2147	H	-3.0315	2.513	2.6444
H	5.5043	-0.687	1.7799	H	-3.8353	0.9614	2.9286
H	2.7784	3.0896	-1.0041	H	-4.9298	-2.3303	-0.4912
H	-3.7633	-0.6767	1.9168	H	3.5592	-1.9454	-1.4204
H	-1.4049	4.9545	2.1721	H	3.6041	4.3153	-1.4831
H	-2.9406	3.9932	2.5245	H	2.3242	3.109	-0.9548
H	0.3891	-2.0203	2.6265	H	-0.5472	-1.101	-3.2397
H	0.0478	4.4252	0.4474	H	5.8643	3.913	-1.3982
1c-17	X axis(Å)	Y axis(Å)	Z axis(Å)	1c-18	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-2.4317	-3.6158	-0.6584	C	2.4383	-3.1422	1.7754
C	-1.865	-3.1148	0.6701	C	2.2	-3.1345	0.2657
C	-1.5934	-1.6016	0.6709	C	1.7562	-1.7619	-0.2648
C	-2.8467	-0.7954	0.221	C	2.7235	-0.6295	0.189
C	-3.3492	-1.2694	-1.1925	C	2.8745	-0.6048	1.7545
C	-3.6326	-2.7958	-1.1404	C	3.3495	-2.0018	2.2393

C	-2.6422	0.7371	0.2272	C	2.3382	0.774	-0.3343
C	-3.9331	1.5052	-0.1561	C	3.3641	1.8584	0.0768
C	-4.5177	1.0012	-1.488	C	3.6138	1.8472	1.5991
C	-4.669	-0.5229	-1.5303	C	3.9499	0.4513	2.1336
C	-2.3516	-1.0006	-2.3507	C	1.5705	-0.2446	2.5163
O	-0.4312	-1.315	-0.1404	O	0.391	-1.5027	0.1357
C	-3.7711	3.0173	-0.1904	C	2.96	3.2159	-0.48
C	6.956	0.5615	-0.8569	C	-6.3573	0.0111	0.488
C	6.1544	1.8374	-0.6355	C	-5.5542	0.7053	1.581
C	4.8285	1.6171	0.0568	C	-4.0674	0.67	1.3194
C	4.2422	0.4014	0.1917	C	-3.5399	0.4542	0.0895
C	4.8935	-0.8699	-0.3947	C	-4.4295	0.3338	-1.1661
C	6.0502	-0.5409	-1.379	C	-5.9411	0.5448	-0.8713
C	2.9257	0.1373	0.9126	C	-2.0665	0.208	-0.1994
C	1.9183	-0.6416	0.0429	C	-1.8582	-1.2053	-0.7887
C	2.5434	-1.9539	-0.4487	C	-2.7437	-1.4206	-2.0305
C	3.8496	-1.6925	-1.196	C	-4.2151	-1.0852	-1.755
C	5.4611	-1.7274	0.7613	C	-4.0524	1.4062	-2.2181
C	4.2413	2.884	0.5971	C	-3.2421	0.8458	2.5559
O	4.7266	3.9875	0.3718	O	-3.7374	1.0185	3.6646
C	0.5951	-0.9225	0.7187	C	-0.3865	-1.4608	-1.0212
C	-1.1167	-1.1765	2.0407	C	1.6275	-1.8255	-1.7697
O	-3.9177	-1.0784	1.1558	O	4.039	-0.9259	-0.3431
C	-2.6336	3.7044	-0.3878	C	2.4423	4.2514	0.2016
O	-1.7958	-1.1099	3.0555	O	2.5404	-1.9719	-2.5694
C	0.29	-0.8084	2.0098	C	0.242	-1.6574	-2.1786
C	-4.9977	3.8364	0.0486	C	3.1988	3.449	-1.9362
O	-6.1005	3.3453	0.2535	O	3.6348	2.5852	-2.6868
H	-2.7345	-4.6638	-0.547	H	2.8883	-4.1001	2.0629
H	-1.642	-3.6106	-1.4178	H	1.4767	-3.094	2.2979
H	-2.5688	-3.3703	1.4729	H	3.1229	-3.4507	-0.2375
H	-0.9409	-3.6683	0.8807	H	1.4437	-3.8949	0.0324
H	-4.4804	-2.9978	-0.4729	H	4.366	-2.2002	1.8751
H	-3.937	-3.1576	-2.1309	H	3.4137	-2.0196	3.3347
H	-2.3532	1.0686	1.2329	H	2.293	0.7462	-1.4296
H	-1.8157	1.0015	-0.4401	H	1.3349	1.0566	0.0053
H	-4.6647	1.2807	0.633	H	4.33	1.6052	-0.3836
H	-5.5048	1.4489	-1.6588	H	4.4421	2.5258	1.84
H	-3.8908	1.3345	-2.3243	H	2.7404	2.2276	2.1399
H	-5.0272	-0.8174	-2.5252	H	4.0604	0.5046	3.2243
H	-5.4621	-0.8159	-0.8303	H	4.9335	0.1528	1.7488
H	-1.4448	-1.6051	-2.2876	H	0.803	-1.0179	2.4469
H	-2.8125	-1.2447	-3.3158	H	1.7764	-0.1161	3.5861
H	-2.036	0.0444	-2.4042	H	1.1165	0.6854	2.1647
H	7.7617	0.755	-1.5745	H	-6.2058	-1.0738	0.5359
H	7.4385	0.2529	0.0775	H	-7.4267	0.1898	0.6481
H	5.9621	2.3161	-1.6044	H	-5.7945	0.208	2.5283

H	6.78	2.5268	-0.0552	H	-5.8724	1.7511	1.6745
H	5.6438	-0.2173	-2.3473	H	-6.5528	0.0774	-1.6532
H	6.6456	-1.4394	-1.5845	H	-6.1848	1.6162	-0.8989
H	3.1467	-0.4208	1.8313	H	-1.6899	0.9739	-0.888
H	2.4383	1.0578	1.2393	H	-1.4446	0.3077	0.6919
H	1.6977	-0.0165	-0.8351	H	-2.1865	-1.9361	-0.0344
H	2.7194	-2.6347	0.3932	H	-2.3861	-0.8131	-2.8703
H	1.8527	-2.4739	-1.1248	H	-2.6764	-2.4663	-2.3567
H	4.2833	-2.6535	-1.5014	H	-4.7797	-1.195	-2.6898
H	3.5988	-1.1618	-2.1251	H	-4.6146	-1.8397	-1.0645
H	4.6818	-2.0808	1.4437	H	-3.03	1.308	-2.5926
H	5.9741	-2.6159	0.3752	H	-4.7162	1.3458	-3.0889
H	6.1815	-1.1657	1.366	H	-4.1449	2.4155	-1.799
H	3.3405	2.7959	1.2162	H	-2.1518	0.8339	2.4376
H	-3.6064	-0.8819	2.0641	H	3.9754	-0.9934	-1.3195
H	-2.6016	4.7907	-0.387	H	2.1958	5.1977	-0.2723
H	-1.6863	3.2094	-0.5709	H	2.2411	4.1975	1.2662
H	0.8746	-0.513	2.8595	H	-0.1139	-1.675	-3.1906
H	-4.857	4.9305	0.0301	H	2.9497	4.4563	-2.3109
1c-19	X axis(Å)	Y axis(Å)	Z axis(Å)	1c-20	X axis(Å)	Y axis(Å)	Z axis(Å)
C	1.4965	-3.2309	1.708	C	1.2568	-3.2971	1.6326
C	1.2904	-3.1851	0.1941	C	1.0684	-3.1918	0.1193
C	1.4147	-1.7661	-0.3817	C	1.2463	-1.7586	-0.4057
C	2.7451	-1.0842	0.0536	C	2.5944	-1.1384	0.0663
C	2.8875	-1.0645	1.621	C	2.7179	-1.1762	1.6346
C	2.7769	-2.5188	2.1552	C	2.5549	-2.6437	2.117
C	2.9339	0.3392	-0.5184	C	2.8402	0.297	-0.452
C	4.2858	0.9629	-0.1008	C	4.2243	0.844	-0.0224
C	4.5315	0.8993	1.4162	C	4.4325	0.7339	1.4986
C	4.2874	-0.4992	1.9919	C	4.1289	-0.6673	2.0385
C	1.8246	-0.1969	2.347	C	1.6751	-0.3012	2.3808
O	0.2554	-0.9866	-0.0106	O	0.1086	-0.9546	-0.0214
C	4.4374	2.371	-0.6395	C	4.5098	2.2605	-0.489
C	-6.2792	1.7788	0.9522	C	-6.3561	1.9614	0.9669
C	-6.514	0.4993	0.1602	C	-6.6177	0.7184	0.1266
C	-5.262	-0.3137	-0.0783	C	-5.3867	-0.1218	-0.1264
C	-4.0062	0.1681	0.0958	C	-4.1199	0.3169	0.079
C	-3.7641	1.6275	0.5403	C	-3.8414	1.7518	0.578
C	-5.0466	2.4982	0.4312	C	-5.097	2.6628	0.486
C	-2.7253	-0.6333	-0.1038	C	-2.8602	-0.514	-0.135
C	-1.7224	0.0768	-1.0315	C	-1.8262	0.199	-1.0256
C	-1.4108	1.4889	-0.5224	C	-1.4805	1.5827	-0.4631
C	-2.6937	2.3008	-0.3606	C	-2.7414	2.4252	-0.2865
C	-3.2886	1.6339	2.0128	C	-3.3837	1.6922	2.055
C	-5.5567	-1.7188	-0.5032	C	-5.7163	-1.5019	-0.604
O	-6.6903	-2.1061	-0.7663	O	-6.8565	-1.845	-0.898
C	-0.4536	-0.7224	-1.1784	C	-0.5794	-0.6313	-1.1867

C	1.282	-1.8182	-1.8876	C	1.1301	-1.7554	-1.9138
O	3.8484	-1.8789	-0.4502	O	3.6758	-1.9539	-0.4538
C	5.3956	2.7254	-1.5113	C	3.6078	3.2026	-0.8108
O	2.0981	-2.2934	-2.6647	O	1.9407	-2.229	-2.6976
C	0.0519	-1.177	-2.3226	C	-0.075	-1.0631	-2.3402
C	3.477	3.4259	-0.1987	C	5.9554	2.6253	-0.6337
O	3.4454	4.5592	-0.6626	O	6.3492	3.7329	-0.9788
H	1.5358	-4.2774	2.0334	H	1.2584	-4.355	1.9214
H	0.6262	-2.7931	2.2092	H	0.396	-2.8485	2.1406
H	2.0231	-3.8493	-0.2822	H	1.7833	-3.8637	-0.3729
H	0.3006	-3.6023	-0.0317	H	0.0676	-3.5672	-0.1302
H	3.6379	-3.1094	1.816	H	3.3999	-3.2502	1.7657
H	2.8225	-2.5227	3.2518	H	2.5886	-2.687	3.2131
H	2.9188	0.3011	-1.6157	H	2.8137	0.3045	-1.5493
H	2.0984	0.9823	-0.2219	H	2.0352	0.9572	-0.1134
H	5.0718	0.3476	-0.563	H	4.9729	0.1991	-0.5049
H	5.567	1.1931	1.6319	H	5.4705	0.9834	1.7535
H	3.9015	1.6221	1.9465	H	3.8112	1.4736	2.0183
H	4.4042	-0.4605	3.0826	H	4.2303	-0.6574	3.1314
H	5.0775	-1.1707	1.6322	H	4.901	-1.3577	1.675
H	0.8154	-0.6083	2.2836	H	0.6531	-0.6733	2.287
H	2.0565	-0.125	3.4168	H	1.8931	-0.2813	3.4558
H	1.7775	0.8248	1.9615	H	1.6698	0.7367	2.0382
H	-7.157	2.4296	0.8652	H	-7.2137	2.6402	0.8936
H	-6.1679	1.547	2.0176	H	-6.2645	1.6885	2.0243
H	-6.9513	0.7525	-0.8142	H	-7.0351	1.0189	-0.8431
H	-7.26	-0.0951	0.7021	H	-7.3873	0.1272	0.638
H	-5.2303	2.7727	-0.6168	H	-5.2599	2.9798	-0.5533
H	-4.9155	3.4426	0.9742	H	-4.9455	3.583	1.0643
H	-2.2751	-0.8107	0.8815	H	-2.4273	-0.7393	0.8483
H	-2.9111	-1.6257	-0.5198	H	-3.0695	-1.4851	-0.5883
H	-2.1907	0.1715	-2.0221	H	-2.2796	0.3422	-2.0174
H	-0.8695	1.4518	0.4308	H	-0.7961	2.1035	-1.1451
H	-0.7494	2.0045	-1.2305	H	-0.9519	1.4961	0.494
H	-2.4399	3.2928	0.0349	H	-2.464	3.3948	0.147
H	-3.1103	2.4689	-1.3635	H	-3.1409	2.6407	-1.2873
H	-2.3353	1.1136	2.1486	H	-2.4475	1.1398	2.1826
H	-3.148	2.6589	2.375	H	-3.2181	2.6992	2.4551
H	-4.0127	1.1455	2.6741	H	-4.1295	1.202	2.6904
H	-4.7085	-2.4106	-0.5733	H	-4.8881	-2.2165	-0.6846
H	3.7138	-2.0363	-1.4089	H	3.5402	-2.0814	-1.4168
H	5.4796	3.7432	-1.8856	H	3.9178	4.1899	-1.1481
H	6.125	2.0098	-1.8769	H	2.5393	3.0384	-0.7442
H	-0.2965	-1.0877	-3.3337	H	-0.4096	-0.9311	-3.3513
H	2.7696	3.1178	0.5879	H	6.6659	1.8137	-0.4033
1d-1	X axis(Å)	Y axis(Å)	Z axis(Å)	1d-2	X axis(Å)	Y axis(Å)	Z axis(Å)
C	4.1763	-2.7931	-0.5817	C	4.1097	-2.8742	-0.4578

C	2.6537	-2.8408	-0.4818	C	2.5845	-2.8802	-0.3948
C	2.0303	-1.594	0.16	C	1.9783	-1.6034	0.2025
C	2.6087	-0.2743	-0.4247	C	2.606	-0.312	-0.3955
C	4.1713	-0.2232	-0.4779	C	4.17	-0.3034	-0.4103
C	4.6937	-1.491	-1.2032	C	4.676	-1.6002	-1.0948
C	2.0288	1.0106	0.2084	C	2.0463	1.0014	0.1963
C	2.4746	2.2889	-0.5428	C	2.5449	2.2519	-0.5682
C	4.0108	2.3329	-0.6931	C	4.0848	2.2507	-0.6836
C	4.5908	1.0408	-1.2844	C	4.643	0.9309	-1.2329
C	4.8641	-0.135	0.9041	C	4.8303	-0.2032	0.9868
O	0.5989	-1.6274	-0.1856	O	0.5559	-1.6084	-0.1796
C	1.8636	3.5293	0.0937	C	1.9551	3.5209	0.0319
C	-6.3372	0.0579	-0.8323	C	-6.3457	-0.3491	0.132
C	-5.7424	1.137	0.0634	C	-5.7669	1.0601	0.1891
C	-4.2475	1.024	0.2464	C	-4.2587	1.0663	0.1779
C	-3.5318	-0.0876	-0.0547	C	-3.5182	0.009	-0.2329
C	-4.2123	-1.3467	-0.6305	C	-4.1637	-1.2377	-0.8722
C	-5.7579	-1.3014	-0.4753	C	-5.7081	-1.1218	-1.0104
C	-2.0241	-0.2201	0.1169	C	-2.0153	-0.1219	-0.0391
C	-1.6196	-1.4944	0.884	C	-1.6819	-1.3586	0.825
C	-2.2092	-2.743	0.2218	C	-2.3162	-2.6383	0.2612
C	-3.7277	-2.6231	0.1089	C	-3.8189	-2.4643	0.0121
C	-3.8698	-1.4545	-2.1357	C	-3.6238	-1.4557	-2.3074
C	-3.6264	2.2841	0.7638	C	-3.6525	2.3334	0.6924
O	-4.2914	3.2031	1.2322	O	-4.3105	3.205	1.2512
C	-0.121	-1.5994	1.0006	C	-0.1925	-1.5177	0.9857
C	1.952	-1.6872	1.6723	C	1.8581	-1.6581	1.7139
O	2.1564	-0.2472	-1.8142	O	2.1884	-0.3026	-1.796
C	2.5064	4.483	0.788	C	2.61	4.4705	0.7205
O	2.8765	-1.8001	2.4616	O	2.7577	-1.7864	2.5293
C	0.5713	-1.6416	2.1337	C	0.4689	-1.5489	2.1375
C	0.3971	3.746	-0.1019	C	0.499	3.7739	-0.196
O	-0.3303	2.9356	-0.6647	O	-0.24	2.9755	-0.7607
H	4.6137	-2.9439	0.4106	H	4.5188	-3.0137	0.5482
H	4.52	-3.6383	-1.1904	H	4.4457	-3.7414	-1.039
H	2.2415	-2.9728	-1.4916	H	2.1939	-3.0251	-1.4114
H	2.3566	-3.7427	0.0688	H	2.2504	-3.761	0.1685
H	4.3979	-1.4692	-2.2601	H	4.4063	-1.5945	-2.1589
H	5.7911	-1.5036	-1.1975	H	5.7722	-1.6411	-1.0619
H	0.9356	0.9594	0.1765	H	0.9534	0.9793	0.1373
H	2.3005	1.0827	1.2677	H	2.2932	1.0881	1.2606
H	2.0748	2.2424	-1.5661	H	2.1668	2.1968	-1.5992
H	4.2923	3.1727	-1.3412	H	4.404	3.0681	-1.3426
H	4.4876	2.519	0.2759	H	4.5445	2.4451	0.2921
H	5.6848	1.1238	-1.3175	H	5.7394	0.9837	-1.241
H	4.2698	0.955	-2.3303	H	4.3449	0.8309	-2.2844
H	4.4231	0.6242	1.5546	H	4.3959	0.5835	1.6084

H	4.8525	-1.0783	1.4488	H	4.7767	-1.1326	1.5523
H	5.9243	0.1217	0.7859	H	5.9002	0.0198	0.89
H	-7.4268	0.0428	-0.7131	H	-6.1778	-0.8671	1.0838
H	-6.1429	0.2938	-1.8848	H	-7.4307	-0.2947	-0.0132
H	-6.2156	1.0872	1.0525	H	-6.1513	1.5369	1.0985
H	-6.0035	2.1111	-0.3683	H	-6.1294	1.6486	-0.663
H	-6.0406	-1.5299	0.5616	H	-6.1625	-2.1181	-1.0796
H	-6.2273	-2.0748	-1.0963	H	-5.9661	-0.6079	-1.9471
H	-1.5628	-0.2085	-0.879	H	-1.5253	-0.1748	-1.0185
H	-1.5924	0.6272	0.6541	H	-1.5794	0.7478	0.4575
H	-2.041	-1.4214	1.8974	H	-2.119	-1.1897	1.8205
H	-1.7703	-2.9055	-0.7699	H	-1.8189	-2.94	-0.6686
H	-1.9651	-3.6327	0.8162	H	-2.1678	-3.4668	0.9657
H	-4.1193	-3.5183	-0.3912	H	-4.2059	-3.3825	-0.4481
H	-4.1401	-2.6369	1.1274	H	-4.3198	-2.3737	0.9851
H	-2.7963	-1.5734	-2.3135	H	-2.5461	-1.638	-2.342
H	-4.3684	-2.3182	-2.5905	H	-4.1088	-2.3193	-2.7778
H	-4.1843	-0.5622	-2.688	H	-3.8204	-0.58	-2.9377
H	-2.5338	2.3616	0.71	H	-2.5748	2.4681	0.5328
H	1.1894	-0.3921	-1.7985	H	1.2182	-0.4246	-1.8013
H	1.9972	5.3504	1.1994	H	2.1168	5.3592	1.1052
H	3.5736	4.4366	0.9781	H	3.6717	4.3995	0.9327
H	0.2476	-1.6326	3.1569	H	0.1199	-1.4957	3.151
H	-0.0097	4.6871	0.3063	H	0.1107	4.7322	0.1894
1d-3	X axis(Å)	Y axis(Å)	Z axis(Å)	1d-4	X axis(Å)	Y axis(Å)	Z axis(Å)
C	3.8768	-3.0742	-0.455	C	3.6341	-3.3704	-0.7989
C	2.3541	-3.0143	-0.3621	C	2.1879	-2.9291	-1.0074
C	1.8177	-1.6783	0.1713	C	1.8126	-1.6406	-0.2625
C	2.4686	-0.4582	-0.5419	C	2.873	-0.5186	-0.4473
C	4.0335	-0.5074	-0.5868	C	4.3461	-0.9771	-0.1837
C	4.4787	-1.8684	-1.1848	C	4.6425	-2.2404	-1.0337
C	1.9584	0.9153	-0.0509	C	2.5515	0.7923	0.3054
C	2.5287	2.0828	-0.8913	C	3.5263	1.9369	-0.0651
C	4.0582	2.0212	-1.0433	C	4.9954	1.4917	0.0984
C	4.5423	0.6416	-1.5051	C	5.3011	0.1717	-0.6214
C	4.7224	-0.3284	0.788	C	4.6694	-1.3014	1.2957
O	0.3808	-1.6489	-0.1574	O	0.5627	-1.1642	-0.8766
C	2.0532	3.4363	-0.399	C	3.1643	3.2113	0.6836
C	-6.4918	0.2773	-0.8385	C	-6.6342	1.4031	-0.3279
C	-5.8509	1.3917	-0.0215	C	-6.6775	-0.1179	-0.262
C	-4.3596	1.2349	0.1714	C	-5.3771	-0.753	0.1765
C	-3.6857	0.0834	-0.0727	C	-4.193	-0.0924	0.2166
C	-4.4195	-1.1867	-0.556	C	-4.0841	1.3814	-0.2312
C	-5.9604	-1.0741	-0.3911	C	-5.349	1.8611	-0.9959
C	-2.1804	-0.0976	0.0749	C	-2.8729	-0.6829	0.6979
C	-1.8104	-1.3218	0.9326	C	-1.7317	-0.5073	-0.3244
C	-2.4595	-2.5938	0.3778	C	-1.571	0.9752	-0.6911

C	-3.9737	-2.4236	0.2705	C	-2.8853	1.5632	-1.199
C	-4.0995	-1.4148	-2.0527	C	-3.8937	2.2788	1.0147
C	-3.6997	2.4961	0.6365	C	-5.5416	-2.1857	0.58
O	-4.3309	3.5091	0.9193	O	-6.6106	-2.7804	0.49
C	-0.3154	-1.4781	1.0324	C	-0.4005	-1.0694	0.1223
C	1.7583	-1.6444	1.6871	C	1.3402	-1.8978	1.1542
O	2.0142	-0.541	-1.931	O	2.8071	-0.1657	-1.8636
C	1.2961	4.2618	-1.1412	C	3.8437	3.7773	1.695
O	2.6788	-1.7926	2.4745	O	1.971	-2.3944	2.074
C	0.393	-1.4564	2.1562	C	-0.0459	-1.4874	1.3333
C	2.4212	3.9136	0.9628	C	1.9443	3.9448	0.2277
O	3.0626	3.2405	1.7591	O	1.2079	3.5329	-0.6607
H	4.3027	-3.1636	0.5497	H	3.7497	-3.7839	0.2082
H	4.1659	-3.9904	-0.984	H	3.8579	-4.1947	-1.4869
H	1.9334	-3.2031	-1.3592	H	2.0181	-2.7874	-2.0835
H	1.9977	-3.8451	0.2605	H	1.5163	-3.7474	-0.7171
H	4.1913	-1.9255	-2.2428	H	4.6367	-1.9859	-2.1015
H	5.573	-1.9489	-1.1649	H	5.6523	-2.612	-0.8178
H	0.8652	0.9588	-0.138	H	1.5359	1.1124	0.0473
H	2.1893	1.0419	1.0105	H	2.5554	0.6316	1.3896
H	2.125	1.9559	-1.907	H	3.4008	2.1613	-1.1342
H	4.3843	2.7711	-1.7755	H	5.6607	2.27	-0.2966
H	4.5576	2.2838	-0.1044	H	5.2497	1.3792	1.1583
H	5.6394	0.6425	-1.5413	H	6.3447	-0.1072	-0.4265
H	4.2136	0.4797	-2.5397	H	5.2369	0.3355	-1.7046
H	4.309	0.5028	1.3646	H	4.3141	-0.534	1.9877
H	4.6691	-1.2196	1.4118	H	4.2563	-2.2543	1.6245
H	5.7932	-0.1276	0.6585	H	5.7534	-1.387	1.4417
H	-7.5803	0.3113	-0.7134	H	-7.5002	1.7702	-0.8908
H	-6.2965	0.4333	-1.9055	H	-6.716	1.826	0.6799
H	-6.3235	1.4306	0.9685	H	-6.9378	-0.5145	-1.2519
H	-6.0756	2.3417	-0.5217	H	-7.4902	-0.3976	0.4196
H	-6.2403	-1.2187	0.6616	H	-5.3417	1.4717	-2.0234
H	-6.4647	-1.8709	-0.9522	H	-5.3508	2.9547	-1.0855
H	-1.7469	-0.1904	-0.9295	H	-2.6102	-0.1969	1.6463
H	-1.6946	0.7733	0.5193	H	-2.9517	-1.7467	0.9289
H	-2.2099	-1.1545	1.9437	H	-2.0201	-1.0568	-1.2325
H	-2.0416	-2.8515	-0.6028	H	-1.2103	1.5474	0.1726
H	-2.2421	-3.4433	1.0377	H	-0.8117	1.0928	-1.4749
H	-4.4052	-3.3373	-0.1584	H	-2.7373	2.6288	-1.4173
H	-4.3734	-2.3468	1.2913	H	-3.1135	1.0832	-2.1609
H	-3.0349	-1.5957	-2.2313	H	-2.9637	2.0632	1.5498
H	-4.6416	-2.2845	-2.4415	H	-3.8619	3.3379	0.734
H	-4.3799	-0.5497	-2.6634	H	-4.71	2.1512	1.734
H	-2.6062	2.4908	0.7176	H	-4.6562	-2.7038	0.9673
H	1.0613	-0.7549	-1.9017	H	1.8687	0.0264	-2.0623
H	0.9593	5.2313	-0.7856	H	3.5249	4.7018	2.1685

H	0.9907	3.987	-2.1473	H	4.7507	3.3372	2.0963
H	0.0894	-1.3479	3.18	H	-0.5881	-1.5315	2.2583
H	2.0708	4.9257	1.2278	H	1.7302	4.8933	0.749
1d-5	X axis(Å)	Y axis(Å)	Z axis(Å)	1d-6	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-2.9478	-3.5364	0.2548	C	4.1834	-2.7267	-0.6791
C	-1.5674	-2.8861	0.2228	C	2.6629	-2.8342	-0.582
C	-1.5687	-1.4364	-0.2831	C	1.9956	-1.6308	0.0965
C	-2.6815	-0.5786	0.3809	C	2.5213	-0.2758	-0.4613
C	-4.1005	-1.2403	0.3631	C	4.0811	-0.161	-0.5013
C	-3.9994	-2.67	0.9564	C	4.6561	-1.3876	-1.2576
C	-2.7379	0.884	-0.1149	C	1.8854	0.972	0.1892
C	-3.7265	1.7447	0.7101	C	2.2938	2.285	-0.5179
C	-5.1169	1.0787	0.7878	C	3.8274	2.3938	-0.6417
C	-5.0505	-0.3828	1.2493	C	4.458	1.1416	-1.2679
C	-4.7527	-1.3424	-1.0378	C	4.7595	-0.0844	0.8886
O	-0.2734	-0.8642	0.1216	O	0.5629	-1.7093	-0.2324
C	-3.7405	3.1785	0.2015	C	1.6161	3.4651	0.161
C	6.8776	0.7011	0.2525	C	-6.265	0.3197	-0.8274
C	6.1419	0.2655	1.5129	C	-5.5845	1.3808	0.0321
C	4.7727	-0.3234	1.257	C	-4.1154	1.1362	0.2358
C	4.1167	-0.2173	0.0743	C	-3.4829	-0.0185	-0.0714
C	4.7223	0.5697	-1.1071	C	-4.2434	-1.2355	-0.6179
C	5.9319	1.4443	-0.6754	C	-5.7802	-1.0739	-0.4446
C	2.7604	-0.841	-0.2353	C	-1.9839	-0.2178	0.0595
C	1.7473	0.179	-0.7912	C	-1.6352	-1.4781	0.8697
C	2.326	0.8806	-2.0288	C	-2.3066	-2.7154	0.2605
C	3.6672	1.5373	-1.7071	C	-3.8213	-2.517	0.1518
C	5.1984	-0.4272	-2.1904	C	-3.9297	-1.4017	-2.1232
C	4.2265	-1.051	2.4473	C	-3.3854	2.3132	0.7886
O	4.8298	-1.12	3.5134	O	-2.7066	2.2669	1.8079
C	0.4087	-0.4833	-1.0288	C	-0.1415	-1.6493	0.964
C	-1.4522	-1.3426	-1.7914	C	1.9367	-1.7658	1.6069
O	-2.2982	-0.4866	1.7878	O	2.0771	-0.2403	-1.8531
C	-4.719	3.7827	-0.4929	C	2.1887	4.3638	0.9788
O	-2.2466	-1.7395	-2.629	O	2.8698	-1.9269	2.378
C	-0.2008	-0.7123	-2.1877	C	0.5645	-1.6961	2.0886
C	-2.5594	4.0292	0.5402	C	0.1609	3.6689	-0.1207
O	-1.5803	3.6039	1.1415	O	-0.4749	2.9765	-0.9078
H	-3.2652	-3.773	-0.766	H	4.626	-2.8927	0.3086
H	-2.8763	-4.4992	0.7751	H	4.558	-3.5393	-1.3134
H	-1.1445	-2.915	1.2363	H	2.2548	-2.9515	-1.5951
H	-0.8932	-3.5025	-0.386	H	2.3995	-3.7622	-0.0582
H	-3.7506	-2.6181	2.0243	H	4.368	-1.3461	-2.316
H	-4.9733	-3.1726	0.898	H	5.7531	-1.3594	-1.2428
H	-1.7397	1.3294	-0.0285	H	0.7958	0.8914	0.1299
H	-3.0005	0.926	-1.1782	H	2.1337	1.025	1.2555
H	-3.3606	1.7878	1.7461	H	1.9144	2.2551	-1.5492

H	-5.7536	1.639	1.4844	H	4.0847	3.2647	-1.2579
H	-5.6192	1.1164	-0.1852	H	4.2857	2.5651	0.3385
H	-6.0633	-0.806	1.2402	H	5.5484	1.2656	-1.2918
H	-4.7292	-0.4095	2.2983	H	4.1452	1.0747	-2.3177
H	-4.6861	-0.4124	-1.6076	H	4.2736	0.627	1.5609
H	-4.3249	-2.134	-1.652	H	4.7956	-1.0454	1.4
H	-5.8185	-1.5872	-0.9482	H	5.8053	0.2321	0.7885
H	7.7198	1.3477	0.5251	H	-7.3515	0.3856	-0.6973
H	7.3066	-0.1714	-0.2532	H	-6.0671	0.5143	-1.8877
H	6.025	1.1305	2.1786	H	-6.0677	1.4091	1.0171
H	6.7793	-0.458	2.0359	H	-5.7491	2.3611	-0.4312
H	5.5814	2.3459	-0.1543	H	-6.0641	-1.2579	0.6007
H	6.4831	1.7972	-1.5562	H	-6.3129	-1.8246	-1.0418
H	2.9082	-1.6514	-0.9613	H	-1.5583	-0.2827	-0.9505
H	2.3165	-1.3213	0.6382	H	-1.4916	0.6414	0.5215
H	1.5847	0.9517	-0.0252	H	-2.0343	-1.3457	1.886
H	2.4517	0.1729	-2.8568	H	-1.8875	-2.9389	-0.7281
H	1.6304	1.6532	-2.3806	H	-2.1065	-3.5947	0.8857
H	4.0622	2.0048	-2.6184	H	-4.2642	-3.4025	-0.3218
H	3.4759	2.3573	-1.001	H	-4.2259	-2.4817	1.1729
H	4.3769	-1.0156	-2.6106	H	-2.8713	-1.6083	-2.3107
H	5.6743	0.0995	-3.0258	H	-4.4994	-2.2342	-2.5521
H	5.9268	-1.1415	-1.7913	H	-4.1817	-0.5	-2.692
H	3.2467	-1.531	2.3386	H	-3.5445	3.2546	0.2365
H	-1.3833	-0.1418	1.8093	H	1.1132	-0.4048	-1.8437
H	-4.6572	4.821	-0.807	H	1.6338	5.1865	1.4212
H	-5.6262	3.2617	-0.7807	H	3.2386	4.3102	1.2464
H	0.0984	-0.5122	-3.1987	H	0.2541	-1.6582	3.1152
H	-2.6109	5.0797	0.2072	H	-0.3219	4.4981	0.424
1d-7	X axis(Å)	Y axis(Å)	Z axis(Å)	1d-8	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-2.806	-3.5471	-0.4787	C	3.4171	-3.4883	-0.631
C	-1.4274	-2.9028	-0.3585	C	1.9848	-3.0187	-0.8719
C	-1.4432	-1.3729	-0.4912	C	1.6688	-1.6478	-0.2566
C	-2.5403	-0.7179	0.3954	C	2.7588	-0.5891	-0.5897
C	-3.9609	-1.3573	0.2273	C	4.2212	-1.0663	-0.2925
C	-3.8518	-2.8919	0.4297	C	4.4615	-2.4282	-0.9962
C	-2.598	0.8237	0.3048	C	2.4898	0.8134	0.0011
C	-3.6042	1.4275	1.314	C	3.526	1.8564	-0.4823
C	-4.9896	0.7612	1.2531	C	4.9798	1.388	-0.2994
C	-4.9042	-0.768	1.3158	C	5.2151	-0.0161	-0.8678
C	-4.6289	-1.0914	-1.1439	C	4.5522	-1.2281	1.2113
O	-0.1407	-0.9036	0.015	O	0.4178	-1.1923	-0.8882
C	-3.6912	2.9383	1.2149	C	3.288	3.2308	0.1129
C	6.9624	0.8223	0.3854	C	-6.7366	1.5118	-0.421
C	6.2737	0.0576	1.508	C	-6.7863	0.0014	-0.2319
C	4.9195	-0.5004	1.1323	C	-5.4824	-0.6032	0.2381
C	4.2254	-0.1162	0.032	C	-4.2943	0.0505	0.2046

C	4.7734	0.9686	-0.9194	C	-4.1853	1.4818	-0.3636
C	5.9711	1.7443	-0.3041	C	-5.4602	1.9063	-1.1442
C	2.8757	-0.6832	-0.3941	C	-2.9697	-0.5089	0.7102
C	1.8208	0.4123	-0.6464	C	-1.8463	-0.4245	-0.3432
C	2.3432	1.424	-1.6771	C	-1.6819	1.0216	-0.831
C	3.6755	2.0214	-1.2281	C	-3.0017	1.5766	-1.3624
C	5.2441	0.2989	-2.2323	C	-3.9692	2.4761	0.802
C	4.4364	-1.5393	2.097	C	-5.6487	-1.9958	0.7638
O	5.0313	-1.8019	3.1371	O	-6.7174	-2.5961	0.7183
C	0.4914	-0.2087	-1.0121	C	-0.5119	-0.9625	0.1221
C	-1.3596	-0.9196	-1.935	C	1.2259	-1.7533	1.1887
O	-2.1286	-0.9897	1.7732	O	2.6746	-0.3981	-2.0384
C	-3.3476	3.7594	2.2215	C	2.9825	4.3079	-0.63
O	-2.1353	-1.169	-2.8435	O	1.8468	-2.221	2.1295
C	-0.1487	-0.1483	-2.1758	C	-0.133	-1.2593	1.3614
C	-4.1788	3.5842	-0.0351	C	3.392	3.443	1.5831
O	-4.4859	2.957	-1.0405	O	3.6196	2.5407	2.3784
H	-3.135	-3.5184	-1.5226	H	3.5326	-3.7942	0.414
H	-2.7265	-4.61	-0.2201	H	3.6019	-4.3898	-1.2277
H	-0.9941	-3.1788	0.6125	H	1.8051	-2.9811	-1.9549
H	-0.7565	-3.3445	-1.1067	H	1.2881	-3.7776	-0.4927
H	-3.5931	-3.1156	1.4729	H	4.4527	-2.2945	-2.0859
H	-4.8258	-3.3657	0.2524	H	5.4599	-2.8102	-0.7475
H	-1.6114	1.247	0.5358	H	1.5009	1.1678	-0.3172
H	-2.8329	1.1294	-0.7186	H	2.4619	0.7598	1.093
H	-3.2094	1.1981	2.3152	H	3.3805	1.9525	-1.5687
H	-5.603	1.1134	2.0926	H	5.6571	2.0892	-0.8039
H	-5.528	1.0561	0.3459	H	5.2677	1.4032	0.7574
H	-5.9138	-1.1861	1.2117	H	6.25	-0.3166	-0.6586
H	-4.5654	-1.0625	2.3174	H	5.1365	0.0275	-1.9617
H	-4.5594	-0.0459	-1.4541	H	4.2199	-0.3783	1.8127
H	-4.2148	-1.7007	-1.9462	H	4.1225	-2.1282	1.649
H	-5.6958	-1.3449	-1.1076	H	5.6354	-1.3215	1.3589
H	7.7937	1.4067	0.7965	H	-7.6098	1.8376	-0.9981
H	7.4007	0.1212	-0.334	H	-6.7999	2.0151	0.5504
H	6.1446	0.723	2.3714	H	-7.0628	-0.4725	-1.1827
H	6.9471	-0.7493	1.8224	H	-7.5901	-0.2177	0.4817
H	5.6115	2.4723	0.4362	H	-5.4718	1.4353	-2.1368
H	6.4877	2.327	-1.0772	H	-5.4579	2.9891	-1.3217
H	3.0197	-1.2793	-1.3048	H	-2.6878	0.0502	1.6116
H	2.4702	-1.3793	0.3422	H	-3.0507	-1.5504	1.0266
H	1.6638	0.9588	0.2954	H	-2.1567	-1.0424	-1.1987
H	2.4628	0.9543	-2.6606	H	-1.3024	1.6589	-0.0228
H	1.6176	2.2373	-1.8047	H	-0.9356	1.0687	-1.6345
H	4.0302	2.7189	-1.9978	H	-2.8513	2.62	-1.6683
H	3.4836	2.6272	-0.3315	H	-3.2491	1.0225	-2.2787
H	4.4272	-0.1927	-2.7697	H	-3.0315	2.2982	1.3376

H	5.6775	1.038	-2.916	H	-3.9364	3.5087	0.4356
H	6.0055	-0.4664	-2.0461	H	-4.7741	2.4128	1.5424
H	3.5124	-2.0722	1.842	H	-4.7657	-2.4773	1.2006
H	-1.1746	-0.7849	1.8256	H	1.7241	-0.3284	-2.2557
H	-3.4139	4.8409	2.1482	H	2.816	5.2914	-0.2007
H	-2.987	3.363	3.167	H	2.8937	4.2337	-1.7106
H	0.112	0.3148	-3.1083	H	-0.6488	-1.1945	2.3003
H	-4.2449	4.6852	-0.0116	H	3.2424	4.4797	1.9298
1d-9	X axis(Å)	Y axis(Å)	Z axis(Å)	1d-10	X axis(Å)	Y axis(Å)	Z axis(Å)
C	3.7585	-3.1873	-0.6161	C	3.7881	-3.1583	-0.2462
C	2.24	-3.0429	-0.563	C	2.2664	-3.0413	-0.2103
C	1.7579	-1.763	0.1349	C	1.7607	-1.6646	0.2439
C	2.5175	-0.4991	-0.3571	C	2.4797	-0.5013	-0.4979
C	4.0768	-0.6482	-0.3595	C	4.0424	-0.6074	-0.4854
C	4.4591	-1.9306	-1.1442	C	4.4575	-2.0086	-1.0069
C	2.0839	0.8121	0.337	C	2.0038	0.9098	-0.0851
C	2.7368	2.0624	-0.3072	C	2.6449	2.018	-0.9543
C	4.265	1.9147	-0.4237	C	4.1754	1.8954	-1.0507
C	4.688	0.5916	-1.0734	C	4.6235	0.4804	-1.4347
C	4.7267	-0.7271	1.0439	C	4.6908	-0.3908	0.9037
O	0.3459	-1.5926	-0.2538	O	0.3383	-1.6011	-0.1383
C	2.3843	3.3718	0.3812	C	2.205	3.4084	-0.5374
C	-6.4882	0.4961	-0.9156	C	-6.5306	-0.1151	0.1001
C	-5.8967	1.4147	0.1455	C	-5.9248	1.283	0.1179
C	-4.4153	1.2171	0.3702	C	-4.4153	1.2614	0.1307
C	-3.7247	0.1339	-0.0642	C	-3.6889	0.1828	-0.2508
C	-4.4275	-1.01	-0.8277	C	-4.3557	-1.0745	-0.8511
C	-5.9758	-0.9219	-0.7262	C	-5.8959	-0.935	-1.0094
C	-2.229	-0.0831	0.1277	C	-2.1875	0.0273	-0.0613
C	-1.9055	-1.4556	0.7467	C	-1.8796	-1.1742	0.8572
C	-2.5157	-2.5875	-0.0863	C	-2.5464	-2.4647	0.3553
C	-4.0222	-2.3898	-0.2416	C	-4.0433	-2.269	0.0881
C	-4.027	-0.938	-2.3205	C	-3.81	-1.3636	-2.2716
C	-3.7819	2.3598	1.1008	C	-3.804	2.5275	0.6424
O	-4.4361	3.2574	1.6208	O	-4.4726	3.4714	1.0493
C	-0.4187	-1.6412	0.9031	C	-0.3939	-1.3629	1.0177
C	1.615	-1.9337	1.6361	C	1.6498	-1.56	1.7535
O	2.1201	-0.337	-1.7527	O	2.0697	-0.6299	-1.8974
C	2.0535	3.5416	1.6723	C	1.5063	4.2279	-1.3409
O	2.4969	-2.1461	2.4526	O	2.5377	-1.6981	2.5793
C	0.2227	-1.8341	2.05	C	0.2752	-1.3132	2.1645
C	2.3796	4.6033	-0.4646	C	2.5448	3.9312	0.815
O	2.6353	4.5921	-1.662	O	3.1346	3.2714	1.6608
H	4.1369	-3.4479	0.3777	H	4.1761	-3.2167	0.776
H	4.0135	-4.0349	-1.2638	H	4.0616	-4.1071	-0.7236
H	1.8508	-3.0639	-1.5901	H	1.8734	-3.2606	-1.2124
H	1.8109	-3.9283	-0.0764	H	1.8592	-3.8302	0.4354

H	4.2062	-1.8119	-2.2058	H	4.2038	-2.1035	-2.0708
H	5.5451	-2.0854	-1.1084	H	5.547	-2.1263	-0.9452
H	0.9959	0.9344	0.2563	H	0.9163	0.9876	-0.2122
H	2.3166	0.7559	1.4047	H	2.2033	1.0752	0.9774
H	2.3333	2.1194	-1.328	H	2.2704	1.8609	-1.9771
H	4.6758	2.7386	-1.0211	H	4.5528	2.5997	-1.8034
H	4.7279	2.0039	0.567	H	4.6529	2.1822	-0.1076
H	5.7839	0.5289	-1.0728	H	5.7204	0.441	-1.4325
H	4.395	0.6086	-2.131	H	4.3237	0.2839	-2.4721
H	4.3607	0.0436	1.7268	H	4.2891	0.4797	1.4283
H	4.5815	-1.6917	1.5287	H	4.5839	-1.2505	1.5638
H	5.814	-0.5988	0.9711	H	5.7721	-0.234	0.8033
H	-7.582	0.5111	-0.8444	H	-6.3837	-0.6051	1.07
H	-6.2363	0.8656	-1.9162	H	-7.6126	-0.0445	-0.0594
H	-6.4153	1.2476	1.0983	H	-6.3136	1.7968	1.0053
H	-6.1042	2.4489	-0.1558	H	-6.2631	1.8497	-0.7585
H	-6.3115	-1.2763	0.2582	H	-6.3679	-1.9247	-1.0516
H	-6.4459	-1.584	-1.4643	H	-6.1344	-0.4469	-1.9648
H	-1.7381	0.0216	-0.8485	H	-1.7068	-0.0877	-1.04
H	-1.7739	0.6781	0.765	H	-1.722	0.9114	0.3797
H	-2.3653	-1.4886	1.7455	H	-2.3078	-0.9498	1.8456
H	-2.0423	-2.6466	-1.0738	H	-2.0544	-2.8259	-0.556
H	-2.3311	-3.553	0.4018	H	-2.4206	-3.2602	1.1011
H	-4.4247	-3.1967	-0.8675	H	-4.4476	-3.1977	-0.3345
H	-4.4783	-2.5159	0.7503	H	-4.5475	-2.1255	1.0529
H	-2.9533	-1.0847	-2.4742	H	-2.7384	-1.5802	-2.2896
H	-4.5423	-1.7107	-2.9026	H	-4.3166	-2.2301	-2.7131
H	-4.2801	0.0324	-2.7614	H	-3.9753	-0.5074	-2.9366
H	-2.6865	2.3731	1.157	H	-2.7093	2.5974	0.6227
H	1.1493	-0.4391	-1.7885	H	1.1091	-0.8086	-1.8923
H	1.806	4.5152	2.0871	H	1.1956	5.224	-1.0393
H	2.0333	2.7158	2.3751	H	1.2252	3.9205	-2.3446
H	-0.1422	-1.9094	3.0567	H	-0.0611	-1.1547	3.1715
H	2.1268	5.5433	0.0547	H	2.2234	4.9656	1.0245
1d-11	X axis(Å)	Y axis(Å)	Z axis(Å)	1d-12	X axis(Å)	Y axis(Å)	Z axis(Å)
C	3.5489	-3.4057	-0.779	C	-3.037	-3.4374	0.6913
C	2.0991	-2.9585	-0.9458	C	-1.6331	-2.8482	0.5845
C	1.7589	-1.6514	-0.2165	C	-1.5793	-1.4763	-0.1029
C	2.8193	-0.5415	-0.4632	C	-2.66	-0.4998	0.439
C	4.2979	-1.0048	-0.242	C	-4.1028	-1.1054	0.4976
C	4.5556	-2.2884	-1.074	C	-4.0561	-2.4498	1.2699
C	2.5333	0.7877	0.2714	C	-2.661	0.8881	-0.2407
C	3.5018	1.9169	-0.1582	C	-3.6176	1.8837	0.4612
C	4.9728	1.4646	-0.0371	C	-5.032	1.2851	0.6155
C	5.2441	0.1272	-0.7383	C	-5.021	-0.1066	1.2609
C	4.6715	-1.2994	1.2318	C	-4.7568	-1.3621	-0.8825
O	0.4912	-1.1792	-0.7963	O	-0.2639	-0.9055	0.2327

C	3.1751	3.2097	0.5751	C	-3.5774	3.2398	-0.2272
C	-6.1897	1.1313	-1.316	C	6.2088	1.6021	0.2744
C	-6.5443	-0.1068	-0.5019	C	5.9394	0.718	1.4856
C	-5.3433	-0.7198	0.1779	C	4.6873	-0.1121	1.3309
C	-4.192	-0.0391	0.3982	C	4.1224	-0.3782	0.1277
C	-4.0626	1.4642	0.0693	C	4.7866	0.0612	-1.1946
C	-5.3815	2.0921	-0.4621	C	6.1576	0.7653	-0.9914
C	-2.8885	-0.6538	0.8872	C	2.7627	-1.0319	-0.0763
C	-1.7792	-0.498	-0.1779	C	1.7957	-0.0638	-0.7935
C	-1.6204	0.9732	-0.6055	C	2.406	0.4558	-2.1092
C	-2.9549	1.6129	-1.0044	C	3.811	1.0355	-1.9048
C	-3.6872	2.2796	1.3315	C	5.0721	-1.1597	-2.104
C	-5.5352	-2.1591	0.5395	C	4.1127	-0.5659	2.6366
O	-6.5654	-2.7752	0.2886	O	4.6366	-0.3086	3.7155
C	-0.436	-1.0582	0.2332	C	0.4335	-0.7006	-0.9529
C	1.3354	-1.8745	1.2213	C	-1.4577	-1.581	-1.61
O	2.7055	-0.2189	-1.8837	O	-2.2753	-0.2423	1.8247
C	3.8939	3.7923	1.5492	C	-4.5323	3.7862	-0.9982
O	1.9957	-2.3542	2.1294	O	-2.2653	-2.0528	-2.3946
C	-0.0416	-1.4524	1.4399	C	-0.1832	-1.0531	-2.0764
C	1.9445	3.9424	0.147	C	-2.365	4.0821	0.0054
O	1.1739	3.5168	-0.7053	O	-1.4026	3.701	0.6606
H	3.6975	-3.7981	0.2323	H	-3.3618	-3.7911	-0.2926
H	3.7427	-4.2463	-1.4562	H	-3.0021	-4.3275	1.3312
H	1.8921	-2.8389	-2.0181	H	-1.2127	-2.7625	1.5959
H	1.4329	-3.7653	-0.614	H	-0.9818	-3.5621	0.0638
H	4.5136	-2.0571	-2.1463	H	-3.8067	-2.2706	2.3238
H	5.5701	-2.6626	-0.8859	H	-5.0481	-2.9193	1.2705
H	1.5114	1.1095	0.0421	H	-1.6469	1.3036	-0.2063
H	2.5743	0.6505	1.3581	H	-2.9207	0.8029	-1.3021
H	3.3397	2.1192	-1.2267	H	-3.2514	2.046	1.4852
H	5.6287	2.2293	-0.4724	H	-5.648	1.9533	1.2308
H	5.264	1.3732	1.0153	H	-5.5315	1.2161	-0.3573
H	6.2921	-0.155	-0.5744	H	-6.0489	-0.4896	1.3001
H	5.1425	0.268	-1.8219	H	-4.7021	-0.0104	2.3066
H	4.3458	-0.5147	1.919	H	-4.6547	-0.5159	-1.5664
H	4.2643	-2.2419	1.5958	H	-4.3582	-2.2412	-1.3876
H	5.7595	-1.3894	1.3412	H	-5.8311	-1.5537	-0.7686
H	-5.6252	0.8478	-2.2122	H	5.4744	2.4149	0.2261
H	-7.1083	1.6197	-1.6608	H	7.1948	2.0704	0.3733
H	-7.0123	-0.8246	-1.1862	H	5.8641	1.3762	2.3595
H	-7.2909	0.1471	0.2609	H	6.7901	0.047	1.6578
H	-5.1682	3.0033	-1.0351	H	6.3977	1.3939	-1.8581
H	-6.015	2.4067	0.3792	H	6.9605	0.0173	-0.9306
H	-2.5985	-0.1793	1.8318	H	2.8799	-1.9582	-0.6514
H	-2.9849	-1.7162	1.1195	H	2.3046	-1.3444	0.8638
H	-2.1017	-1.069	-1.0614	H	1.6555	0.8131	-0.1435

H	-1.1574	1.5541	0.2018	H	2.4517	-0.3443	-2.8572
H	-0.9338	1.044	-1.4591	H	1.7615	1.2366	-2.5332
H	-2.7819	2.6742	-1.2242	H	4.2145	1.3274	-2.8829
H	-3.2849	1.1545	-1.946	H	3.7183	1.9615	-1.3219
H	-2.7145	2.0086	1.751	H	4.1696	-1.6958	-2.4092
H	-3.6457	3.3513	1.1031	H	5.582	-0.8479	-3.0234
H	-4.4305	2.1374	2.1252	H	5.7187	-1.8845	-1.5948
H	-4.7123	-2.6563	1.0676	H	3.1964	-1.1676	2.5998
H	1.7618	-0.0251	-2.0534	H	-1.3489	0.0704	1.8073
H	3.5983	4.7291	2.0135	H	-4.4313	4.7725	-1.4425
H	4.8116	3.3543	1.9275	H	-5.4585	3.267	-1.2212
H	-0.5513	-1.474	2.3839	H	0.1232	-0.9953	-3.1032
H	1.7556	4.9035	0.6546	H	-2.3769	5.0826	-0.4595
1d-13	X axis(Å)	Y axis(Å)	Z axis(Å)	1d-14	X axis(Å)	Y axis(Å)	Z axis(Å)
C	3.8535	-3.052	-0.5808	C	-2.5894	-3.5967	0.7199
C	2.3303	-3.032	-0.4723	C	-1.2604	-2.856	0.6019
C	1.7695	-1.73	0.1165	C	-1.3558	-1.5098	-0.1312
C	2.3838	-0.4707	-0.5604	C	-2.5445	-0.6442	0.3721
C	3.9486	-0.4783	-0.6201	C	-3.9106	-1.4088	0.4415
C	4.4215	-1.806	-1.2697	C	-3.7183	-2.7123	1.26
C	1.8456	0.8719	-0.019	C	-2.6997	0.7077	-0.3608
C	2.3734	2.0794	-0.8273	C	-3.7819	1.6088	0.2893
C	3.9026	2.0665	-0.9903	C	-5.1153	0.861	0.4745
C	4.4202	0.7158	-1.5011	C	-4.9462	-0.499	1.1622
C	4.6446	-0.3307	0.7548	C	-4.5191	-1.7852	-0.932
O	0.3279	-1.7214	-0.1885	O	-0.1171	-0.7808	0.1975
C	1.8511	3.3952	-0.2862	C	-4.0143	2.9248	-0.4369
C	-6.4742	0.5049	-0.7073	C	6.9804	1.0281	0.2573
C	-5.7816	1.5511	0.1575	C	6.2134	0.7988	1.5529
C	-4.2996	1.3266	0.303	C	4.8748	0.1203	1.3657
C	-3.6751	0.1609	0.0128	C	4.2559	-0.0062	0.1652
C	-4.4524	-1.0536	-0.5253	C	4.8789	0.5796	-1.1196
C	-5.9877	-0.8905	-0.3419	C	6.0465	1.5592	-0.8167
C	-2.1774	-0.0617	0.1667	C	2.9281	-0.7192	-0.065
C	-1.8402	-1.3528	0.936	C	1.907	0.1495	-0.8264
C	-2.5318	-2.5679	0.3094	C	2.5091	0.6367	-2.1526
C	-4.0415	-2.3461	0.2289	C	3.8181	1.3871	-1.9144
C	-4.1488	-1.2104	-2.0343	C	5.4216	-0.5773	-1.992
C	-3.577	2.5515	0.7648	C	4.3161	-0.4145	2.6487
O	-2.4974	2.9215	0.3221	O	4.8602	-0.2315	3.7328
C	-0.3491	-1.553	1.0134	C	0.5968	-0.5902	-0.9805
C	1.7309	-1.7533	1.6331	C	-1.2025	-1.6497	-1.6329
O	1.92	-0.5219	-1.9478	O	-2.2024	-0.294	1.7472
C	1.0364	4.2022	-0.9863	C	-3.8144	3.1733	-1.7421
O	2.6596	-1.9466	2.4016	O	-1.9609	-2.1988	-2.4157
C	0.3751	-1.562	2.1274	C	0.0392	-1.0472	-2.097
C	2.2114	3.8429	1.0868	C	-4.4945	4.0773	0.3835

O	2.9303	3.1974	1.8392	O	-4.7003	4.0011	1.5881
H	4.2911	-3.1684	0.4162	H	-2.863	-4.016	-0.2538
H	4.1588	-3.9409	-1.1461	H	-2.4604	-4.4561	1.3889
H	1.904	-3.1928	-1.4718	H	-0.8625	-2.6901	1.6124
H	1.9994	-3.8937	0.1217	H	-0.5276	-3.5084	0.1097
H	4.1281	-1.8318	-2.3273	H	-3.4992	-2.4702	2.3081
H	5.5176	-1.861	-1.2598	H	-4.6506	-3.2911	1.2728
H	0.7513	0.891	-0.0926	H	-1.751	1.2594	-0.3289
H	2.0864	0.9717	1.0434	H	-2.9242	0.528	-1.4165
H	1.9671	1.9717	-1.8442	H	-3.4031	1.859	1.2903
H	4.2024	2.8492	-1.699	H	-5.804	1.4674	1.0763
H	4.4016	2.3107	-0.0465	H	-5.6077	0.7247	-0.4964
H	5.5166	0.7473	-1.5439	H	-5.9228	-0.9979	1.2096
H	4.0886	0.5803	-2.5386	H	-4.6502	-0.3322	2.2058
H	4.2185	0.4718	1.3621	H	-4.5186	-0.9534	-1.6407
H	4.6147	-1.2432	1.3486	H	-4.0128	-2.6237	-1.4087
H	5.7098	-0.1029	0.6241	H	-5.5625	-2.104	-0.815
H	-7.5589	0.5714	-0.564	H	7.7925	1.7428	0.434
H	-6.2871	0.7104	-1.7674	H	7.453	0.0952	-0.0703
H	-6.2309	1.5486	1.1589	H	6.0436	1.7643	2.0469
H	-5.9757	2.54	-0.2759	H	6.8542	0.2065	2.2176
H	-6.2653	-1.0839	0.7035	H	5.6514	2.5265	-0.4769
H	-6.5253	-1.6351	-0.9424	H	6.6178	1.768	-1.73
H	-1.7275	-0.0819	-0.8343	H	3.1219	-1.6433	-0.6253
H	-1.6952	0.7623	0.6999	H	2.4663	-1.0436	0.8691
H	-2.228	-1.2406	1.9593	H	1.6957	1.0412	-0.2178
H	-2.13	-2.7766	-0.6892	H	2.6851	-0.2035	-2.8347
H	-2.3347	-3.4626	0.9136	H	1.8046	1.3086	-2.6592
H	-4.5055	-3.221	-0.2445	H	4.2312	1.6981	-2.8826
H	-4.4299	-2.3122	1.2562	H	3.5779	2.3127	-1.3728
H	-3.0885	-1.3989	-2.2306	H	4.6332	-1.2611	-2.3212
H	-4.7097	-2.0494	-2.4619	H	5.9086	-0.1919	-2.8953
H	-4.4187	-0.3106	-2.598	H	6.158	-1.1814	-1.4509
H	-4.1188	3.1413	1.5239	H	3.3834	-0.9882	2.5916
H	0.9587	-0.6952	-1.9119	H	-1.2834	0.037	1.7388
H	0.6477	5.1351	-0.5895	H	-3.9983	4.1486	-2.1844
H	0.7133	3.9367	-1.989	H	-3.4728	2.4059	-2.4283
H	0.0886	-1.4579	3.1562	H	0.3699	-1.0223	-3.1179
H	1.7851	4.8103	1.4025	H	-4.6573	5.022	-0.1625
1d-15	X axis(Å)	Y axis(Å)	Z axis(Å)	1d-16	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-2.8894	-3.5491	0.0143	C	3.1662	-3.6208	-0.826
C	-1.4875	-2.9457	0.038	C	1.7768	-3.019	-1.017
C	-1.4493	-1.4501	-0.3086	C	1.5506	-1.7091	-0.2485
C	-2.5143	-0.6372	0.4812	C	2.7265	-0.7077	-0.4252
C	-3.9584	-1.2407	0.4095	C	4.1422	-1.3319	-0.1786
C	-3.9032	-2.7348	0.825	C	4.2913	-2.6053	-1.0517
C	-2.5169	0.8776	0.1754	C	2.5576	0.6148	0.3568

C	-3.4918	1.6538	1.0934	C	3.6624	1.6475	0.013
C	-4.9009	1.0373	1.1313	C	5.0728	1.0426	0.1395
C	-4.8704	-0.4702	1.4078	C	5.2185	-0.2916	-0.6019
C	-4.6283	-1.1452	-0.983	C	4.4384	-1.7157	1.2922
O	-0.1264	-0.9626	0.1216	O	0.3583	-1.0858	-0.8494
C	-3.5246	3.1379	0.7837	C	3.5728	2.9414	0.8071
C	6.2684	1.6785	0.6062	C	-6.745	1.7386	-0.3472
C	6.0537	0.5282	1.582	C	-6.8408	0.2187	-0.3663
C	4.826	-0.2888	1.257	C	-5.5761	-0.4838	0.0742
C	4.2347	-0.2806	0.0373	C	-4.3724	0.1317	0.1841
C	4.8481	0.4821	-1.156	C	-4.2012	1.6227	-0.1785
C	6.206	1.1598	-0.8195	C	-5.4254	2.1869	-0.9517
C	2.885	-0.9076	-0.2841	C	-3.0881	-0.5304	0.6687
C	1.8747	0.1754	-0.7249	C	-1.9125	-0.3392	-0.3109
C	2.4322	1.0093	-1.8942	C	-1.6893	1.154	-0.5889
C	3.8285	1.5665	-1.5914	C	-2.9675	1.8154	-1.0998
C	5.1377	-0.4778	-2.3364	C	-4.0195	2.4438	1.1202
C	4.3032	-1.0679	2.423	C	-5.8012	-1.9294	0.3949
O	4.7928	-0.9914	3.5448	O	-6.8845	-2.4819	0.2345
C	0.5213	-0.4422	-0.9953	C	-0.6156	-0.9752	0.137
C	-1.3622	-1.2076	-1.8019	C	1.0568	-1.9387	1.1661
O	-2.1008	-0.7284	1.882	O	2.6884	-0.3223	-1.8328
C	-3.1423	4.0785	1.6638	C	3.0502	3.1006	2.0345
O	-2.1542	-1.5538	-2.6636	O	1.6505	-2.4715	2.0899
C	-0.1267	-0.5224	-2.1534	C	-0.3042	-1.4498	1.3388
C	-3.9995	3.6201	-0.5427	C	4.099	4.1773	0.1534
O	-4.3382	2.8703	-1.4491	O	4.5816	4.1853	-0.972
H	-3.2261	-3.655	-1.0222	H	3.2412	-4.0603	0.174
H	-2.8462	-4.5674	0.4193	H	3.2934	-4.4539	-1.5279
H	-1.0561	-3.0984	1.0367	H	1.6179	-2.8415	-2.0894
H	-0.8394	-3.5126	-0.6429	H	1.0206	-3.7631	-0.7351
H	-3.6439	-2.8194	1.8885	H	4.3059	-2.3332	-2.1152
H	-4.8951	-3.1925	0.7193	H	5.2554	-3.0898	-0.8511
H	-1.5137	1.2923	0.3412	H	1.5924	1.0746	0.1076
H	-2.7495	1.0454	-0.88	H	2.539	0.4054	1.4306
H	-3.0969	1.5523	2.1155	H	3.5104	1.9092	-1.0436
H	-5.4939	1.5261	1.9152	H	5.33	0.9066	1.1974
H	-5.436	1.2219	0.1936	H	5.817	1.7424	-0.2615
H	-5.8953	-0.861	1.3669	H	6.2249	-0.6909	-0.4218
H	-4.5338	-0.6337	2.4396	H	5.1659	-0.1025	-1.6818
H	-4.5235	-0.1569	-1.4374	H	4.1813	-0.9234	1.9995
H	-4.2437	-1.8761	-1.6932	H	3.9217	-2.6203	1.6104
H	-5.7034	-1.3511	-0.9078	H	5.5066	-1.9283	1.4256
H	5.5122	2.4566	0.764	H	-7.5806	2.1654	-0.9139
H	7.2441	2.1415	0.7932	H	-6.8437	2.1091	0.6795
H	5.9782	0.962	2.5863	H	-7.0834	-0.1147	-1.3836
H	6.9289	-0.1334	1.5804	H	-7.6829	-0.0689	0.2752

H	6.4081	1.9808	-1.5189	H	-5.3996	1.8536	-1.9984
H	7.0285	0.4427	-0.9513	H	-5.3881	3.2831	-0.981
H	3.0049	-1.6673	-1.0656	H	-2.8376	-0.1062	1.6495
H	2.4625	-1.4448	0.5671	H	-3.2093	-1.6019	0.8377
H	1.7368	0.8684	0.1189	H	-2.1949	-0.8263	-1.2559
H	2.4741	0.4101	-2.8113	H	-1.3352	1.6643	0.3153
H	1.7572	1.8485	-2.1055	H	-0.903	1.2865	-1.3431
H	4.1953	2.0937	-2.4815	H	-2.7773	2.8855	-1.2534
H	3.731	2.3251	-0.8036	H	-3.1824	1.3978	-2.0933
H	4.2403	-0.9544	-2.7398	H	-3.1137	2.1674	1.6687
H	5.612	0.0597	-3.1663	H	-3.9445	3.515	0.8997
H	5.8173	-1.282	-2.0296	H	-4.8611	2.3054	1.8077
H	3.4579	-1.7419	2.2358	H	-4.9482	-2.4965	0.7861
H	-1.1402	-0.5511	1.9024	H	1.7593	-0.1068	-2.0453
H	-3.1698	5.1407	1.4399	H	3.0175	4.0654	2.5334
H	-2.7879	3.8052	2.6542	H	2.6474	2.2678	2.6008
H	0.1408	-0.2043	-3.1429	H	-0.8641	-1.4961	2.2533
H	-4.0252	4.7153	-0.6736	H	4.0283	5.1038	0.7482
1d-17	X axis(Å)	Y axis(Å)	Z axis(Å)	1d-18	X axis(Å)	Y axis(Å)	Z axis(Å)
C	3.3284	-3.5241	-0.599	C	3.3384	-2.9046	-1.3427
C	1.8929	-3.0456	-0.8004	C	2.6499	-2.9408	0.0171
C	1.6113	-1.6585	-0.2049	C	1.9729	-1.6095	0.3782
C	2.6987	-0.6183	-0.5991	C	2.5585	-0.3734	-0.377
C	4.1661	-1.1034	-0.3422	C	4.0885	-0.4976	-0.6525
C	4.3692	-2.4827	-1.0234	C	4.3764	-1.7828	-1.4892
C	2.4631	0.7994	-0.031	C	2.1916	0.9787	0.2776
C	3.4914	1.8212	-0.5729	C	2.6725	2.1895	-0.5515
C	4.9464	1.3425	-0.4298	C	4.1879	2.0764	-0.8126
C	5.149	-0.0759	-0.9746	C	4.5646	0.7422	-1.466
C	4.5477	-1.2355	1.1525	C	4.9365	-0.5683	0.6402
O	0.3433	-1.2042	-0.8023	O	0.5544	-1.7006	0.0131
C	3.2868	3.2107	-8.00E-04	C	2.2321	3.4936	0.0966
C	-6.3083	1.169	-1.3865	C	-6.3212	0.1178	-0.9449
C	-6.6577	6.00E-04	-0.4731	C	-5.7199	1.2594	-0.1349
C	-5.4502	-0.5655	0.2355	C	-4.2314	1.1325	0.0885
C	-4.2911	0.1214	0.3834	C	-3.5363	-0.0165	-0.099
C	-4.1569	1.5925	-0.0649	C	-4.2351	-1.3089	-0.5704
C	-5.4803	2.1872	-0.6228	C	-5.782	-1.216	-0.4545
C	-2.9843	-0.4642	0.8985	C	-2.0359	-0.1658	0.1142
C	-1.893	-0.4022	-0.1948	C	-1.679	-1.3692	1.0089
C	-1.7294	1.0285	-0.7398	C	-2.2833	-2.6625	0.4549
C	-3.0661	1.6471	-1.165	C	-3.7959	-2.5211	0.2955
C	-3.7547	2.5016	1.1227	C	-3.8655	-1.5647	-2.051
C	-5.6463	-1.9695	0.715	C	-3.5943	2.4211	0.5091
O	-6.6772	-2.6019	0.5123	O	-4.252	3.3863	0.8859
C	-0.5483	-0.9439	0.2345	C	-0.1858	-1.486	1.1693
C	1.2183	-1.7284	1.257	C	1.8724	-1.4539	1.8852

O	2.5658	-0.4584	-2.0479	O	1.9233	-0.3339	-1.6892
C	2.9657	4.2741	-0.7568	C	3.0172	4.4015	0.6998
O	1.8677	-2.1815	2.1857	O	2.7942	-1.3899	2.6845
C	-0.1293	-1.2178	1.466	C	0.4835	-1.3631	2.3114
C	3.4435	3.4543	1.4598	C	0.7769	3.832	0.0264
O	3.69	2.5676	2.2669	O	-0.0641	3.0774	-0.4493
H	3.4773	-3.8083	0.4479	H	3.8226	-3.8691	-1.537
H	3.4839	-4.4401	-1.1817	H	2.5753	-2.7945	-2.1236
H	1.6759	-3.0296	-1.8772	H	1.9117	-3.7529	0.0137
H	1.2029	-3.789	-0.3808	H	3.3971	-3.2144	0.7714
H	4.3238	-2.3727	-2.1148	H	4.4433	-1.5413	-2.5581
H	5.3721	-2.8691	-0.8008	H	5.3654	-2.1809	-1.2266
H	1.4671	1.1565	-0.3229	H	2.6038	1.0489	1.2909
H	2.4726	0.7702	1.0623	H	1.1022	1.0341	0.3801
H	3.3092	1.8948	-1.6556	H	2.1867	2.1562	-1.5371
H	5.6122	2.0257	-0.9727	H	4.5115	2.8928	-1.4705
H	5.2707	1.378	0.6159	H	4.7508	2.1868	0.1215
H	6.1877	-0.3819	-0.7947	H	5.6526	0.7068	-1.6069
H	5.0327	-0.0555	-2.0659	H	4.1316	0.7213	-2.4748
H	4.2439	-0.3697	1.7461	H	4.6961	0.231	1.3461
H	4.1258	-2.1218	1.6245	H	4.8171	-1.5205	1.1618
H	5.6345	-1.3358	1.2647	H	6.0049	-0.4802	0.408
H	-5.7603	0.8123	-2.2666	H	-7.4131	0.1372	-0.8501
H	-7.2293	1.6361	-1.7539	H	-6.0989	0.2542	-2.0093
H	-7.1398	-0.7652	-1.0925	H	-6.2131	1.3067	0.8445
H	-7.3914	0.3184	0.2781	H	-5.9509	2.1966	-0.6561
H	-5.2705	3.0494	-1.2684	H	-6.0912	-1.3436	0.5922
H	-6.098	2.5711	0.2013	H	-6.2571	-2.0319	-1.0137
H	-2.6749	0.0808	1.7977	H	-1.5569	-0.2632	-0.8686
H	-3.0844	-1.5044	1.2148	H	-1.5916	0.7206	0.5725
H	-2.2378	-1.0372	-1.0247	H	-2.1208	-1.1906	2.0003
H	-1.2472	1.6669	0.0109	H	-1.8282	-2.9283	-0.5067
H	-1.0576	1.0243	-1.6079	H	-2.0724	-3.4962	1.1366
H	-2.8891	2.6864	-1.4701	H	-4.1978	-3.4505	-0.1281
H	-3.4156	1.1195	-2.0623	H	-4.2299	-2.4308	1.301
H	-2.7766	2.2568	1.5457	H	-2.7921	-1.7248	-2.1932
H	-3.7103	3.5517	0.81	H	-4.3764	-2.4555	-2.4346
H	-4.4851	2.428	1.9374	H	-4.1467	-0.7209	-2.6906
H	-4.8257	-2.4225	1.2851	H	-2.4994	2.4751	0.4681
H	1.609	-0.3844	-2.2338	H	0.9705	-0.4977	-1.5455
H	2.8231	5.2685	-0.3442	H	2.6261	5.3203	1.1282
H	2.8388	4.1769	-1.8317	H	4.0893	4.2618	0.7938
H	-0.6112	-1.1278	2.4207	H	0.1404	-1.1858	3.3127
H	3.3158	4.4999	1.788	H	0.4899	4.812	0.4444
1d-19	X axis(Å)	Y axis(Å)	Z axis(Å)				
C	3.648	-3.2851	-0.4709				
C	2.1361	-3.0764	-0.4643				

C	1.6896	-1.7582	0.1841
C	2.5153	-0.5413	-0.32
C	4.0664	-0.7553	-0.2748
C	4.4148	-2.0742	-1.0135
C	2.1194	0.8056	0.3269
C	2.8422	2.0092	-0.3312
C	4.3652	1.7945	-0.4027
C	4.7484	0.4372	-1.0047
C	4.6745	-0.8217	1.1478
O	0.2974	-1.541	-0.25
C	2.5292	3.3503	0.314
C	-6.5736	-0.0586	-0.086
C	-5.9708	1.2984	0.2569
C	-4.4637	1.2621	0.3339
C	-3.7179	0.2789	-0.2258
C	-4.3519	-0.8211	-1.1048
C	-5.8816	-0.6342	-1.3094
C	-2.2289	0.0717	0.0084
C	-1.9747	-1.2954	0.6784
C	-2.6097	-2.4483	-0.1151
C	-4.0898	-2.1867	-0.4172
C	-3.732	-0.8178	-2.5241
C	-3.8754	2.3904	1.1201
O	-4.5589	3.196	1.7422
C	-0.5012	-1.5302	0.8846
C	1.498	-1.8794	1.6847
O	2.1625	-0.4014	-1.73
C	2.1779	3.5685	1.5923
O	2.3478	-2.1013	2.5321
C	0.0995	-1.7152	2.0547
C	2.5945	4.5576	-0.5635
O	2.8747	4.5035	-1.7543
H	3.9882	-3.5326	0.5399
H	3.8843	-4.1607	-1.0877
H	1.7742	-3.1108	-1.501
H	1.6572	-3.929	0.0343
H	4.1952	-1.9752	-2.0846
H	5.4919	-2.2727	-0.9436
H	1.0402	0.971	0.2126
H	2.3206	0.7688	1.4018
H	2.4681	2.0559	-1.3636
H	4.8257	2.5835	-1.0108
H	4.806	1.892	0.5973
H	5.8403	0.3288	-0.9722
H	4.4844	0.4368	-2.0701
H	4.3243	-0.0169	1.7989
H	4.4747	-1.765	1.6547

H	5.7679	-0.742	1.1018
H	-6.4772	-0.7427	0.7654
H	-7.646	0.055	-0.282
H	-6.4019	1.616	1.2138
H	-6.2682	2.0408	-0.4942
H	-6.3507	-1.5877	-1.5829
H	-6.0692	0.0464	-2.1518
H	-1.6941	0.1528	-0.9452
H	-1.7895	0.8413	0.647
H	-2.4612	-1.2729	1.6651
H	-2.0672	-2.618	-1.053
H	-2.5242	-3.3817	0.4561
H	-4.469	-3.0042	-1.0438
H	-4.6465	-2.2406	0.5277
H	-2.6609	-1.0376	-2.5305
H	-4.2144	-1.5695	-3.1602
H	-3.862	0.1585	-3.0063
H	-2.7824	2.4892	1.1068
H	1.1896	-0.4636	-1.7899
H	1.9623	4.5622	1.976
H	2.1082	2.7634	2.3159
H	-0.2967	-1.7497	3.0518
H	2.3708	5.521	-0.0746

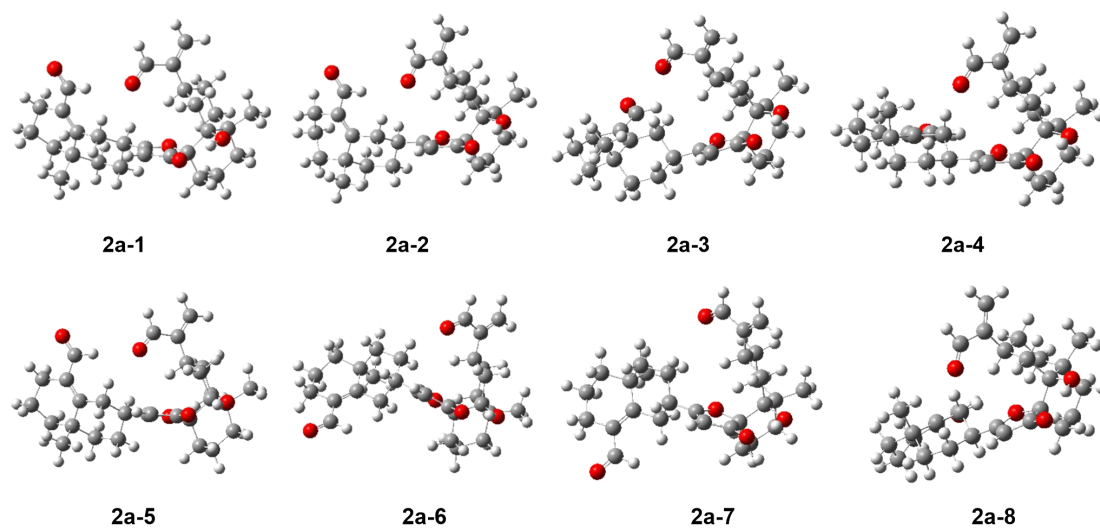


Figure S11. Optimized geometries of predominant conformers for **2a** at the B3LYP/6-31G (d,p) level

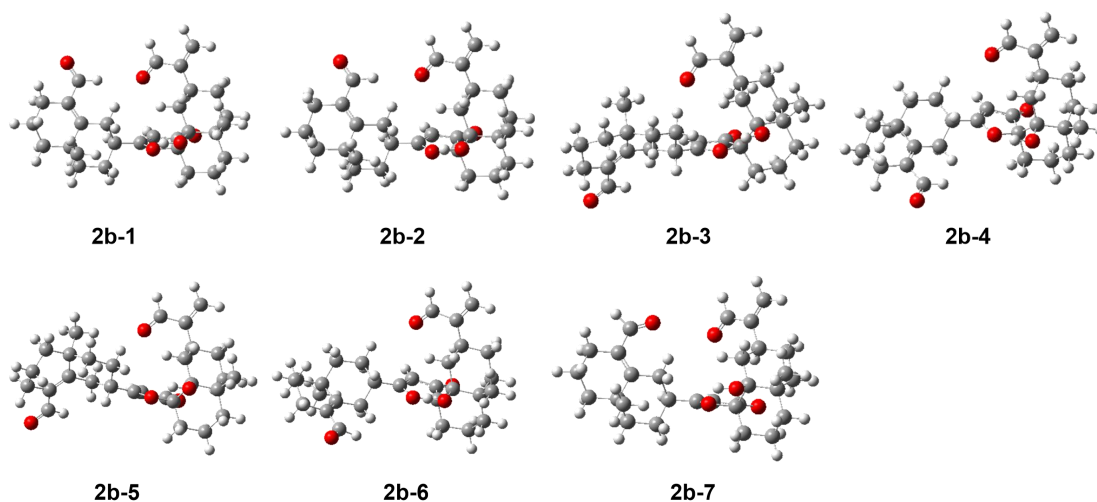


Figure S12. Optimized geometries of predominant conformers for **2b** at the B3LYP/6-31G (d,p) level

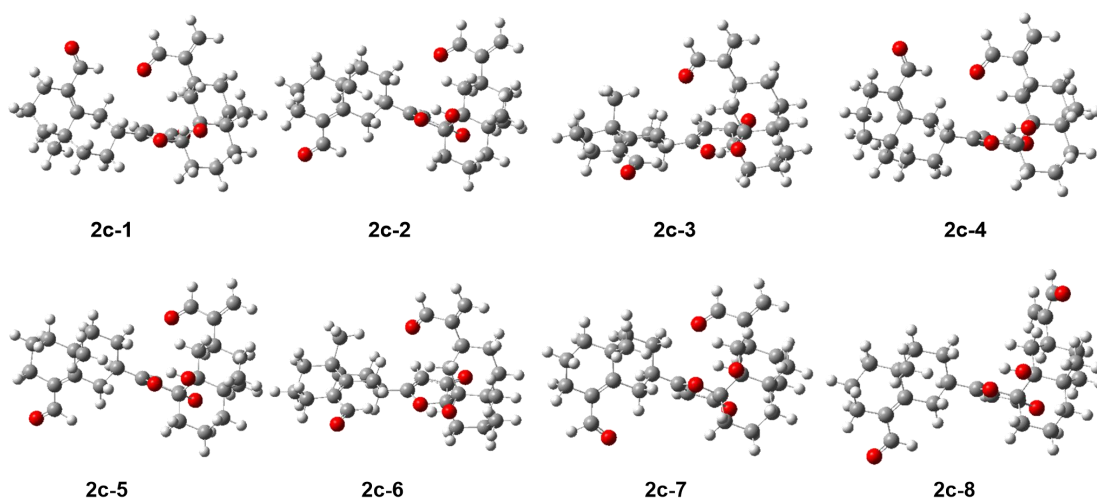


Figure S13. Optimized geometries of predominant conformers for **2c** at the B3LYP/6-31G (d,p) level

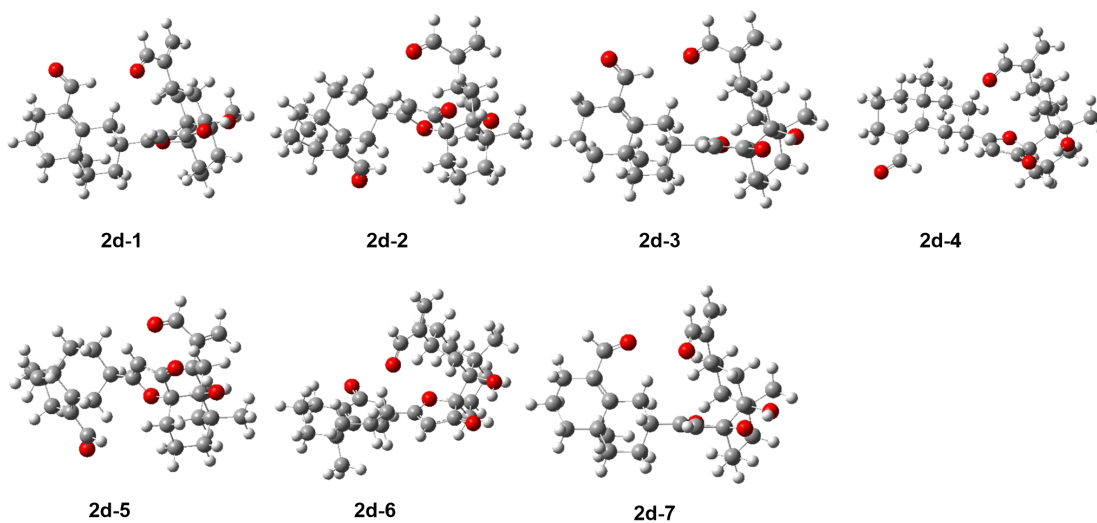


Figure S14. Optimized geometries of predominant conformers for **2d** at the B3LYP/6-31G (d,p) level

Table S4. Conformational analysis of the optimized **2a-2d** at the B3LYP/6-31G(d,p) level in the gas phase

	<i>Conformers</i>	G (Hartree)	ΔG (Kcal/mol)	Population
2a	2a-1	-1503.56707	0	32.74%
	2a-2	-1503.56598	0.68210337	10.31%
	2a-3	-1503.56436	1.70180712	1.84%
	2a-4	-1503.56542	1.03664652	5.67%
	2a-5	-1503.56707	-0.00062751	32.67%
	2a-6	-1503.56551	0.98079813	6.23%
	2a-7	-1503.56588	0.74799192	9.23%
	2a-8	-1503.56404	1.90449285	1.31%
	<i>Conformers</i>	G (Hartree)	ΔG (Kcal/mol)	Population
2b	2b-1	-1503.55999	0	32.74%
	2b-2	-1503.55862	0.85843368	7.68%
	2b-3	-1503.55957	0.26292669	21.00%
	2b-4	-1503.55968	0.19264557	23.65%
	2b-5	-1503.55742	1.61019066	2.16%
	2b-6	-1503.55907	0.58044675	12.29%
	2b-7	-1503.55599	2.51129502	0.47%
	<i>Conformers</i>	G (Hartree)	ΔG (Kcal/mol)	Population
2c	2c-1	-1503.55986	0	29.73%
	2c-2	-1503.55983	0.0188253	28.80%
	2c-3	-1503.55888	0.60993972	10.61%
	2c-4	-1503.55820	1.03978407	5.14%
	2c-5	-1503.55883	0.64257024	10.05%
	2c-6	-1503.55751	1.47339348	2.47%
	2c-7	-1503.55761	1.40938746	2.75%
	2c-8	-1503.55887	0.61872486	10.46%
	<i>Conformers</i>	G (Hartree)	ΔG (Kcal/mol)	Population
2d	2d-1	-1503.56686	0.34262046	30.70%
	2d-2	-1503.56489	1.57944267	3.80%

2d-3	-1503.56741	0	54.76%
2d-4	-1503.56425	1.98544164	1.92%
2d-5	-1503.56492	1.56312741	3.91%
2d-6	-1503.56511	1.44201798	4.80%
2d-7	-1503.56162	3.63077286	0.12%

Functional mPW1PW91		Solvent? PCM		Basis Set 6-311+G(d, p)			Type of Data Unscaled Shifts	
		DP4+	100.00%	0.00%	0.00%	0.00%	-	
Nuclei	sp2?	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	
C		17.8	21.79144	19.32576	19.66939	21.98157		
C		32.4	36.58948	34.43455	34.42308	36.88207		
C		93	99.91618	101.66301	101.97703	100.17876		
C		74.5	81.14559	82.31426	82.4668	81.04481		
C		37.4	43.21026	45.35631	45.59831	43.20041		
C		35.9	38.50166	38.51452	38.93547	38.65965		
C		38.9	43.14244	38.8055	38.55492	43.7994		
C		31.9	36.3865	37.66566	38.63409	35.79981		
C		25.3	27.34715	26.76923	27.0323	27.16		
C		32.8	35.62858	34.08509	34.25058	35.69729		
C		23.3	23.84116	25.15494	25.37836	23.918		
C	x	154.6	163.88979	163.52575	163.70674	164.03568		
C		17.8	21.30092	21.42837	21.50497	21.32356		
C		24	27.39453	27.39394	27.77938	27.50378		
C	x	134.2	142.66947	142.37139	142.5019	142.42689		
C	x	160.3	176.64615	177.13083	177.32481	176.96322		
C		36.7	43.05925	43.23182	43.44446	43.08861		
C		39.4	41.77093	41.76948	41.82879	41.8151		
C		26.3	29.4719	30.933	30.17548	30.78609		
C		41.8	47.60592	46.81796	47.28239	47.52158		
C		26	30.60885	27.86613	29.42013	27.81382		
C		40.8	44.53219	43.82744	44.30614	44.10792		
C		25.1	26.60765	26.68197	26.72074	26.58974		
C	x	191.4	200.41716	198.92073	199.03546	198.7145		
C	x	196.3	208.11332	201.88341	202.35973	207.25919		
C	x	210.4	219.41183	213.34085	213.50027	219.64035		
C	x	133	146.0152	146.04031	146.3107	146.25945		
C	x	101.9	107.62434	111.57571	111.53378	108.73719		
C	x	194.5	205.24959	205.48995	205.51808	205.23919		
H	x	9.41	9.71641	9.73309	9.7942	9.691		
H		1.52	1.51809	1.41645	1.53852	1.53592		
H		1.79	1.93426	2.5383	2.42015	1.98209		
H		1.35	1.36654	1.57752	1.60105	1.36473		
H		2.15	2.20125	2.40978	2.4085	2.20438		
H		1.27	1.25451	1.28063	1.28242	1.27747		
H		1.91	2.03291	1.91482	1.91218	2.04862		
H		1.4	1.33293	1.97651	1.88683	1.31196		
H		1.47	1.33247	1.02179	1.22796	1.28543		
H		2.81	3.04076	2.54575	2.56863	3.09366		
H		1.51	1.33465	1.36476	1.33528	1.30556		
H		1.58	1.8547	1.75042	1.86257	1.90232		
H		1.16	1.18677	1.04153	1.03465	1.22127		
H		2.29	2.43402	3.33778	3.33177	2.45305		
H		1.06	1.45077	1.41834	1.42851	1.44668		
H		1.06	0.367	0.40756	0.41724	0.37532		
H		1.06	1.53041	1.54155	1.58852	1.56977		
H		1.54	1.62247	1.62749	1.68298	1.66467		
H		1.65	1.64976	1.64114	1.63562	1.60762		
H		2.39	2.59854	2.49463	2.14845	2.08515		
H		2.08	2.04023	2.19913	2.54362	2.56605		
H		1.61	1.60629	1.61851	1.4387	1.41099		
H		1.4	1.38965	1.43505	1.66542	1.62226		
H		3.92	4.53639	4.1444	2.71652	2.40121		
H		2.37	2.59932	2.48508	4.01364	4.20716		
H		2.73	2.7689	2.74135	2.76665	2.97864		
H		1.87	2.05322	2.04735	2.07529	2.18147		
H		2.06	2.03921	2.22164	2.11197	2.28157		
H		1.61	1.62106	1.65347	1.85974	1.91614		
H		1.78	1.89443	1.83729	1.65604	1.65361		
H		1.25	0.81848	0.82421	1.66168	1.91519		
H		1.25	1.95591	1.99862	1.4671	0.80636		
H		1.25	1.34313	1.25116	0.91419	1.27245		
H	x	10.26	10.86402	10.71334	10.73513	10.6126		
H		5.09	5.5181	2.03546	2.03308	5.50219		
H	x	5.93	6.48762	6.44414	6.41283	6.48695		
H	x	6.22	6.81074	6.78455	6.79859	6.85275		
H	x	5.59	5.76835	5.72117	5.73777	5.74329		

Functional	Solvent?		Basis Set		Type of Data	
mPW1PW91	PCM		6-311+G(d,p)		Unscaled Shifts	
	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	100.00%	0.00%	0.00%	0.00%	-	-
sDP4+ (C data)	90.64%	0.00%	0.00%	9.36%	-	-
sDP4+ (all data)	100.00%	0.00%	0.00%	0.00%	-	-
uDP4+ (H data)	100.00%	0.00%	0.00%	0.00%	-	-
uDP4+ (C data)	67.02%	0.00%	0.00%	32.98%	-	-
uDP4+ (all data)	100.00%	0.00%	0.00%	0.00%	-	-
DP4+ (H data)	100.00%	0.00%	0.00%	0.00%	-	-
DP4+ (C data)	95.16%	0.00%	0.00%	4.84%	-	-
DP4+ (all data)	100.00%	0.00%	0.00%	0.00%	-	-

Figure S15. DP4+ analysis of experimental NMR data of **2** and unscaled shifts of **2a-2d** (Isomer 1-4)

Table S5. The Cartesian coordinates of the lowest energy conformers for **2a-2d** in the gas phase at the B3LYP/6-31G(d,p) level

2a-1	X axis(Å)	Y axis(Å)	Z axis(Å)	2a-2	X axis(Å)	Y axis(Å)	Z axis(Å)
C	3.5441	-2.7128	-1.0641	C	3.4703	-2.6563	-1.2382
C	2.9984	-2.6068	0.354	C	2.968	-2.6214	0.1992
C	2.3839	-1.2251	0.6024	C	2.3566	-1.2566	0.5333
C	3.411	-0.0641	0.3459	C	3.3704	-0.0785	0.3009
C	4.0989	-0.1787	-1.0679	C	4.0153	-0.1224	-1.1371
C	4.5843	-1.6327	-1.3344	C	4.4981	-1.5594	-1.4871
C	2.8013	1.3516	0.5359	C	2.7604	1.3234	0.5757
C	1.8896	1.8363	-0.6085	C	1.8124	1.8561	-0.517
C	2.5816	1.6859	-1.9733	C	2.464	1.7746	-1.9071
C	3.1286	0.2725	-2.1897	C	3.0096	0.376	-2.2065
C	5.3783	0.7058	-1.1517	C	5.2881	0.7719	-1.2174
O	1.185	-1.1242	-0.1984	O	1.1325	-1.1229	-0.223
C	1.3692	3.2341	-0.3134	C	1.2921	3.2346	-0.142
C	-6.3658	-0.3628	-0.923	C	-5.6148	-0.0283	-1.7907
C	-5.7376	0.9702	-0.5356	C	-5.5094	1.0511	-0.72
C	-4.4108	0.8369	0.1756	C	-4.3288	0.8475	0.1984
C	-3.6904	-0.3113	0.2071	C	-3.7043	-0.3469	0.3409
C	-4.1487	-1.5729	-0.5551	C	-4.2073	-1.6235	-0.3648
C	-5.3169	-1.2756	-1.5364	C	-5.5304	-1.4028	-1.1496
C	-2.3781	-0.5006	0.955	C	-2.394	-0.5612	1.0817
C	-1.2524	-0.9726	0.0167	C	-1.296	-0.9744	0.0788
C	-1.6561	-2.2906	-0.6581	C	-1.713	-2.2377	-0.6949
C	-2.9797	-2.1378	-1.4095	C	-3.0955	-2.0845	-1.3456
C	-4.6205	-2.6416	0.4587	C	-4.5048	-2.7487	0.6564
C	-3.978	2.1061	0.8446	C	-3.8778	2.1016	0.8827
O	-4.6131	3.152	0.7458	O	-4.3957	3.194	0.6713
C	0.0981	-1.1103	0.6789	C	0.0743	-1.1512	0.6884
C	1.8222	-1.1732	2.0052	C	1.8399	-1.2764	1.9541
O	4.4786	-0.187	1.3186	O	4.4678	-0.2409	1.2337

C	1.8348	4.391	-0.8117	C	1.7318	4.4168	-0.6031
O	2.4728	-1.1346	3.0406	O	2.5231	-1.287	2.9691
C	0.37	-1.1411	1.9822	C	0.3877	-1.247	1.9791
C	0.1931	3.3363	0.6024	C	0.1453	3.2851	0.8145
H	-0.1794	4.3561	0.799	H	-0.2344	4.2911	1.0619
O	-0.3386	2.3562	1.1123	O	-0.355	2.2785	1.3042
H	4.0028	-3.6989	-1.2022	H	3.9279	-3.6324	-1.4377
H	2.728	-2.6469	-1.7923	H	2.6321	-2.5593	-1.9372
H	2.2454	-3.3932	0.4933	H	2.2223	-3.4173	0.3232
H	3.7997	-2.8084	1.076	H	3.7917	-2.8538	0.8857
H	4.9324	-1.727	-2.3712	H	4.8155	-1.6024	-2.5371
H	5.4571	-1.8475	-0.7027	H	5.3901	-1.7997	-0.8925
H	2.2633	1.3939	1.4914	H	2.2514	1.3173	1.5479
H	3.6193	2.0736	0.6712	H	3.5788	2.043	0.7203
H	1.0067	1.1941	-0.6627	H	0.9317	1.2114	-0.5756
H	1.8674	1.9153	-2.7746	H	1.7256	2.0379	-2.6752
H	3.4006	2.4047	-2.0818	H	3.2766	2.5022	-2.0051
H	3.6413	0.2435	-3.1601	H	3.4927	0.3954	-3.1922
H	2.2866	-0.4203	-2.2848	H	2.1678	-0.3159	-2.3085
H	6.1562	0.3603	-0.4614	H	6.0881	0.3981	-0.5684
H	5.8086	0.6716	-2.1597	H	5.6874	0.7883	-2.2385
H	5.1842	1.7552	-0.9155	H	5.0972	1.8079	-0.9253
H	-6.8198	-0.835	-0.0443	H	-6.5661	0.0765	-2.3249
H	-7.1773	-0.1906	-1.6395	H	-4.8186	0.0967	-2.5341
H	-6.4573	1.5073	0.0944	H	-6.4257	1.0711	-0.1169
H	-5.5866	1.5747	-1.4392	H	-5.4414	2.0163	-1.2358
H	-5.7888	-2.2099	-1.8654	H	-6.3909	-1.5113	-0.4745
H	-4.9355	-0.7915	-2.446	H	-5.6516	-2.1755	-1.9193
H	-2.0515	0.405	1.4655	H	-2.0632	0.326	1.6214
H	-2.5388	-1.2335	1.7559	H	-2.5295	-1.3243	1.8566
H	-1.1413	-0.2074	-0.766	H	-1.2065	-0.1546	-0.6502
H	-0.8827	-2.6055	-1.3704	H	-0.9797	-2.456	-1.4819
H	-1.7359	-3.0933	0.0853	H	-1.7104	-3.1081	-0.0273
H	-2.7961	-1.4712	-2.2638	H	-3.0034	-1.3621	-2.1673
H	-3.2617	-3.109	-1.8362	H	-3.3732	-3.0402	-1.8085
H	-5.0112	-3.5264	-0.0573	H	-4.927	-3.6273	0.1539
H	-3.8127	-2.9867	1.1114	H	-3.6171	-3.0915	1.1949
H	-5.4153	-2.2592	1.1084	H	-5.2306	-2.4148	1.4075
H	-3.0538	2.0767	1.4336	H	-3.0618	2.0106	1.6099
H	4.0843	-0.2411	2.2147	H	4.1016	-0.3403	2.1377
H	1.3976	5.3535	-0.5602	H	1.2951	5.363	-0.2948
H	2.6831	4.4245	-1.4875	H	2.5566	4.4883	-1.3044
H	-0.2683	-1.0981	2.8432	H	-0.2225	-1.2442	2.8614
2a-3	X axis(Å)	Y axis(Å)	Z axis(Å)	2a-4	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-3.0766	-1.4535	2.6402	C	2.9871	-0.9388	-2.9185
C	-2.9065	-2.2806	1.3717	C	2.8386	-1.9605	-1.7974
C	-2.3839	-1.4111	0.2203	C	2.3295	-1.2886	-0.5157

C	-3.3422	-0.2036	-0.0742	C	3.2932	-0.1416	-0.0424
C	-3.6393	0.6449	1.2192	C	3.575	0.9044	-1.1858
C	-4.0205	-0.279	2.412	C	3.9341	0.1864	-2.5191
C	-2.8585	0.7238	-1.2193	C	2.8155	0.5811	1.2429
C	-1.6834	1.6543	-0.8604	C	1.6378	1.5519	1.0462
C	-1.9477	2.4225	0.4439	C	1.9157	2.5395	-0.1
C	-2.4155	1.5201	1.5884	C	2.3509	1.8341	-1.3883
C	-4.8624	1.5876	1.0199	C	4.8081	1.7958	-0.8532
O	-1.0256	-1.0295	0.5407	O	0.9677	-0.8637	-0.7627
C	-1.2872	2.6229	-1.9658	C	1.2603	2.1988	2.3692
C	6.1865	0.2471	0.3539	C	-6.198	0.5	-0.3332
C	5.2656	1.0566	1.2576	C	-5.2857	1.3358	-1.2215
C	3.7973	0.8963	0.9396	C	-3.8111	1.1166	-0.9702
C	3.2976	-0.0991	0.1654	C	-3.3165	0.0743	-0.2568
C	4.2192	-1.1627	-0.4612	C	-4.2471	-1.0038	0.3352
C	5.6391	-1.1586	0.1698	C	-5.6845	-0.9276	-0.25
C	1.8225	-0.2723	-0.1762	C	-1.8416	-0.153	0.0543
C	1.2971	-1.6986	0.08	C	-1.3532	-1.5641	-0.327
C	2.1736	-2.7296	-0.646	C	-2.2333	-2.627	0.3488
C	3.6384	-2.5837	-0.2397	C	-3.7073	-2.4205	0.0047
C	4.352	-0.8796	-1.9767	C	-4.3296	-0.8163	1.8689
C	2.9534	1.9753	1.5476	C	-2.9552	2.1867	-1.5751
O	3.3883	2.7446	2.4	O	-3.4159	3.0941	-2.2605
C	-0.1762	-1.8006	-0.2578	C	0.1279	-1.7271	-0.0522
C	-2.1677	-2.2717	-1.0031	C	2.1307	-2.3318	0.5597
O	-4.6178	-0.743	-0.5038	O	4.5738	-0.7394	0.2799
C	-2.0681	3.0833	-2.9571	C	1.5292	3.4539	2.7638
O	-3.0373	-2.6918	-1.7538	O	3.0164	-2.8932	1.19
C	-0.753	-2.5457	-1.1994	C	0.7169	-2.6015	0.7624
C	0.1284	3.0996	-1.9753	C	0.4752	1.3604	3.3252
H	0.3906	3.8205	-2.7682	H	0.215	1.8372	4.2855
O	0.9631	2.7184	-1.1634	O	0.1303	0.2121	3.0706
H	-3.4789	-2.091	3.4363	H	3.3763	-1.4381	-3.8136
H	-2.1034	-1.0951	2.9938	H	2.0081	-0.5304	-3.1937
H	-2.208	-3.0995	1.5867	H	2.1388	-2.7377	-2.1306
H	-3.8613	-2.7482	1.1005	H	3.7985	-2.4607	-1.618
H	-4.0837	0.3098	3.3363	H	3.9817	0.9173	-3.3367
H	-5.0261	-0.6898	2.2471	H	4.9421	-0.2436	-2.4406
H	-2.5961	0.1253	-2.1013	H	2.5718	-0.164	2.0104
H	-3.7184	1.3189	-1.5517	H	3.6624	1.1285	1.6804
H	-0.8182	1.0076	-0.6989	H	0.7606	0.9821	0.734
H	-1.0347	2.9397	0.7658	H	1.0112	3.1259	-0.307
H	-2.6899	3.2118	0.2715	H	2.6881	3.2621	0.185
H	-2.6578	2.1536	2.4519	H	2.5844	2.5989	-2.1407
H	-1.5729	0.902	1.913	H	1.4977	1.2812	-1.7932
H	-5.7847	1.0234	0.842	H	5.7313	1.2077	-0.8004
H	-5.0298	2.1994	1.9145	H	4.9578	2.5559	-1.6293

H	-4.7374	2.2737	0.1782	H	4.7081	2.3206	0.1004
H	6.2966	0.7469	-0.6152	H	-6.2605	0.9452	0.6663
H	7.1883	0.2033	0.7966	H	-7.2152	0.5087	-0.7417
H	5.5625	2.1097	1.1787	H	-5.5485	2.3899	-1.0692
H	5.4272	0.7549	2.3005	H	-5.4938	1.1018	-2.2736
H	6.3329	-1.745	-0.4457	H	-6.3753	-1.5321	0.3512
H	5.6174	-1.647	1.1539	H	-5.7056	-1.3566	-1.2613
H	1.196	0.4113	0.3989	H	-1.2045	0.5718	-0.4529
H	1.6745	-0.0058	-1.2305	H	-1.6851	0.0195	1.1256
H	1.3837	-1.9013	1.1578	H	-1.4788	-1.6807	-1.4137
H	1.8404	-3.7454	-0.3979	H	-1.9341	-3.629	0.0158
H	2.0788	-2.6265	-1.7334	H	-2.1009	-2.6064	1.4372
H	3.7196	-2.854	0.8224	H	-3.8296	-2.6197	-1.0691
H	4.2352	-3.3228	-0.7896	H	-4.3039	-3.1802	0.526
H	5.0271	-1.6003	-2.4524	H	-5.0184	-1.5424	2.316
H	3.3933	-0.9432	-2.501	H	-3.3614	-0.9494	2.3615
H	4.7497	0.1229	-2.1685	H	-4.6848	0.185	2.1358
H	1.9144	2.0556	1.2051	H	-1.8765	2.1373	-1.3845
H	-4.461	-1.3604	-1.2493	H	4.4246	-1.4662	0.9216
H	-1.7043	3.7695	-3.7172	H	1.2113	3.8445	3.7267
H	-3.1124	2.8021	-3.0458	H	2.0882	4.1448	2.1411
H	-0.341	-3.2108	-1.9335	H	0.3118	-3.3507	1.4147
2a-5	X axis(Å)	Y axis(Å)	Z axis(Å)	2a-6	X axis(Å)	Y axis(Å)	Z axis(Å)
C	3.323	-2.0747	-2.1764	C	1.6904	-2.9217	-1.6318
C	2.9394	-2.5503	-0.7812	C	1.6057	-2.9081	-0.11
C	2.3522	-1.3998	0.048	C	1.8114	-1.4872	0.4311
C	3.3525	-0.1951	0.1647	C	3.1973	-0.8959	-0.0108
C	3.8756	0.2813	-1.2432	C	3.3998	-0.9668	-1.571
C	4.3257	-0.9299	-2.1098	C	3.0289	-2.3769	-2.1157
C	2.7844	1.0067	0.9636	C	3.4491	0.5453	0.5
C	1.7498	1.8681	0.2141	C	2.6588	1.6452	-0.2314
C	2.2687	2.2824	-1.1735	C	2.8376	1.5345	-1.7558
C	2.7828	1.0914	-1.9858	C	2.5555	0.1231	-2.2804
C	5.1388	1.1824	-1.1071	C	4.8918	-0.7532	-1.9636
O	1.0713	-1.0507	-0.5286	O	0.6678	-0.7011	0.0187
C	1.298	3.0274	1.0904	C	2.9913	3.0097	0.3523
C	-6.3315	0.1268	-0.5986	C	-6.1838	1.1434	-1.1276
C	-5.4077	1.2512	-1.049	C	-6.2632	-0.0975	-0.2482
C	-3.9813	1.1032	-0.5734	C	-4.922	-0.7308	0.0445
C	-3.4686	-0.0488	-0.074	C	-3.7343	-0.112	-0.1697
C	-4.33	-1.3226	0.0473	C	-3.6712	1.3304	-0.7172
C	-5.6471	-1.2194	-0.7705	C	-5.051	2.0429	-0.6629
C	-2.0386	-0.2172	0.4249	C	-2.3647	-0.7329	0.0795
C	-1.3319	-1.4436	-0.1771	C	-1.4578	0.1567	0.9512
C	-2.1523	-2.7165	0.0673	C	-1.3224	1.555	0.34
C	-3.5642	-2.5595	-0.4953	C	-2.6948	2.1906	0.1291
C	-4.6886	-1.5429	1.5364	C	-3.1951	1.2916	-2.1891

C	-3.1962	2.3739	-0.6792	C	-5.0443	-2.1257	0.5747
O	-3.6273	3.3734	-1.2454	O	-6.1254	-2.6367	0.8483
C	0.0876	-1.5518	0.3266	C	-0.1137	-0.4957	1.1552
C	1.9389	-1.9278	1.404	C	1.6543	-1.4894	1.9362
O	4.5204	-0.6537	0.8907	O	4.239	-1.7207	0.5685
C	1.6571	4.3168	0.9789	C	3.7535	3.9662	-0.2026
O	2.6905	-2.2091	2.3275	O	2.462	-1.9298	2.7425
C	0.4948	-2.0711	1.4837	C	0.3855	-0.8942	2.3233
C	0.3232	2.7127	2.1772	C	2.3785	3.341	1.6747
H	0.0241	3.5585	2.8193	H	2.628	4.333	2.0878
O	-0.1325	1.5887	2.353	O	1.6403	2.5696	2.2761
H	3.7637	-2.9092	-2.7345	H	1.5673	-3.95	-1.9916
H	2.4306	-1.7677	-2.7331	H	0.8667	-2.3425	-2.0642
H	2.2102	-3.3643	-0.8842	H	0.621	-3.2947	0.1829
H	3.8165	-2.9786	-0.2798	H	2.3493	-3.5954	0.3122
H	4.552	-0.5964	-3.1308	H	3.0321	-2.3667	-3.2133
H	5.2653	-1.3353	-1.7099	H	3.8042	-3.0967	-1.8191
H	2.3636	0.647	1.911	H	3.2548	0.587	1.5788
H	3.6192	1.6472	1.2823	H	4.5233	0.7671	0.4275
H	0.857	1.266	0.0244	H	1.592	1.4967	-0.049
H	1.4629	2.772	-1.7354	H	2.1612	2.2388	-2.257
H	3.0717	3.0224	-1.0876	H	3.8518	1.8239	-2.0518
H	3.1796	1.4663	-2.9384	H	2.7582	0.1072	-3.3594
H	1.9339	0.4556	-2.2552	H	1.4848	-0.0817	-2.1847
H	5.9882	0.6295	-0.6904	H	5.5317	-1.5542	-1.5766
H	5.4535	1.5599	-2.0873	H	5.0091	-0.7493	-3.0539
H	4.9743	2.0493	-0.462	H	5.2984	0.1901	-1.5899
H	-6.6251	0.2779	0.4464	H	-6.0405	0.854	-2.1749
H	-7.2556	0.1543	-1.1877	H	-7.1352	1.686	-1.082
H	-5.8351	2.1966	-0.6927	H	-6.9263	-0.8157	-0.746
H	-5.4015	1.2953	-2.1458	H	-6.7352	0.1665	0.707
H	-6.3387	-2.0217	-0.4842	H	-5.0344	2.9564	-1.2706
H	-5.4402	-1.3622	-1.8401	H	-5.2713	2.3647	0.3644
H	-1.4225	0.6522	0.1958	H	-2.4293	-1.7103	0.5619
H	-2.0613	-0.2927	1.5196	H	-1.8913	-0.921	-0.8931
H	-1.2792	-1.3014	-1.2669	H	-1.9412	0.2662	1.9331
H	-1.6676	-3.5723	-0.4193	H	-0.7345	2.1985	1.0046
H	-2.2043	-2.9557	1.1357	H	-0.7816	1.5157	-0.6129
H	-3.4827	-2.4914	-1.589	H	-3.1321	2.376	1.1201
H	-4.1339	-3.4745	-0.2879	H	-2.5629	3.1761	-0.3359
H	-5.3346	-2.42	1.6586	H	-3.1798	2.2981	-2.6228
H	-3.8045	-1.706	2.1607	H	-2.1848	0.8836	-2.2933
H	-5.2174	-0.6812	1.9582	H	-3.8516	0.6731	-2.8108
H	-2.2014	2.39	-0.2172	H	-4.1165	-2.6935	0.7145
H	4.2246	-1.0512	1.7373	H	4.0891	-1.7747	1.5364
H	1.2763	5.0896	1.6412	H	3.9325	4.9232	0.2797
H	2.3547	4.6567	0.2204	H	4.2395	3.8289	-1.1629

H	-0.0543	-2.4919	2.3035	H	-0.0098	-0.8291	3.3184
2a-7	X axis(Å)	Y axis(Å)	Z axis(Å)	2a-8	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-1.753	-2.7825	1.824	C	2.8308	-0.5929	-3.0683
C	-1.662	-2.9404	0.3113	C	2.6872	-1.7478	-2.0841
C	-1.8496	-1.5885	-0.3904	C	2.2511	-1.2343	-0.7061
C	-3.2236	-0.9279	-0.0202	C	3.2721	-0.1893	-0.1283
C	-3.4311	-0.8231	1.5378	C	3.5493	0.9881	-1.1372
C	-3.0868	-2.1709	2.2353	C	3.8324	0.4401	-2.566
C	-3.4572	0.4549	-0.6829	C	2.8677	0.3732	1.2582
C	-2.658	1.6244	-0.0725	C	1.7197	1.3977	1.2371
C	-2.8148	1.6734	1.4555	C	1.9924	2.5184	0.2194
C	-2.5672	0.3201	2.1262	C	2.3535	1.9746	-1.1666
C	-4.9183	-0.5384	1.9014	C	4.8258	1.7891	-0.7431
O	-0.6964	-0.7714	-0.0813	O	0.8973	-0.7386	-0.8387
C	-2.9746	2.9853	-0.6776	C	1.4133	1.8757	2.6474
C	6.1327	1.2177	0.9011	C	-6.0176	-0.0224	-1.0633
C	6.2135	-0.1716	0.2823	C	-5.2877	1.3002	-1.2626
C	4.8695	-0.8331	0.0802	C	-3.8245	1.2161	-0.9001
C	3.688	-0.1692	0.13	C	-3.317	0.245	-0.1022
C	3.6362	1.3541	0.3835	C	-4.2234	-0.7911	0.594
C	5.0304	2.0242	0.2355	C	-5.7375	-0.5582	0.3297
C	2.3151	-0.8097	-0.04	C	-1.8349	-0.0106	0.1322
C	1.4548	-0.093	-1.0975	C	-1.4294	-1.4088	-0.385
C	1.3253	1.397	-0.771	C	-2.3266	-2.5028	0.2269
C	2.7009	2.0461	-0.6444	C	-3.8195	-2.1909	0.0643
C	3.1177	1.609	1.819	C	-4.0509	-0.7357	2.1322
C	4.9788	-2.3072	-0.1557	C	-2.989	2.278	-1.5434
O	6.0547	-2.8731	-0.3198	O	-3.4573	3.1247	-2.2975
C	0.1	-0.7421	-1.2253	C	0.0543	-1.6566	-0.2046
C	-1.6939	-1.7725	-1.8843	C	2.0556	-2.4022	0.2328
O	-4.2788	-1.7944	-0.5084	O	4.5415	-0.8632	0.0611
C	-4.0948	3.3429	-1.3275	C	1.7464	3.0567	3.193
O	-2.5241	-2.2534	-2.643	O	2.9436	-3.0703	0.7447
C	-0.3998	-1.2846	-2.3333	C	0.6418	-2.648	0.4642
C	-1.9203	4.039	-0.5716	C	0.6279	0.9459	3.5146
H	-2.1738	5.0203	-1.0075	H	0.4198	1.2998	4.5386
O	-0.8335	3.845	-0.0412	O	0.2285	-0.1455	3.1252
H	-1.6448	-3.7654	2.2974	H	3.1679	-0.9825	-4.0361
H	-0.9235	-2.1689	2.193	H	1.8578	-0.1217	-3.2471
H	-0.6811	-3.3696	0.0693	H	1.9475	-2.4524	-2.4858
H	-2.4124	-3.6625	-0.0342	H	3.6343	-2.2968	-2.0114
H	-3.0965	-2.0417	3.3253	H	3.8762	1.2699	-3.2832
H	-3.8714	-2.907	2.0121	H	4.8262	-0.0279	-2.5859
H	-3.2531	0.3935	-1.7598	H	3.7492	0.8319	1.7282
H	-4.5318	0.6711	-0.63	H	2.6251	-0.4579	1.932
H	-1.606	1.4321	-0.2958	H	0.8116	0.9024	0.8882
H	-2.1125	2.4002	1.8828	H	1.1035	3.1557	0.1277

H	-3.8151	2.0385	1.7193	H	2.801	3.1719	0.5642
H	-2.7689	0.424	3.2005	H	2.587	2.8236	-1.8224
H	-1.5009	0.0843	2.0548	H	1.4663	1.5065	-1.6041
H	-5.5755	-1.3592	1.5932	H	5.7282	1.1706	-0.8059
H	-5.0371	-0.424	2.9855	H	4.974	2.6396	-1.4193
H	-5.3022	0.3731	1.4361	H	4.7805	2.1867	0.274
H	5.9548	1.1396	1.9796	H	-7.095	0.1291	-1.1958
H	7.095	1.7287	0.7805	H	-5.7032	-0.748	-1.8229
H	6.8506	-0.7873	0.9291	H	-5.758	2.0837	-0.6555
H	6.7146	-0.1046	-0.692	H	-5.4121	1.5869	-2.3137
H	5.0138	3.0386	0.6535	H	-6.1398	0.1646	1.0534
H	5.2857	2.1371	-0.8273	H	-6.301	-1.4865	0.4871
H	2.3759	-1.8621	-0.3248	H	-1.2074	0.7332	-0.3605
H	1.8088	-0.8006	0.9341	H	-1.6102	0.0894	1.199
H	1.972	-0.181	-2.0643	H	-1.6097	-1.4229	-1.4705
H	0.7613	1.9061	-1.5627	H	-2.1179	-3.4665	-0.2551
H	0.7615	1.5429	0.1576	H	-2.0982	-2.6352	1.2913
H	3.17	2.0311	-1.638	H	-4.0721	-2.2739	-1.0011
H	2.5726	3.1044	-0.3827	H	-4.3972	-2.9699	0.5781
H	3.1065	2.6811	2.0472	H	-4.7301	-1.4422	2.6244
H	2.0985	1.2397	1.9696	H	-3.04	-0.9843	2.4664
H	3.7461	1.1173	2.5697	H	-4.2782	0.2661	2.516
H	4.0453	-2.8827	-0.1766	H	-1.9195	2.2912	-1.3001
H	-4.1266	-1.9667	-1.4617	H	4.3899	-1.6639	0.6071
H	-4.2381	4.3374	-1.7415	H	1.4777	3.3268	4.2106
H	-4.9246	2.6579	-1.4669	H	2.312	3.8034	2.6452
H	0.0057	-1.37	-3.323	H	0.2355	-3.4607	1.0343
2b-1	X axis(Å)	Y axis(Å)	Z axis(Å)	2b-2	X axis(Å)	Y axis(Å)	Z axis(Å)
C	4.1559	-2.7297	-0.3015	C	-4.1038	-2.7382	0.4966
C	2.6358	-2.7994	-0.2892	C	-2.5842	-2.7891	0.434
C	1.9965	-1.4071	-0.2903	C	-1.9649	-1.3901	0.3541
C	2.5505	-0.4878	0.8553	C	-2.5711	-0.5272	-0.809
C	4.112	-0.4931	1.0081	C	-4.1367	-0.5585	-0.9062
C	4.6813	-1.9336	0.8856	C	-4.6812	-1.9995	-0.7034
C	1.9971	0.9602	0.8292	C	-2.0376	0.9274	-0.8634
C	2.6773	1.9024	-0.1822	C	-2.6946	1.9026	0.132
C	4.2075	1.8634	-0.0195	C	-4.2289	1.838	0.0252
C	4.7707	0.4387	-0.038	C	-4.7715	0.4085	0.1228
C	4.5476	0.004	2.4202	C	-4.6282	-0.127	-2.3215
O	0.5605	-1.6019	-0.0286	O	-0.5362	-1.5775	0.0507
C	2.0642	3.2936	-0.1082	C	-2.1033	3.2968	-0.0199
C	-6.4333	-0.1819	0.8818	C	6.398	-0.3278	0.1748
C	-5.8275	1.1257	0.3867	C	5.8559	1.0398	-0.2232
C	-4.3267	1.0819	0.2132	C	4.3476	1.0718	-0.2724
C	-3.6047	-0.0658	0.2167	C	3.592	-0.0461	-0.3992
C	-4.2851	-1.4463	0.3344	C	4.2229	-1.4418	-0.5934
C	-5.8239	-1.3586	0.1373	C	5.7734	-1.4028	-0.6976

C	-2.0882	-0.1444	0.1167	C	2.0785	-0.096	-0.2699
C	-1.6337	-1.0614	-1.0306	C	1.6822	-0.9569	0.9456
C	-2.2216	-2.4668	-0.859	C	2.2947	-2.3644	0.8626
C	-3.7469	-2.4077	-0.7626	C	3.8101	-2.3152	0.6224
C	-4.0015	-2.039	1.7349	C	3.7286	-2.1001	-1.9053
C	-3.7177	2.4408	0.0457	C	3.774	2.4457	-0.1113
O	-4.3811	3.4723	0.089	O	4.4752	3.45	-0.0361
C	-0.1317	-1.0974	-1.1227	C	0.1858	-1.0133	1.0952
C	1.9535	-0.8599	-1.7052	C	-1.8809	-0.7824	1.7421
O	2.0215	-1.0585	2.0899	O	-2.0773	-1.1432	-2.0365
C	2.6237	4.3999	0.4087	C	-2.6964	4.3748	-0.5584
O	2.9024	-0.634	-2.441	O	-2.8068	-0.54	2.5017
C	0.5848	-0.6531	-2.1496	C	-0.5011	-0.5344	2.1268
C	0.7067	3.4674	-0.7097	C	-0.727	3.5108	0.5232
H	0.2946	4.4907	-0.685	H	-0.3308	4.5376	0.445
O	0.0717	2.5392	-1.1981	O	-0.0608	2.61	1.0214
H	4.5617	-3.7475	-0.2585	H	-4.4963	-3.7619	0.5105
H	4.5163	-2.2965	-1.24	H	-4.4376	-2.2704	1.4283
H	2.2923	-3.3822	-1.1538	H	-2.2027	-3.3302	1.3097
H	2.2992	-3.3625	0.5913	H	-2.2703	-3.3848	-0.4334
H	5.7773	-1.8998	0.8339	H	-5.7751	-1.9773	-0.6145
H	4.4404	-2.5001	1.7956	H	-4.4641	-2.601	-1.5969
H	0.9134	0.9327	0.6674	H	-0.9485	0.9203	-0.7403
H	2.0914	1.3956	1.8346	H	-2.174	1.319	-1.8819
H	2.4783	1.5491	-1.1975	H	-2.4556	1.5942	1.1533
H	4.6779	2.4383	-0.8275	H	-4.5709	2.2796	-0.9175
H	4.5107	2.3483	0.9151	H	-4.6788	2.4405	0.8248
H	5.8526	0.4939	0.1421	H	-5.8597	0.4428	-0.0213
H	4.6726	0.0296	-1.0448	H	-4.6329	0.0434	1.1417
H	4.2123	-0.6754	3.2119	H	-4.3109	-0.8349	-3.0955
H	5.6403	0.0608	2.4923	H	-5.7235	-0.0875	-2.3573
H	4.1532	0.9951	2.6598	H	-4.2568	0.8581	-2.616
H	-6.2732	-0.2855	1.9611	H	7.4878	-0.3389	0.0581
H	-7.5186	-0.1635	0.7284	H	6.1898	-0.5255	1.2331
H	-6.1089	1.9128	1.0969	H	6.2488	1.3289	-1.2058
H	-6.2781	1.3882	-0.5791	H	6.2367	1.7667	0.5043
H	-6.3056	-2.2892	0.463	H	6.0762	-1.2082	-1.7361
H	-6.0645	-1.2485	-0.9291	H	6.1992	-2.3803	-0.4383
H	-1.623	0.832	-0.0179	H	1.6291	0.8908	-0.1566
H	-1.6965	-0.5108	1.0746	H	1.643	-0.4926	-1.1946
H	-2.0275	-0.6454	-1.9698	H	2.0988	-0.4734	1.8421
H	-1.9417	-3.0968	-1.7128	H	2.1007	-2.9084	1.7959
H	-1.8112	-2.9559	0.0327	H	1.8157	-2.9479	0.0671
H	-4.1282	-2.0931	-1.7441	H	4.2873	-1.9313	1.5338
H	-4.1332	-3.4214	-0.5958	H	4.1777	-3.3411	0.4926
H	-4.5219	-2.9944	1.869	H	4.2239	-3.0653	-2.0657
H	-2.9371	-2.2307	1.9023	H	2.6524	-2.2927	-1.9163

H	-4.3328	-1.3664	2.5336	H	3.9512	-1.4644	-2.7707
H	-2.6363	2.4902	-0.1294	H	2.6814	2.5343	-0.0767
H	1.076	-1.2459	1.9276	H	-1.1245	-1.3126	-1.8994
H	2.1212	5.3635	0.4094	H	-2.2076	5.3437	-0.6158
H	3.6105	4.3888	0.8598	H	-3.6992	4.3339	-0.9711
H	0.281	-0.2111	-3.0792	H	-0.1718	-0.046	3.024
2b-3	X axis(Å)	Y axis(Å)	Z axis(Å)	2b-4	X axis(Å)	Y axis(Å)	Z axis(Å)
C	3.9236	-3.0955	-0.0971	C	-3.1096	-2.9566	1.5968
C	2.4713	-2.917	0.3196	C	-1.6925	-2.5369	1.2362
C	1.9985	-1.4691	0.1581	C	-1.6451	-1.1354	0.6191
C	2.9461	-0.4371	0.8668	C	-2.6348	-0.9689	-0.5875
C	4.4782	-0.6661	0.6125	C	-4.0772	-1.538	-0.3428
C	4.8406	-2.1746	0.6963	C	-4.0224	-2.9127	0.379
C	2.5579	1.0457	0.6305	C	-2.6912	0.4699	-1.163
C	3.0175	1.6346	-0.7169	C	-3.583	1.4528	-0.3801
C	4.5195	1.3861	-0.9378	C	-4.9842	0.8604	-0.1518
C	4.9026	-0.0864	-0.7592	C	-4.9352	-0.5383	0.4705
C	5.3463	0.0283	1.7056	C	-4.8177	-1.807	-1.6882
O	0.6877	-1.3805	0.8212	O	-0.2824	-0.9586	0.0903
C	2.586	3.0883	-0.8322	C	-3.5699	2.821	-1.0441
C	-6.6177	0.955	0.8104	C	6.8823	0.4683	-0.4116
C	-6.5718	-0.379	0.0771	C	6.2623	-0.7278	-1.1217
C	-5.2102	-0.7279	-0.4798	C	4.8648	-1.0662	-0.6539
C	-4.0646	-0.1003	-0.1146	C	4.0984	-0.2327	0.093
C	-4.0699	1.0205	0.9464	C	4.6025	1.1693	0.4967
C	-5.4126	1.0901	1.7256	C	5.8679	1.5936	-0.2991
C	-2.6817	-0.3929	-0.6855	C	2.703	-0.5569	0.6153
C	-1.6274	-0.6719	0.4061	C	1.6649	0.5249	0.258
C	-1.5797	0.4935	1.4055	C	2.1355	1.8974	0.7617
C	-2.959	0.769	1.9993	C	3.5162	2.2387	0.2047
C	-3.8352	2.382	0.2495	C	4.9479	1.1683	2.0049
C	-5.2655	-1.8266	-1.4957	C	4.4251	-2.4303	-1.0894
O	-6.298	-2.4366	-1.7543	O	5.1056	-3.141	-1.8222
C	-0.2393	-0.9523	-0.1264	C	0.2939	0.1224	0.7523
C	1.5983	-1.2092	-1.2797	C	-1.6577	-0.086	1.7123
O	2.7369	-0.6472	2.2954	O	-2.0616	-1.7725	-1.662
C	3.3649	4.1761	-0.7146	C	-4.5482	3.3756	-1.7782
O	2.3026	-1.3091	-2.2732	O	-2.5305	0.1013	2.5469
C	0.1946	-0.8408	-1.3785	C	-0.4324	0.6979	1.7059
C	1.1469	3.34	-1.1488	C	-2.352	3.6597	-0.828
H	0.8542	4.3985	-1.2545	H	-2.365	4.6593	-1.2946
O	0.327	2.4385	-1.2828	O	-1.3871	3.2747	-0.1774
H	4.2214	-4.1361	0.0781	H	-3.0906	-3.9784	1.9943
H	4.0429	-2.92	-1.171	H	-3.5091	-2.3247	2.3965
H	1.8393	-3.5965	-0.267	H	-1.0606	-2.5851	2.1326
H	2.346	-3.2342	1.3634	H	-1.2592	-3.265	0.5376
H	5.875	-2.3301	0.3634	H	-5.0328	-3.2177	0.6808

H	4.8097	-2.5003	1.7452	H	-3.6734	-3.6813	-0.3242
H	1.4758	1.1663	0.757	H	-1.6726	0.8648	-1.2606
H	2.977	1.6567	1.4431	H	-3.0468	0.4232	-2.2026
H	2.5118	1.1131	-1.5335	H	-3.1642	1.6065	0.6178
H	4.7997	1.7029	-1.9506	H	-5.5593	1.5206	0.51
H	5.1203	1.9934	-0.2519	H	-5.5441	0.8094	-1.092
H	5.9902	-0.1769	-0.8813	H	-5.9636	-0.9137	0.556
H	4.4753	-0.6668	-1.5789	H	-4.5757	-0.4584	1.4979
H	5.1857	-0.4153	2.6948	H	-4.3316	-2.5993	-2.2686
H	6.414	-0.0779	1.4796	H	-5.8485	-2.1339	-1.5063
H	5.1367	1.0974	1.7958	H	-4.864	-0.9225	-2.3291
H	-6.648	1.78	0.0896	H	7.2408	0.1725	0.5809
H	-7.5419	1.0192	1.3965	H	7.761	0.8109	-0.9704
H	-7.3172	-0.3419	-0.7268	H	6.9328	-1.5839	-0.9776
H	-6.8788	-1.1791	0.7631	H	6.225	-0.5271	-2.2003
H	-5.4813	2.0301	2.2875	H	6.3389	2.4676	0.1681
H	-5.4603	0.2853	2.4722	H	5.5901	1.9047	-1.3157
H	-2.687	-1.2459	-1.3665	H	2.3355	-1.5149	0.2436
H	-2.3771	0.4676	-1.2951	H	2.7581	-0.6748	1.7056
H	-1.9469	-1.5744	0.9473	H	1.5983	0.5861	-0.8383
H	-0.8885	0.2627	2.2262	H	1.4278	2.6749	0.4478
H	-1.1904	1.398	0.9232	H	2.1632	1.9238	1.8574
H	-3.231	-0.0949	2.6217	H	3.4137	2.3728	-0.8812
H	-2.8877	1.6261	2.6815	H	3.8305	3.2116	0.6042
H	-3.8799	3.2051	0.9721	H	5.3496	2.1397	2.3157
H	-2.8583	2.4409	-0.2404	H	4.0766	0.9666	2.6355
H	-4.5886	2.5769	-0.5216	H	5.6971	0.407	2.2482
H	-4.3334	-2.0786	-2.0153	H	3.4531	-2.7857	-0.7271
H	1.7701	-0.7072	2.4288	H	-1.1113	-1.5474	-1.7015
H	2.9796	5.1859	-0.8258	H	-4.4642	4.37	-2.208
H	4.4251	4.1021	-0.4956	H	-5.4765	2.8536	-1.986
H	-0.3017	-0.532	-2.2785	H	-0.2325	1.5421	2.3377
2b-5	X axis(Å)	Y axis(Å)	Z axis(Å)	2b-6	X axis(Å)	Y axis(Å)	Z axis(Å)
C	3.815	-3.1534	-0.1322	C	-3.1966	-2.8899	1.6186
C	2.3552	-2.9475	0.2436	C	-1.7587	-2.5181	1.289
C	1.9266	-1.483	0.1114	C	-1.6531	-1.1277	0.6543
C	2.8778	-0.4992	0.8811	C	-2.6061	-0.9492	-0.5797
C	4.4107	-0.7625	0.6687	C	-4.071	-1.471	-0.3646
C	4.73	-2.2822	0.7176	C	-4.0765	-2.8361	0.3771
C	2.537	1.0001	0.6781	C	-2.6041	0.4821	-1.1762
C	3.0556	1.616	-0.6353	C	-3.4852	1.5026	-0.4302
C	4.5569	1.3331	-0.8159	C	-4.9092	0.956	-0.2303
C	4.8949	-0.154	-0.6704	C	-4.9187	-0.4343	0.4122
C	5.2608	-0.1252	1.8096	C	-4.7848	-1.7372	-1.725
O	0.5977	-1.3779	0.7351	O	-0.2726	-0.9992	0.159
C	2.6666	3.0838	-0.7197	C	-3.4132	2.86	-1.1122
C	-6.2548	0.2899	1.5901	C	6.2568	0.9006	-1.2204

C	-6.4768	-0.4572	0.2809	C	6.0695	-0.6066	-1.3416
C	-5.1954	-0.6828	-0.4852	C	4.7846	-1.0853	-0.709
C	-4.0685	0.0384	-0.2683	C	4.1022	-0.3635	0.2133
C	-4.0452	1.2346	0.7066	C	4.6545	0.9638	0.7753
C	-5.4341	1.5415	1.3338	C	6.0619	1.3266	0.2238
C	-2.6993	-0.2742	-0.855	C	2.7064	-0.6929	0.7249
C	-1.6851	-0.6015	0.2657	C	1.7122	0.4299	0.3539
C	-1.6423	0.5208	1.3203	C	2.2145	1.7997	0.8487
C	-3.037	0.8958	1.8336	C	3.6519	2.0847	0.3971
C	-3.6132	2.5347	-0.016	C	4.812	0.8906	2.3144
C	-5.2805	-1.8051	-1.471	C	4.3188	-2.4067	-1.235
O	-6.2853	-2.4953	-1.6059	O	4.9157	-3.0175	-2.1154
C	-0.2871	-0.9002	-0.2289	C	0.3185	0.0747	0.8197
C	1.5805	-1.1697	-1.3298	C	-1.6619	-0.0628	1.7323
O	2.6166	-0.7457	2.2953	O	-2.0306	-1.7853	-1.6277
C	3.4697	4.1458	-0.5444	C	-4.3545	3.4328	-1.88
O	2.3144	-1.2579	-2.3028	O	-2.5493	0.1619	2.5419
C	0.1901	-0.7631	-1.4625	C	-0.4145	0.6851	1.746
C	1.2456	3.3839	-1.0736	C	-2.1767	3.6651	-0.8748
H	0.9843	4.4527	-1.1557	H	-2.1468	4.6575	-1.3558
O	0.407	2.5095	-1.2611	O	-1.2419	3.2613	-0.1925
H	4.0792	-4.2067	0.0204	H	-3.2187	-3.9059	2.0303
H	3.9738	-2.9495	-1.1959	H	-3.5969	-2.2349	2.399
H	1.7248	-3.5917	-0.3833	H	-1.1516	-2.5723	2.2021
H	2.1877	-3.292	1.2727	H	-1.33	-3.2689	0.6119
H	5.7701	-2.4562	0.413	H	-5.103	-3.1062	0.6569
H	4.6564	-2.638	1.7545	H	-3.7332	-3.625	-0.3062
H	1.455	1.1464	0.7737	H	-1.5719	0.8449	-1.253
H	2.9453	1.5749	1.522	H	-2.9345	0.431	-2.2239
H	2.5631	1.1331	-1.4832	H	-3.0876	1.6579	0.5761
H	4.8783	1.6721	-1.8092	H	-5.4807	1.6429	0.4071
H	5.1509	1.903	-0.093	H	-5.4462	0.9083	-1.184
H	5.9832	-0.2707	-0.7604	H	-5.9599	-0.7773	0.4762
H	4.4795	-0.6979	-1.5207	H	-4.5832	-0.3503	1.4475
H	5.0564	-0.5934	2.7791	H	-4.3084	-2.5521	-2.2817
H	6.3322	-0.2539	1.6145	H	-5.8294	-2.0303	-1.5653
H	5.0769	0.9462	1.9258	H	-4.7878	-0.8611	-2.379
H	-7.2227	0.5606	2.0272	H	7.2629	1.1741	-1.5583
H	-5.7489	-0.3579	2.3159	H	5.5489	1.4252	-1.8732
H	-7.1752	0.1008	-0.3552	H	6.9115	-1.1285	-0.8703
H	-6.9561	-1.4123	0.5271	H	6.093	-0.8534	-2.4098
H	-6.0146	2.1917	0.6644	H	6.8406	0.8369	0.8253
H	-5.3161	2.1021	2.2698	H	6.2438	2.4047	0.3172
H	-2.7224	-1.1203	-1.5447	H	2.327	-1.6344	0.3234
H	-2.3613	0.5775	-1.4566	H	2.7351	-0.842	1.8109
H	-2.0423	-1.5139	0.7662	H	1.6674	0.489	-0.7441
H	-1.0316	0.2077	2.177	H	1.5622	2.5944	0.4651

H	-1.149	1.4094	0.9084	H	2.1614	1.8596	1.9421
H	-3.4162	0.058	2.4336	H	3.6467	2.2292	-0.6914
H	-2.9396	1.7457	2.5212	H	3.9722	3.0402	0.832
H	-3.6468	3.3895	0.6701	H	5.2442	1.8196	2.7049
H	-2.5972	2.4923	-0.4175	H	3.8669	0.7352	2.8416
H	-4.2819	2.7565	-0.8564	H	5.478	0.0679	2.6012
H	-4.4003	-1.9856	-2.1005	H	3.4143	-2.8344	-0.7851
H	1.6448	-0.7834	2.396	H	-1.0735	-1.588	-1.6474
H	3.115	5.1686	-0.6368	H	-4.2292	4.4178	-2.321
H	4.52	4.0363	-0.2945	H	-5.2923	2.9356	-2.1056
H	-0.2688	-0.4167	-2.3685	H	-0.207	1.533	2.3703
2b-7	X axis(Å)	Y axis(Å)	Z axis(Å)	2b-8	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-4.1886	-2.6765	0.1661	C	-3.9577	-2.9331	-0.5328
C	-2.6732	-2.8233	0.188	C	-2.582	-2.8442	0.1279
C	-1.9688	-1.4654	0.2599	C	-2.0205	-1.41	0.231
C	-2.4435	-0.4836	-0.8691	C	-2.6576	-0.429	-0.8034
C	-3.9982	-0.3986	-1.0624	C	-4.2339	-0.3814	-0.7264
C	-4.6463	-1.8097	-0.9997	C	-4.8243	-1.727	-0.205
C	-1.816	0.9293	-0.7819	C	-2.0218	0.9857	-0.8531
C	-2.4725	1.8713	0.242	C	-2.5717	1.9947	0.1643
C	-3.9939	1.9351	0.0279	C	-4.0933	2.0975	-0.0032
C	-4.6348	0.5415	-0.0079	C	-4.7567	0.7422	0.2123
C	-4.3672	0.1616	-2.4703	C	-4.8361	-0.1221	-2.1366
O	-0.5343	-1.7112	0.0374	O	-0.5847	-1.5105	-0.0611
C	-1.7544	3.2102	0.2255	C	-1.8397	3.3225	0.0503
C	6.3952	0.0713	-0.8316	C	6.4362	-0.2345	-0.8393
C	5.724	1.3268	-0.2863	C	5.8309	1.0816	-0.3664
C	4.2306	1.1971	-0.1584	C	4.3277	1.0478	-0.2149
C	3.5654	0.0189	-0.1781	C	3.5982	-0.095	-0.2222
C	4.3011	-1.3209	-0.3483	C	4.2716	-1.4806	-0.315
C	5.8359	-1.1694	-0.1479	C	5.8076	-1.4003	-0.0934
C	2.0566	-0.0994	-0.038	C	2.0792	-0.1638	-0.1501
C	1.6444	-1.1126	1.0452	C	1.5996	-1.0601	1.0032
C	2.2829	-2.4808	0.7848	C	2.1814	-2.4717	0.8572
C	3.8048	-2.3554	0.6986	C	3.7085	-2.4256	0.7835
C	4.0392	-1.8567	-1.7755	C	4.0078	-2.087	-1.7134
C	3.5408	2.5172	-0.0359	C	3.7235	2.4099	-0.0619
O	2.5567	2.8406	-0.6894	O	4.3878	3.4399	-0.1233
C	0.1442	-1.2015	1.1384	C	0.0961	-1.0985	1.0785
C	-1.948	-0.9715	1.6949	C	-1.9953	-0.9446	1.672
O	-1.9128	-1.0461	-2.107	O	-2.2959	-0.9943	-2.1038
C	-2.1511	4.3306	-0.3994	C	-2.2886	4.4442	-0.5365
O	-2.9095	-0.7694	2.4216	O	-2.9543	-0.7812	2.4105
C	-0.5859	-0.779	2.1652	C	-0.6311	-0.7441	2.1335
C	-0.4749	3.2958	0.9959	C	-0.4936	3.4098	0.6903
H	0.0915	4.2363	0.8875	H	0.0038	4.3935	0.6393
O	-0.0752	2.3914	1.7216	O	0.0451	2.4529	1.2354

H	-4.643	-3.6702	0.0738	H	-4.4569	-3.851	-0.2003
H	-4.5521	-2.2617	1.1117	H	-3.8458	-3.0269	-1.6192
H	-2.3813	-3.4545	1.0374	H	-2.6523	-3.2886	1.1297
H	-2.3413	-3.3685	-0.7054	H	-1.8918	-3.4935	-0.4264
H	-5.7396	-1.7181	-0.9671	H	-4.9525	-1.6964	0.8843
H	-4.418	-2.357	-1.9247	H	-5.8318	-1.8835	-0.6109
H	-0.7403	0.8469	-0.5921	H	-0.9317	0.9069	-0.7691
H	-1.8607	1.3989	-1.7754	H	-2.1729	1.3993	-1.8621
H	-2.3403	1.4682	1.249	H	-2.3931	1.6247	1.18
H	-4.4547	2.5159	0.8371	H	-4.5027	2.8102	0.7238
H	-4.2378	2.4621	-0.9008	H	-4.3563	2.4763	-0.9978
H	-5.7068	0.6603	-0.2137	H	-5.8417	0.8575	0.0883
H	-4.5838	0.1004	0.9893	H	-4.6202	0.4662	1.2617
H	-4.0468	-0.5121	-3.2731	H	-4.6659	-0.9677	-2.812
H	-5.4529	0.2795	-2.5692	H	-5.9214	0.0242	-2.0831
H	-3.9139	1.1361	-2.6698	H	-4.4086	0.7703	-2.6047
H	6.2495	0.0087	-1.9161	H	6.2925	-0.3476	-1.9199
H	7.4769	0.1332	-0.6654	H	7.519	-0.2214	-0.6689
H	5.9775	2.1679	-0.9433	H	6.1274	1.8601	-1.0798
H	6.1376	1.5591	0.7033	H	6.2686	1.351	0.6035
H	6.3591	-2.0598	-0.5184	H	6.2888	-2.3369	-0.4019
H	6.0716	-1.1011	0.9231	H	6.0313	-1.281	0.9757
H	1.5985	0.859	0.2176	H	1.616	0.8166	-0.045
H	1.6376	-0.3851	-1.0114	H	1.7054	-0.5451	-1.1093
H	2.0281	-0.7451	2.0086	H	1.9816	-0.6335	1.9424
H	2.0268	-3.1737	1.5962	H	1.8846	-3.0899	1.7139
H	1.8917	-2.9268	-0.1374	H	1.7801	-2.9682	-0.0347
H	4.1723	-2.0742	1.6954	H	4.0769	-2.1034	1.7675
H	4.2326	-3.3428	0.483	H	4.0893	-3.4441	0.6338
H	4.5778	-2.7959	-1.9466	H	4.5264	-3.0458	-1.8291
H	2.9787	-2.0565	-1.9591	H	2.9454	-2.2769	-1.8955
H	4.3647	-1.1445	-2.5417	H	4.3543	-1.4242	-2.5138
H	4.0225	3.2187	0.6661	H	2.6439	2.4633	0.1206
H	-0.9698	-1.2421	-1.9393	H	-1.3347	-1.1678	-2.0771
H	-1.5779	5.2526	-0.3602	H	-1.7084	5.3626	-0.5647
H	-3.0622	4.3665	-0.9871	H	-3.2584	4.4882	-1.0221
H	-0.2956	-0.3272	3.0946	H	-0.3358	-0.3828	3.0999
2c-1	X axis(Å)	Y axis(Å)	Z axis(Å)	2c-2	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-4.2084	-2.7589	0.5418	C	3.0818	-3.4131	-0.0549
C	-2.7314	-2.8199	0.1807	C	1.6688	-2.8669	0.0836
C	-2.1026	-1.4258	0.0957	C	1.6221	-1.3424	-0.062
C	-2.8983	-0.4596	-0.8516	C	2.6342	-0.6096	0.8881
C	-4.4536	-0.467	-0.6444	C	4.0756	-1.2304	0.9233
C	-4.9866	-1.9147	-0.4586	C	4.0169	-2.7821	0.9676
C	-2.346	0.9891	-0.8877	C	2.6922	0.9266	0.6849
C	-2.777	1.8836	0.2904	C	3.5603	1.3973	-0.4979
C	-4.3041	1.8424	0.478	C	4.961	0.7646	-0.4362

C	-4.852	0.4142	0.5644	C	4.9097	-0.7595	-0.2931
C	-5.1973	0.0888	-1.8969	C	4.8445	-0.809	2.2125
O	-0.7652	-1.6002	-0.4928	O	0.269	-0.9274	0.3449
C	-2.1915	3.2797	0.1348	C	3.5501	2.9154	-0.5894
C	6.7401	-0.161	-0.5033	C	-6.6481	0.8373	1.0913
C	5.9724	1.1435	-0.6782	C	-6.6086	-0.0504	-0.1456
C	4.5571	1.0982	-0.1498	C	-5.2445	-0.6299	-0.4435
C	3.9137	-0.0514	0.1718	C	-4.0957	-0.1792	0.1192
C	4.5765	-1.4302	-0.0306	C	-4.1009	1.0067	1.1086
C	5.8653	-1.3406	-0.8944	C	-5.4521	1.7742	1.1019
C	2.5089	-0.133	0.7518	C	-2.7097	-0.7633	-0.1298
C	1.5883	-1.0448	-0.0816	C	-1.681	0.3079	-0.5343
C	2.1961	-2.4496	-0.1844	C	-1.621	1.4295	0.5089
C	3.6071	-2.3921	-0.7715	C	-3.004	2.038	0.7291
C	4.9495	-2.0242	1.3483	C	-3.8457	0.4727	2.5382
C	3.9445	2.4588	-0.0078	C	-5.2996	-1.7722	-1.4101
O	4.5236	3.4824	-0.3591	O	-6.3338	-2.1086	-1.9776
C	0.1661	-1.1161	0.4221	C	-0.3184	-0.2983	-0.7456
C	-1.7341	-0.9384	1.4825	C	1.6034	-0.9607	-1.5303
O	-2.6677	-0.9727	-2.198	O	2.0872	-0.7816	2.2302
C	-2.8461	4.3983	-0.2181	C	4.5387	3.7555	-0.2421
O	-2.4852	-0.7622	2.4301	O	2.4573	-1.209	-2.3685
C	-0.3018	-0.7177	1.6012	C	0.373	-0.2682	-1.8799
C	-0.7374	3.4417	0.4415	C	2.3224	3.5444	-1.1643
H	-0.3343	4.4642	0.344	H	2.3385	4.6441	-1.2511
O	-0.0197	2.5066	0.779	O	1.3463	2.8933	-1.519
H	-4.618	-3.7761	0.5481	H	3.063	-4.4988	0.0981
H	-4.3436	-2.3689	1.5557	H	3.4611	-3.2537	-1.0692
H	-2.2024	-3.4372	0.9186	H	1.0203	-3.3453	-0.6619
H	-2.6069	-3.343	-0.7766	H	1.2546	-3.1597	1.0576
H	-6.0418	-1.8893	-0.1574	H	5.0235	-3.199	0.8337
H	-4.9617	-2.4397	-1.4234	H	3.6865	-3.1074	1.9637
H	-1.2531	0.9621	-0.9745	H	1.6735	1.3231	0.5994
H	-2.6626	1.4666	-1.8264	H	3.0698	1.393	1.6064
H	-2.3552	1.4892	1.2187	H	3.1204	1.0437	-1.434
H	-4.5762	2.3802	1.3954	H	5.518	1.0144	-1.3484
H	-4.8109	2.3638	-0.3415	H	5.5398	1.1785	0.3967
H	-5.9462	0.4692	0.6402	H	5.9389	-1.1324	-0.2058
H	-4.5255	-0.0365	1.5031	H	4.5287	-1.1912	-1.2204
H	-5.0559	-0.5546	-2.7727	H	4.3754	-1.2139	3.1163
H	-6.2773	0.1444	-1.7148	H	5.8737	-1.1869	2.1925
H	-4.862	1.0908	-2.1777	H	4.8974	0.2759	2.3372
H	7.642	-0.1412	-1.1261	H	-7.5781	1.4176	1.096
H	7.0798	-0.2615	0.5339	H	-6.6617	0.2204	1.997
H	5.9344	1.3995	-1.7449	H	-6.9337	0.5312	-1.018
H	6.5432	1.9354	-0.1778	H	-7.3433	-0.8523	-0.0028
H	5.6039	-1.233	-1.9562	H	-5.5172	2.4193	0.2148

H	6.4441	-2.2696	-0.8168	H	-5.517	2.4429	1.9695
H	2.5834	-0.5051	1.7816	H	-2.3854	-1.2777	0.7842
H	2.0354	0.8448	0.8339	H	-2.7102	-1.5299	-0.9073
H	1.5399	-0.6171	-1.0942	H	-2.015	0.7509	-1.484
H	2.2166	-2.9322	0.8004	H	-1.2197	1.0593	1.4601
H	1.5748	-3.0863	-0.827	H	-0.9355	2.2176	0.1728
H	4.0266	-3.4062	-0.7907	H	-2.933	2.813	1.5031
H	3.5142	-2.0806	-1.8213	H	-3.291	2.5559	-0.1967
H	5.6017	-1.3513	1.9157	H	-4.5901	-0.2764	2.8296
H	4.072	-2.2182	1.9728	H	-2.8642	-6.00E-04	2.6407
H	5.4765	-2.9786	1.2346	H	-3.8875	1.2846	3.2734
H	2.938	2.5171	0.424	H	-4.3657	-2.3145	-1.6011
H	-1.7088	-1.1503	-2.2674	H	1.1338	-0.5744	2.1696
H	-2.3542	5.3643	-0.2938	H	4.456	4.8331	-0.3537
H	-3.9054	4.395	-0.453	H	5.4748	3.3993	0.1753
H	0.1907	-0.2913	2.454	H	0.139	0.1633	-2.8344
2c-3	X axis(Å)	Y axis(Å)	Z axis(Å)	2c-4	X axis(Å)	Y axis(Å)	Z axis(Å)
C	4.1266	-2.5594	-1.1136	C	-4.1439	-2.8144	0.4013
C	2.6058	-2.6022	-1.1381	C	-2.657	-2.8416	0.0781
C	1.9853	-1.2669	-0.7153	C	-2.0484	-1.4362	0.0565
C	2.5372	-0.7513	0.6608	C	-2.8333	-0.452	-0.8811
C	4.0964	-0.8344	0.82	C	-4.393	-0.4879	-0.7158
C	4.6447	-2.1787	0.2668	C	-4.9089	-1.9484	-0.5907
C	2.0079	0.6473	1.0697	C	-2.302	1.0046	-0.8576
C	2.7235	1.837	0.4017	C	-2.7756	1.8546	0.3368
C	4.2487	1.7207	0.5675	C	-4.3063	1.7862	0.4833
C	4.7874	0.3593	0.1166	C	-4.8358	0.3486	0.5093
C	4.5175	-0.8031	2.3208	C	-5.1121	0.0975	-1.9693
O	0.5439	-1.5105	-0.538	O	-0.6926	-1.5695	-0.4995
C	2.1267	3.1505	0.8833	C	-2.2062	3.2626	0.2403
C	-6.4825	0.2543	0.532	C	6.1571	-0.2237	-1.4822
C	-5.7511	-0.6829	1.4839	C	5.8162	1.1358	-0.8835
C	-4.2493	-0.6893	1.3097	C	4.506	1.1276	-0.1339
C	-3.6145	-0.1683	0.2301	C	3.9291	-0.0092	0.3262
C	-4.4063	0.4547	-0.9388	C	4.6196	-1.3839	0.2059
C	-5.9213	0.1157	-0.8729	C	6.0413	-1.3	-0.4167
C	-2.1023	-0.1191	0.0401	C	2.5255	-0.102	0.9023
C	-1.6466	-0.7103	-1.3095	C	1.6372	-0.9791	-0.007
C	-2.3729	-0.0082	-2.4666	C	2.2628	-2.3704	-0.207
C	-3.888	-0.0948	-2.2944	C	3.72	-2.2843	-0.6823
C	-4.2445	1.9931	-0.8973	C	4.8059	-2.0384	1.5969
C	-3.536	-1.314	2.4689	C	3.8837	2.4836	3.00E-04
O	-4.1299	-1.841	3.4041	O	4.3957	3.4959	-0.4679
C	-0.1386	-0.6735	-1.4176	C	0.2044	-1.0984	0.4557
C	1.9633	-0.3105	-1.8906	C	-1.7265	-0.9903	1.4687
O	1.9805	-1.6588	1.6587	O	-2.5598	-0.9191	-2.2363
C	2.6772	4.0246	1.7417	C	-2.8682	4.3834	-0.0912

O	2.9228	0.1112	-2.519	O	-2.5059	-0.8581	2.4004
C	0.6017	0.0502	-2.2521	C	-0.302	-0.7502	1.6347
C	0.7997	3.535	0.3131	C	-0.7615	3.4336	0.5846
H	0.393	4.5045	0.6477	H	-0.3697	4.4634	0.5257
O	0.1845	2.8263	-0.4756	O	-0.0395	2.4982	0.912
H	4.5173	-3.5478	-1.3833	H	-4.5377	-3.837	0.3628
H	4.5068	-1.864	-1.8687	H	-4.3118	-2.4607	1.4235
H	2.2669	-2.8837	-2.1436	H	-2.1381	-3.4754	0.809
H	2.2489	-3.4035	-0.4776	H	-2.499	-3.3304	-0.8924
H	5.7418	-2.153	0.2401	H	-5.9717	-1.9476	-0.3162
H	4.3794	-2.9927	0.9554	H	-4.8518	-2.441	-1.5712
H	0.927	0.6954	0.8929	H	-2.6022	1.5073	-1.7884
H	2.0908	0.7541	2.1611	H	-1.2071	0.9958	-0.9177
H	2.5426	1.811	-0.676	H	-2.3717	1.4365	1.2629
H	4.7432	2.5067	-0.0176	H	-4.6095	2.2901	1.41
H	4.5409	1.8881	1.61	H	-4.7994	2.327	-0.332
H	5.8673	0.3335	0.3141	H	-5.9323	0.3863	0.5573
H	4.6956	0.2816	-0.9682	H	-4.528	-0.1278	1.4416
H	4.1613	-1.6871	2.8617	H	-4.9377	-0.5148	-2.8612
H	5.6097	-0.7903	2.418	H	-6.1972	0.1312	-1.8145
H	4.1327	0.073	2.8495	H	-4.7852	1.1129	-2.2085
H	-7.5524	0.0155	0.5329	H	5.4902	-0.4455	-2.3239
H	-6.3945	1.2893	0.8814	H	7.1772	-0.203	-1.8826
H	-6.1191	-1.7065	1.336	H	5.7889	1.858	-1.7082
H	-6.0175	-0.391	2.5072	H	6.6126	1.4553	-0.1999
H	-6.094	-0.9162	-1.2085	H	6.3313	-2.2697	-0.8405
H	-6.4875	0.7574	-1.5597	H	6.7821	-1.0786	0.3645
H	-1.7778	0.9261	0.1189	H	2.0511	0.8731	1.0109
H	-1.5699	-0.6432	0.8357	H	2.5738	-0.5082	1.9191
H	-1.9395	-1.7702	-1.3349	H	1.6034	-0.4858	-0.9904
H	-2.0705	1.0434	-2.5376	H	2.2082	-2.9474	0.7243
H	-2.0992	-0.4775	-3.4201	H	1.6875	-2.9379	-0.9497
H	-4.3713	0.437	-3.1242	H	4.1333	-3.2999	-0.7305
H	-4.1758	-1.1502	-2.3985	H	3.7187	-1.9051	-1.7128
H	-3.2056	2.3108	-1.0304	H	3.862	-2.2642	2.1004
H	-4.8291	2.4703	-1.6923	H	5.3518	-2.9856	1.5103
H	-4.5822	2.41	0.0579	H	5.3795	-1.3842	2.2644
H	-2.4399	-1.2873	2.4592	H	2.9408	2.5514	0.557
H	1.0412	-1.7904	1.4241	H	-1.5965	-1.0785	-2.2863
H	2.1885	4.9528	2.0247	H	-2.3881	5.3577	-0.1247
H	3.6423	3.8452	2.2042	H	-3.9218	4.3739	-0.3501
H	0.3282	0.759	-3.0101	H	0.1588	-0.3426	2.514
2c-5	X axis(Å)	Y axis(Å)	Z axis(Å)	2c-6	X axis(Å)	Y axis(Å)	Z axis(Å)
C	3.1685	-3.3649	-0.1389	C	3.9903	-2.5295	-1.4208
C	1.7411	-2.8704	0.0394	C	2.4688	-2.5133	-1.4047
C	1.6383	-1.3465	-0.0818	C	1.913	-1.204	-0.836
C	2.646	-0.5925	0.8561	C	2.5197	-0.8477	0.5673

C	4.1085	-1.1631	0.8497	C	4.0779	-1.003	0.6717
C	4.1044	-2.7164	0.872	C	4.5585	-2.3055	-0.0258
C	2.6464	0.9476	0.6746	C	2.0564	0.5219	1.1268
C	3.4707	1.465	-0.5199	C	2.7998	1.7449	0.5567
C	4.8934	0.8805	-0.4991	C	4.3231	1.5576	0.665
C	4.8977	-0.6463	-0.378	C	4.7967	0.2284	0.0682
C	4.8916	-0.7336	2.1275	C	4.5385	-1.1352	2.1554
O	0.2814	-0.9852	0.3619	O	0.468	-1.4092	-0.6418
C	3.4063	2.983	-0.5884	C	2.2672	3.0254	1.1815
C	-6.3032	1.4907	0.3994	C	-6.4095	-0.533	-0.128
C	-6.5124	0.1255	-0.2443	C	-5.7919	-0.9815	1.1907
C	-5.2206	-0.633	-0.4322	C	-4.2881	-0.8463	1.2041
C	-4.0871	-0.3426	0.2515	C	-3.6113	-0.0435	0.3469
C	-4.0647	0.719	1.3729	C	-4.3437	0.8901	-0.6397
C	-5.4606	1.3427	1.654	C	-5.8908	0.8463	-0.494
C	-2.7122	-0.9249	-0.0442	C	-2.0988	-0.0231	0.1735
C	-1.73	0.1928	-0.4526	C	-1.7067	-0.448	-1.2602
C	-1.6814	1.3222	0.5898	C	-2.4374	0.411	-2.3103
C	-3.0809	1.8381	0.9427	C	-3.9519	0.4509	-2.0742
C	-3.6029	0.0971	2.7142	C	-3.9411	2.3678	-0.4079
C	-5.3033	-1.7036	-1.4741	C	-3.6214	-1.7169	2.2221
O	-6.3123	-1.9033	-2.142	O	-4.2444	-2.4826	2.9501
C	-0.3525	-0.361	-0.7051	C	-0.202	-0.4616	-1.4125
C	1.5722	-0.9445	-1.5433	C	1.9002	-0.1364	-1.9113
O	2.1362	-0.8023	2.2074	O	1.9535	-1.8285	1.4874
C	4.3729	3.8518	-0.2503	C	2.8751	3.7922	2.1015
O	2.4145	-1.1507	-2.4043	O	2.8595	0.3079	-2.5242
C	0.3108	-0.2905	-1.8543	C	0.5459	0.3115	-2.1941
C	2.1451	3.5771	-1.1268	C	0.9396	3.5097	0.6946
H	2.1214	4.6777	-1.1976	H	0.5799	4.4555	1.134
O	1.1843	2.8974	-1.4695	O	0.2751	2.9032	-0.1382
H	3.5188	-3.1777	-1.159	H	4.3343	-3.5005	-1.7965
H	3.1908	-4.4526	-0.0021	H	4.3783	-1.778	-2.1157
H	1.0926	-3.3604	-0.6986	H	2.0934	-2.6819	-2.4224
H	1.3597	-3.1914	1.0179	H	2.0973	-3.3619	-0.815
H	5.1214	-3.096	0.7093	H	5.6547	-2.3173	-0.0824
H	3.8081	-3.0672	1.8702	H	4.2794	-3.173	0.5879
H	1.6129	1.3096	0.6176	H	0.9739	0.626	0.9886
H	3.0285	1.4138	1.5944	H	2.1725	0.5174	2.2203
H	3.022	1.1097	-1.4512	H	2.5899	1.8319	-0.5125
H	5.4205	1.1625	-1.4196	H	4.8326	2.3788	0.1446
H	5.4765	1.3023	0.3268	H	4.6485	1.611	1.7098
H	5.9408	-0.9845	-0.3195	H	5.8795	0.144	0.2308
H	4.5104	-1.0776	-1.3028	H	4.6747	0.2612	-1.0158
H	4.4577	-1.1676	3.0354	H	4.1614	-2.0543	2.6179
H	5.9326	-1.075	2.0788	H	5.6324	-1.1726	2.221
H	4.9098	0.3505	2.2674	H	4.2027	-0.3017	2.7781

H	-5.8193	2.1741	-0.3083	H	-6.1757	-1.253	-0.9213
H	-7.2749	1.9306	0.6515	H	-7.5011	-0.5088	-0.033
H	-7.0098	0.2911	-1.2074	H	-6.0903	-2.0241	1.353
H	-7.1908	-0.4788	0.3706	H	-6.2072	-0.3934	2.0186
H	-5.3524	2.3195	2.142	H	-6.3725	1.1871	-1.4191
H	-6.0196	0.7133	2.3608	H	-6.2158	1.545	0.2897
H	-2.3499	-1.4694	0.8357	H	-1.715	0.9779	0.4011
H	-2.7285	-1.6649	-0.8473	H	-1.5905	-0.6836	0.8785
H	-2.1032	0.6317	-1.39	H	-2.0451	-1.4845	-1.4074
H	-1.1729	0.9865	1.5017	H	-2.0468	1.4355	-2.3116
H	-1.0842	2.1576	0.2028	H	-2.2486	0.0087	-3.3138
H	-2.9872	2.5863	1.7403	H	-4.4031	1.1264	-2.8122
H	-3.4802	2.3695	0.0687	H	-4.3578	-0.5477	-2.2832
H	-2.5827	-0.2949	2.6831	H	-2.8784	2.5614	-0.5769
H	-3.632	0.8425	3.518	H	-4.4955	3.0313	-1.0823
H	-4.257	-0.7331	3.0069	H	-4.1634	2.6775	0.6203
H	-4.417	-2.3354	-1.6129	H	-2.5315	-1.6344	2.3151
H	1.1751	-0.6275	2.1712	H	1.004	-1.9017	1.2687
H	4.2508	4.9274	-0.3438	H	2.4302	4.705	2.4881
H	5.3299	3.5225	0.1412	H	3.8459	3.5354	2.5128
H	0.0396	0.1462	-2.7966	H	0.2835	1.1027	-2.87
2c-7	X axis(Å)	Y axis(Å)	Z axis(Å)	2c-8	X axis(Å)	Y axis(Å)	Z axis(Å)
C	3.0485	-3.3772	-0.0344	C	-2.7164	-3.5236	-0.4007
C	1.6323	-2.8413	0.1111	C	-1.3495	-2.8577	-0.4473
C	1.5741	-1.3169	-0.0335	C	-1.4121	-1.382	-0.0388
C	2.5851	-0.5781	0.9126	C	-2.492	-0.5749	-0.8396
C	4.0309	-1.1886	0.9423	C	-3.8859	-1.2856	-0.9724
C	3.9834	-2.7408	0.9851	C	-3.7129	-2.7958	-1.2935
C	2.6304	0.9587	0.7112	C	-2.6545	0.8964	-0.3744
C	3.4923	1.4389	-0.4723	C	-3.5573	1.0903	0.8582
C	4.8969	0.8136	-0.4181	C	-4.8985	0.3545	0.7327
C	4.8574	-0.7107	-0.2763	C	-4.7278	-1.1078	0.3145
C	4.8011	-0.763	2.2293	C	-4.7107	-0.6985	-2.1571
O	0.222	-0.9109	0.3826	O	-0.1013	-0.7994	-0.3792
C	3.4757	2.9577	-0.5565	C	-3.7311	2.5529	1.2243
C	-6.7502	0.6468	1.0589	C	6.7465	1.2692	-0.9134
C	-6.6605	-0.194	-0.2098	C	6.7597	0.1397	0.1082
C	-5.272	-0.6992	-0.4982	C	5.4167	-0.5259	0.3042
C	-4.1564	-0.2554	0.1252	C	4.2432	0.0058	-0.1194
C	-4.2072	0.9001	1.1399	C	4.1966	1.3752	-0.8322
C	-5.5842	1.6233	1.1288	C	5.5328	2.1571	-0.6963
C	-2.7635	-0.828	-0.0968	C	2.8774	-0.6528	0.0362
C	-1.7621	0.2642	-0.5041	C	1.8425	0.2833	0.6868
C	-1.7332	1.3866	0.5447	C	1.7285	1.5986	-0.0919
C	-3.1316	1.9613	0.7795	C	3.0923	2.2746	-0.2137
C	-3.9526	0.3518	2.5631	C	3.9085	1.1512	-2.3359
C	-5.2414	-1.7549	-1.553	C	5.5226	-1.8502	0.9943

O	-4.4307	-1.7756	-2.4699	O	6.5693	-2.2556	1.4888
C	-0.3853	-0.3087	-0.7125	C	0.4967	-0.3836	0.802
C	1.5461	-0.936	-1.502	C	-1.3832	-1.2601	1.4738
O	2.0446	-0.7545	2.2575	O	-1.9568	-0.4823	-2.1941
C	4.4643	3.8003	-0.2151	C	-3.2858	3.0753	2.3798
O	2.408	-1.1622	-2.3385	O	-2.2155	-1.6666	2.27
C	0.2989	-0.2751	-1.8513	C	-0.1666	-0.604	1.9314
C	2.2406	3.5855	-1.1163	C	-4.4263	3.4892	0.2971
H	2.253	4.6855	-1.1991	H	-4.5225	4.53	0.6505
O	1.2624	2.9339	-1.4633	O	-4.8693	3.1532	-0.7931
H	3.0383	-4.4631	0.1171	H	-2.6215	-4.5616	-0.7409
H	3.4222	-3.2134	-1.0502	H	-3.0876	-3.571	0.6281
H	0.9838	-3.3242	-0.6316	H	-0.6557	-3.4087	0.201
H	1.2248	-3.1376	1.0869	H	-0.9314	-2.9456	-1.4589
H	4.9924	-3.1504	0.8465	H	-4.6832	-3.3055	-1.2325
H	3.6594	-3.0695	1.9821	H	-3.376	-2.913	-2.3327
H	1.608	1.3465	0.6278	H	-1.6697	1.3429	-0.1857
H	3.0057	1.427	1.6327	H	-3.0441	1.4815	-1.217
H	3.05	1.0877	-1.4083	H	-3.0448	0.6279	1.7068
H	5.4483	1.0683	-1.3324	H	-5.425	0.3855	1.6955
H	5.4771	1.2299	0.4127	H	-5.5596	0.8568	0.0188
H	5.8897	-1.0758	-0.1923	H	-5.7255	-1.5436	0.1706
H	4.4775	-1.1449	-1.2027	H	-4.293	-1.6658	1.1457
H	4.3383	-1.1725	3.1343	H	-4.2307	-0.893	-3.1229
H	5.8331	-1.1331	2.2053	H	-5.7074	-1.1537	-2.2006
H	4.8463	0.3221	2.3551	H	-4.849	0.3831	-2.0786
H	-7.6989	1.1959	1.0678	H	7.6645	1.8605	-0.8175
H	-6.7579	-0.0039	1.941	H	6.7457	0.858	-1.9293
H	-6.9933	0.4074	-1.0655	H	7.0945	0.5324	1.077
H	-7.3613	-1.0325	-0.1178	H	7.5077	-0.594	-0.2166
H	-5.6523	2.2962	0.2629	H	5.6114	2.6018	0.3054
H	-5.6898	2.2595	2.0165	H	5.5595	2.9953	-1.4039
H	-2.4386	-1.3124	0.8335	H	2.5342	-0.9709	-0.9567
H	-2.7478	-1.6272	-0.8423	H	2.9172	-1.5648	0.6354
H	-2.1055	0.7005	-1.4536	H	2.1984	0.5228	1.6997
H	-1.3195	1.0228	1.4932	H	1.3054	1.4282	-1.0893
H	-1.0693	2.1936	0.2099	H	1.038	2.2793	0.4223
H	-3.0769	2.7234	1.5674	H	2.9828	3.1941	-0.8031
H	-3.4299	2.4895	-0.1368	H	3.3977	2.5915	0.7933
H	-2.955	-0.0844	2.6736	H	2.934	0.685	-2.5116
H	-4.0356	1.1492	3.3107	H	3.9114	2.1019	-2.8816
H	-4.6731	-0.429	2.8301	H	4.6587	0.5012	-2.7994
H	-6.0454	-2.5062	-1.4771	H	4.6148	-2.4637	1.0455
H	1.0873	-0.5642	2.1957	H	-1.0333	-0.1759	-2.113
H	4.376	4.878	-0.321	H	-3.4161	4.1215	2.6408
H	5.406	3.4463	0.1913	H	-2.7769	2.4575	3.1147
H	0.0435	0.1352	-2.8095	H	0.0863	-0.384	2.951

2d-1	X axis(Å)	Y axis(Å)	Z axis(Å)	2d-2	X axis(Å)	Y axis(Å)	Z axis(Å)
C	3.0609	-2.7955	-1.0405	C	3.0145	-2.8753	-0.8589
C	2.9008	-2.5322	0.4517	C	2.8029	-2.5461	0.6138
C	2.3561	-1.1193	0.6989	C	2.2928	-1.1089	0.7812
C	3.29	-0.0198	0.0781	C	3.285	-0.064	0.1565
C	3.5865	-0.2857	-1.4461	C	3.6341	-0.4007	-1.3424
C	3.9865	-1.7706	-1.6845	C	3.9965	-1.9054	-1.5047
C	2.7679	1.4261	0.282	C	2.8005	1.4038	0.2811
C	1.5892	1.8325	-0.6211	C	1.6721	1.807	-0.6853
C	1.8855	1.525	-2.0989	C	2.018	1.4316	-2.1363
C	2.3562	0.0837	-2.3138	C	2.452	-0.0305	-2.2746
C	4.8001	0.553	-1.9459	C	4.8925	0.3804	-1.8243
O	0.9941	-1.0881	0.2095	O	0.9536	-1.0582	0.234
C	1.1852	3.2722	-0.3411	C	1.301	3.2674	-0.4781
C	-6.0376	-0.569	-1.1293	C	-6.0785	-0.9472	-0.1651
C	-5.7002	0.6515	-0.2818	C	-5.7438	0.5395	-0.1694
C	-4.233	0.78	0.0585	C	-4.264	0.7994	-0.0222
C	-3.3322	-0.2185	-0.1158	C	-3.3221	-0.1336	-0.3025
C	-3.7601	-1.6077	-0.6332	C	-3.6883	-1.5124	-0.8918
C	-5.3025	-1.7923	-0.6065	C	-5.2081	-1.6729	-1.1761
C	-1.8374	-0.1028	0.1477	C	-1.8386	0.0043	-2.00E-04
C	-1.3193	-1.2069	1.083	C	-1.3956	-1.0689	1.0127
C	-1.6578	-2.5917	0.5166	C	-1.7619	-2.4831	0.5305
C	-3.1598	-2.7248	0.2644	C	-3.2391	-2.5905	0.13
C	-3.2679	-1.7844	-2.0893	C	-2.9785	-1.7447	-2.2488
C	-3.8749	2.1324	0.5958	C	-3.948	2.1633	0.509
O	-4.6933	3.0415	0.6946	O	-4.8144	3.0066	0.7191
C	0.1625	-1.0821	1.3292	C	0.0778	-0.9784	1.3164
C	2.1523	-0.9105	2.1839	C	2.0354	-0.832	2.2465
O	4.5708	-0.0896	0.7535	O	4.5347	-0.1438	0.8867
C	1.4644	4.3519	-1.0894	C	1.6483	4.3088	-1.2519
O	3.0337	-0.7267	3.0122	O	2.8879	-0.6414	3.1031
C	0.7397	-0.9557	2.5223	C	0.6094	-0.8183	2.5264
C	0.3625	3.5162	0.8819	C	0.4315	3.582	0.6955
H	0.0945	4.5673	1.0834	H	0.1885	4.6477	0.8461
O	-0.0068	2.6122	1.6229	O	-1.00E-04	2.7182	1.4506
H	3.4751	-3.7998	-1.1882	H	3.403	-3.8965	-0.9491
H	2.0833	-2.7886	-1.5357	H	2.0583	-2.86	-1.394
H	2.2181	-3.2871	0.8627	H	2.0811	-3.2629	1.026
H	3.8628	-2.6708	0.9607	H	3.7389	-2.6918	1.1673
H	4.0465	-1.9738	-2.7615	H	4.093	-2.1544	-2.5694
H	4.9967	-1.9436	-1.2887	H	4.9843	-2.0918	-1.0612
H	2.5057	1.574	1.3372	H	2.5009	1.6028	1.3178
H	3.5984	2.129	0.1251	H	3.658	2.0749	0.1306
H	0.7213	1.2207	-0.365	H	0.7765	1.231	-0.4418
H	0.981	1.6941	-2.6973	H	2.8134	2.0741	-2.529
H	2.6446	2.2067	-2.4971	H	1.1441	1.603	-2.7779

H	2.5973	-0.0476	-3.3769	H	2.7317	-0.2119	-3.3207
H	1.5187	-0.5937	-2.121	H	1.5866	-0.6746	-2.0904
H	5.7296	0.2595	-1.4452	H	5.7915	0.0803	-1.274
H	4.9566	0.4061	-3.0212	H	5.0877	0.1848	-2.8854
H	4.6723	1.6257	-1.7793	H	4.7917	1.4624	-1.706
H	-7.1195	-0.7438	-1.1048	H	-5.9313	-1.3668	0.8373
H	-5.7765	-0.3826	-2.1772	H	-7.1365	-1.0861	-0.4153
H	-6.2679	0.6058	0.6566	H	-6.3032	1.0031	0.6521
H	-6.0479	1.5391	-0.8244	H	-6.0939	1.0013	-1.1009
H	-5.6443	-1.9824	0.4203	H	-5.4826	-2.7349	-1.2028
H	-5.593	-2.6738	-1.1918	H	-5.4492	-1.2746	-2.1717
H	-1.3159	-0.1447	-0.8172	H	-1.2689	-0.0717	-0.9336
H	-1.5634	0.8592	0.5772	H	-1.5822	0.9815	0.4058
H	-1.8395	-1.1015	2.0464	H	-1.9501	-0.889	1.9459
H	-1.1053	-2.7787	-0.4123	H	-1.1292	-2.7777	-0.3157
H	-1.3452	-3.3716	1.2226	H	-1.5579	-3.2103	1.3271
H	-3.3611	-3.7095	-0.1767	H	-3.4196	-3.5942	-0.2759
H	-3.6619	-2.7192	1.2419	H	-3.8465	-2.5143	1.0416
H	-2.1764	-1.77	-2.1687	H	-1.888	-1.7666	-2.1713
H	-3.605	-2.7416	-2.5036	H	-3.2836	-2.7023	-2.6873
H	-3.6437	-0.9897	-2.743	H	-3.2343	-0.9545	-2.9649
H	-2.8369	2.2907	0.9122	H	-2.8931	2.4003	0.6938
H	4.4167	-0.0256	1.7202	H	4.3439	-0.0364	1.8428
H	1.1267	5.3501	-0.8237	H	1.3309	5.3261	-1.0394
H	2.0521	4.285	-1.999	H	2.2751	4.1891	-2.1295
H	0.3185	-0.9033	3.5075	H	0.15	-0.7108	3.4898
2d-3	X axis(Å)	Y axis(Å)	Z axis(Å)	2d-4	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-2.1656	-3.1488	-0.8354	C	3.0021	-2.7369	-1.1679
C	-2.0588	-2.0759	-1.9117	C	2.8142	-2.6124	0.3392
C	-2.0232	-0.6769	-1.2867	C	2.3259	-1.2062	0.7121
C	-3.2838	-0.3976	-0.3924	C	3.3237	-0.0986	0.2237
C	-3.5186	-1.5317	0.6769	C	3.6392	-0.224	-1.3144
C	-3.4045	-2.9409	0.0271	C	3.9833	-1.6944	-1.6908
C	-3.2537	0.9933	0.295	C	2.8764	1.348	0.5588
C	-2.2971	1.1112	1.4974	C	1.73	1.9021	-0.3102
C	-2.5383	-0.0206	2.5096	C	2.0097	1.7062	-1.8084
C	-2.5105	-1.4013	1.8478	C	2.4418	0.2799	-2.1586
C	-4.9574	-1.4657	1.27	C	4.8931	0.6086	-1.7134
O	-0.7689	-0.5432	-0.5806	O	0.9817	-1.0605	0.1982
C	-2.3579	2.513	2.0817	C	1.38	3.3575	-0.0316
C	6.4111	-0.0867	0.6285	C	-6.0407	-1.0199	-0.1777
C	5.5269	-1.0384	1.4236	C	-5.742	0.4583	0.0439
C	4.1476	-1.2333	0.8359	C	-4.268	0.7328	0.2092
C	3.617	-0.4306	-0.1201	C	-3.3052	-0.1349	-0.1849
C	4.3889	0.7939	-0.6557	C	-3.6399	-1.4161	-0.9752
C	5.6208	1.1461	0.2237	C	-5.156	-1.5631	-1.2868
C	2.2496	-0.6222	-0.7661	C	-1.8293	-0.0116	0.1648

C	1.3759	0.6452	-0.6933	C	-1.3573	-1.2336	0.9794
C	2.1162	1.8325	-1.3268	C	-1.694	-2.5575	0.2742
C	3.4739	2.048	-0.6602	C	-3.1696	-2.6301	-0.1334
C	4.8802	0.4959	-2.0922	C	-2.9225	-1.4162	-2.348
C	3.4355	-2.4178	1.4131	C	-3.9665	2.0363	0.8781
O	3.9066	-3.0939	2.3221	O	-4.8326	2.7264	1.4063
C	0.0102	0.3782	-1.2853	C	0.1169	-1.1619	1.2866
C	-1.8723	0.357	-2.3796	C	2.0846	-1.1332	2.204
O	-4.4524	-0.4088	-1.2494	O	4.5837	-0.3012	0.912
C	-3.0104	2.9002	3.1897	C	2.1927	4.304	0.4667
O	-2.7333	0.6831	-3.1854	O	2.9432	-1.0349	3.0697
C	-0.5487	0.9552	-2.3477	C	0.6617	-1.1847	2.5009
C	-1.5815	3.5706	1.3662	C	-0.0222	3.7871	-0.3143
H	-1.6317	4.5834	1.8007	H	-0.2472	4.8522	-0.1344
O	-0.923	3.3434	0.3577	O	-0.8862	3.0156	-0.7136
H	-2.2182	-4.1348	-1.3119	H	3.3796	-3.7388	-1.4038
H	-1.2642	-3.1544	-0.2123	H	2.0382	-2.6416	-1.6805
H	-1.1464	-2.2609	-2.4932	H	2.0888	-3.3717	0.6586
H	-2.8997	-2.1656	-2.6108	H	3.7553	-2.8441	0.8534
H	-3.4292	-3.715	0.805	H	4.0585	-1.7938	-2.7814
H	-4.2834	-3.1224	-0.6067	H	4.9768	-1.9479	-1.296
H	-3.0238	1.7647	-0.4507	H	2.6001	1.4197	1.6188
H	-4.2717	1.2498	0.6213	H	3.7577	1.9961	0.473
H	-1.2674	0.9769	1.1561	H	0.8411	1.3194	-0.0567
H	-1.767	0.013	3.2898	H	1.111	1.9461	-2.3909
H	-3.4967	0.1089	3.0238	H	2.7775	2.4146	-2.1435
H	-2.7283	-2.1577	2.6133	H	2.6995	0.2487	-3.2255
H	-1.4896	-1.6113	1.5139	H	1.578	-0.3834	-2.0526
H	-5.7196	-1.6678	0.509	H	5.7979	0.2436	-1.2146
H	-5.0871	-2.2166	2.0585	H	5.0746	0.5424	-2.7929
H	-5.1916	-0.4912	1.7064	H	4.795	1.6689	-1.4667
H	7.2747	0.2055	1.2371	H	-5.8799	-1.5828	0.7496
H	6.8113	-0.595	-0.2561	H	-7.096	-1.145	-0.4461
H	5.4147	-0.6566	2.4466	H	-6.2993	0.7762	0.933
H	6.0523	-1.9987	1.4952	H	-6.1185	1.047	-0.8018
H	5.2986	1.66	1.1399	H	-5.4079	-2.6139	-1.4773
H	6.2792	1.8484	-0.303	H	-5.406	-1.0216	-2.21
H	2.3961	-0.9143	-1.8143	H	-1.2466	0.102	-0.7565
H	1.6935	-1.4471	-0.3179	H	-1.6121	0.876	0.7626
H	1.2162	0.8881	0.3676	H	-1.9078	-1.2241	1.9321
H	2.2535	1.6767	-2.4035	H	-1.4698	-3.3996	0.9418
H	1.5221	2.7483	-1.2165	H	-1.0598	-2.6973	-0.6097
H	3.985	2.8836	-1.1556	H	-3.3335	-3.562	-0.6895
H	3.2889	2.3723	0.3734	H	-3.7744	-2.7069	0.7798
H	4.0556	0.3317	-2.7928	H	-1.8319	-1.4054	-2.268
H	5.4718	1.3307	-2.4853	H	-3.1906	-2.3086	-2.9261
H	5.5086	-0.4008	-2.1271	H	-3.2086	-0.5384	-2.9398

H	2.4545	-2.67	0.9929	H	-2.9211	2.3698	0.8688
H	-4.2991	0.2055	-1.9981	H	4.4116	-0.3283	1.877
H	-2.994	3.9254	3.5491	H	1.8617	5.3233	0.647
H	-3.5984	2.2059	3.781	H	3.2316	4.1035	0.7077
H	-0.1861	1.7095	-3.0189	H	0.2149	-1.2439	3.4745
2d-5	X axis(Å)	Y axis(Å)	Z axis(Å)	2d-6	X axis(Å)	Y axis(Å)	Z axis(Å)
C	2.8786	-2.7534	-1.8109	C	-2.2896	-3.1761	-0.5458
C	2.354	-2.8881	-0.386	C	-2.1594	-2.212	-1.7181
C	2.1108	-1.5062	0.2329	C	-2.0441	-0.7653	-1.2255
C	3.4225	-0.6416	0.2486	C	-3.2684	-0.3453	-0.3358
C	4.0805	-0.5384	-1.1782	C	-3.5293	-1.3647	0.838
C	4.1662	-1.9388	-1.8523	C	-3.4962	-2.831	0.3185
C	3.2289	0.7708	0.8565	C	-3.1575	1.0994	0.2199
C	2.487	1.7721	-0.0457	C	-2.1672	1.28	1.3869
C	3.1218	1.8318	-1.446	C	-2.4357	0.258	2.5037
C	3.2847	0.4442	-2.0754	C	-2.488	-1.1769	1.9715
C	5.5509	-0.0314	-1.0943	C	-4.9486	-1.1756	1.4511
O	1.0027	-0.9058	-0.479	O	-0.7684	-0.6286	-0.5596
C	2.3541	3.1149	0.655	C	-2.1484	2.7304	1.8406
C	-6.3965	1.1243	-0.8508	C	5.8042	0.6501	1.1994
C	-6.3715	-0.3713	-0.5649	C	5.327	-0.7118	1.6884
C	-5.0792	-0.858	0.0508	C	4.0427	-1.15	1.0263
C	-3.9329	-0.1329	0.0663	C	3.6015	-0.6298	-0.1451
C	-3.8616	1.2628	-0.5876	C	4.4412	0.3834	-0.9515
C	-5.0895	1.5549	-1.4942	C	5.8319	0.6694	-0.3187
C	-2.6239	-0.5723	0.713	C	2.2259	-0.8762	-0.7488
C	-1.4125	-0.4758	-0.2395	C	1.4245	0.4423	-0.821
C	-1.3062	0.9423	-0.8174	C	2.2129	1.5243	-1.5834
C	-2.6078	1.3662	-1.4937	C	3.6313	1.704	-1.0281
C	-3.8013	2.3413	0.5202	C	4.7289	-0.1449	-2.3786
C	-5.208	-2.2185	0.6628	C	3.2846	-2.1716	1.8148
O	-6.2249	-2.8967	0.5593	O	3.6668	-2.5866	2.904
C	-0.0998	-0.9128	0.3812	C	0.0352	0.187	-1.3607
C	1.5315	-1.6617	1.6196	C	-1.8718	0.1562	-2.4117
O	4.3917	-1.3159	1.0901	O	-4.4567	-0.3781	-1.1647
C	3.0506	4.2344	0.3999	C	-2.7524	3.2478	2.9227
O	2.1387	-2.0284	2.6165	O	-2.7356	0.4483	-3.2274
C	0.1201	-1.3137	1.6328	C	-0.5217	0.6909	-2.4606
C	1.3134	3.2147	1.7235	C	-1.3439	3.6801	1.0135
H	1.2297	4.1935	2.2257	H	-1.3353	4.7292	1.3544
O	0.5873	2.2774	2.0344	O	-0.7246	3.3309	0.0149
H	3.0693	-3.7518	-2.2218	H	-2.3993	-4.1977	-0.9283
H	2.1196	-2.2944	-2.4543	H	-1.3746	-3.1685	0.0571
H	1.4223	-3.4677	-0.4153	H	-1.2709	-2.493	-2.2982
H	3.0625	-3.466	0.2204	H	-3.0203	-2.3243	-2.3892
H	4.4852	-1.8321	-2.8971	H	-3.5377	-3.5289	1.1647
H	4.9473	-2.5328	-1.3582	H	-4.3977	-3.0268	-0.2782

H	2.7249	0.6836	1.827	H	-2.9107	1.7877	-0.5982
H	4.2129	1.1848	1.1187	H	-4.1542	1.4332	0.5418
H	1.4664	1.418	-0.2026	H	-1.1535	1.0656	1.0387
H	2.4979	2.4477	-2.1063	H	-1.6449	0.3252	3.2618
H	4.1015	2.3205	-1.4102	H	-3.3742	0.4799	3.0228
H	3.7915	0.5593	-3.0425	H	-2.7218	-1.8491	2.8075
H	2.2937	0.0462	-2.3139	H	-1.4863	-1.4656	1.638
H	6.1936	-0.738	-0.5573	H	-5.7376	-1.409	0.7273
H	5.9772	0.0891	-2.0974	H	-5.0936	-1.8445	2.3077
H	5.6396	0.9321	-0.5858	H	-5.1268	-0.1553	1.8006
H	-7.2358	1.356	-1.5167	H	5.1481	1.4417	1.5805
H	-6.5712	1.6821	0.0763	H	6.8067	0.8515	1.594
H	-6.5358	-0.9209	-1.5008	H	5.2009	-0.6421	2.7754
H	-7.2193	-0.5978	0.0934	H	6.0979	-1.4693	1.5001
H	-4.9898	1.0237	-2.4509	H	6.22	1.6347	-0.6674
H	-5.1365	2.6226	-1.7432	H	6.5592	-0.0851	-0.65
H	-2.4553	0.0518	1.6002	H	2.3308	-1.3213	-1.7454
H	-2.6738	-1.5985	1.0813	H	1.6457	-1.6042	-0.179
H	-1.6011	-1.165	-1.076	H	1.2949	0.8109	0.2077
H	-1.0435	1.6587	-0.0316	H	2.2699	1.2792	-2.6506
H	-0.5023	0.9897	-1.5627	H	1.6865	2.4848	-1.5159
H	-2.4969	2.3933	-1.865	H	4.161	2.4358	-1.6515
H	-2.7422	0.7331	-2.3819	H	3.5527	2.1519	-0.0287
H	-2.9057	2.2547	1.1433	H	3.8265	-0.293	-2.9778
H	-3.7925	3.3482	0.087	H	5.3646	0.5571	-2.9314
H	-4.6629	2.278	1.1937	H	5.2514	-1.1083	-2.3417
H	-4.3456	-2.6026	1.2208	H	2.3607	-2.5628	1.3713
H	3.9794	-1.4858	1.9637	H	-4.2934	0.1578	-1.9694
H	2.8858	5.1614	0.9423	H	-2.6794	4.2994	3.1857
H	3.8246	4.2687	-0.3598	H	-3.3551	2.6391	3.5888
H	-0.5319	-1.3986	2.4803	H	-0.1418	1.3639	-3.2047
2d-7	X axis(Å)	Y axis(Å)	Z axis(Å)				
C	2.9877	-2.7323	-1.3035				
C	2.874	-2.5867	0.2094				
C	2.3192	-1.2059	0.5805				
C	3.223	-0.0482	0.0174				
C	3.4683	-0.1897	-1.5322				
C	3.8761	-1.6463	-1.8988				
C	2.696	1.3719	0.3508				
C	1.465	1.8086	-0.4622				
C	1.7139	1.6386	-1.9709				
C	2.205	0.2312	-2.3262				
C	4.654	0.7018	-2.0069				
O	0.9425	-1.1637	0.134				
C	0.9888	3.1884	-0.0437				
C	-6.11	-0.3249	-0.9627				
C	-5.6636	0.8765	-0.1373				

C	-4.1786	0.92	0.099
C	-3.348	-0.1339	-0.0748
C	-3.8664	-1.4945	-0.5672
C	-5.416	-1.5911	-0.478
C	-1.8497	-0.0771	0.1813
C	-1.3511	-1.2321	1.0685
C	-1.7713	-2.5861	0.4844
C	-3.2873	-2.6465	0.2963
C	-3.4423	-1.6848	-2.0427
C	-3.6943	2.2712	0.5122
O	-2.742	2.8426	-0.0042
C	0.1424	-1.1842	1.2761
C	2.1603	-1.1093	2.0822
O	4.5271	-0.1566	0.642
C	1.1123	4.3323	-0.7363
O	3.0687	-1.0175	2.8969
C	0.7564	-1.1381	2.4565
C	0.2458	3.2784	1.2516
H	-0.215	4.2554	1.4752
O	0.1603	2.3413	2.0387
H	3.4105	-3.7156	-1.5412
H	1.994	-2.7041	-1.7645
H	2.2143	-3.3803	0.5832
H	3.854	-2.7493	0.6751
H	3.8989	-1.7651	-2.9898
H	4.9023	-1.8343	-1.5539
H	2.4942	1.4391	1.4265
H	3.504	2.1012	0.1988
H	0.6367	1.1398	-0.2297
H	0.7857	1.8363	-2.5224
H	2.4446	2.372	-2.3295
H	2.4136	0.198	-3.4037
H	1.3862	-0.4776	-2.1682
H	5.6026	0.3887	-1.5565
H	4.7791	0.6338	-3.0942
H	4.5159	1.758	-1.7617
H	-7.197	-0.441	-0.8817
H	-5.8936	-0.1525	-2.0233
H	-6.1684	0.8552	0.837
H	-5.9946	1.7893	-0.6476
H	-5.7234	-1.7693	0.5617
H	-5.7785	-2.4515	-1.0546
H	-1.337	-0.0877	-0.7886
H	-1.5649	0.8556	0.6722
H	-1.8368	-1.1284	2.0502
H	-1.2656	-2.7729	-0.4707
H	-1.4651	-3.3961	1.1586

H	-3.5538	-3.6162	-0.1435
H	-3.7482	-2.6263	1.2936
H	-2.3547	-1.697	-2.167
H	-3.8227	-2.6326	-2.4408
H	-3.8242	-0.8808	-2.6814
H	-4.3013	2.7529	1.2974
H	4.4036	-0.164	1.615
H	0.7156	5.2765	-0.3743
H	1.6144	4.3704	-1.6969
H	0.3631	-1.1149	3.4541

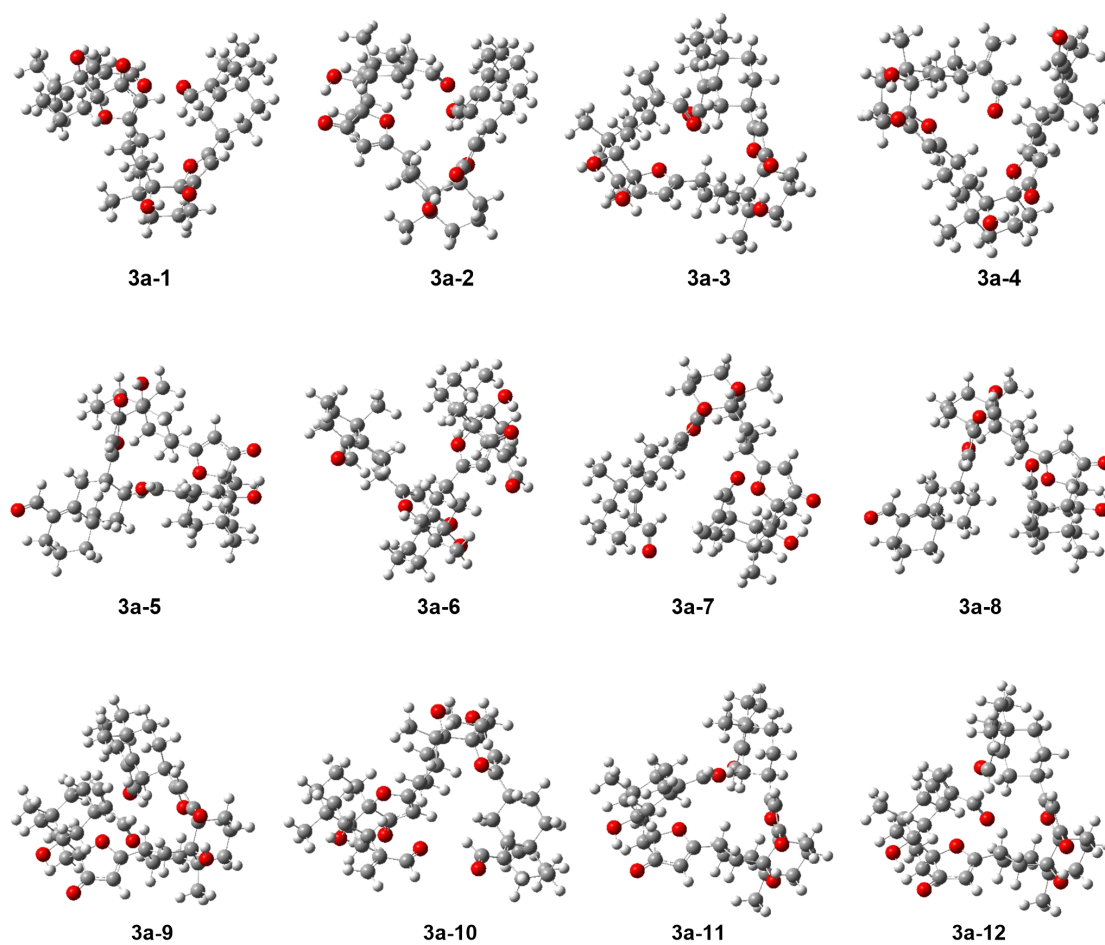
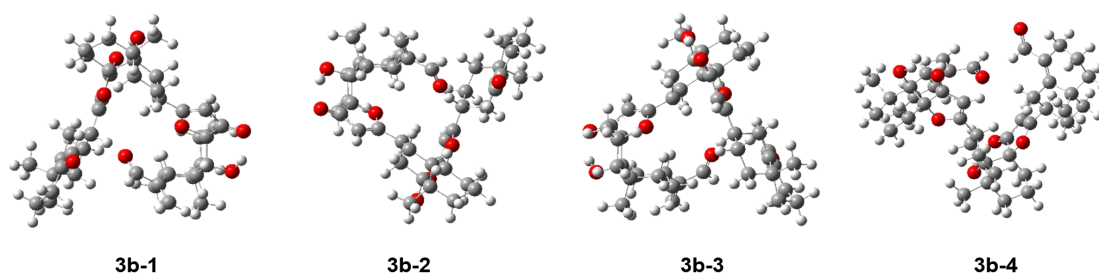


Figure S16. Optimized geometries of predominant conformers for **3a** at the B3LYP/6-31G (d,p) level



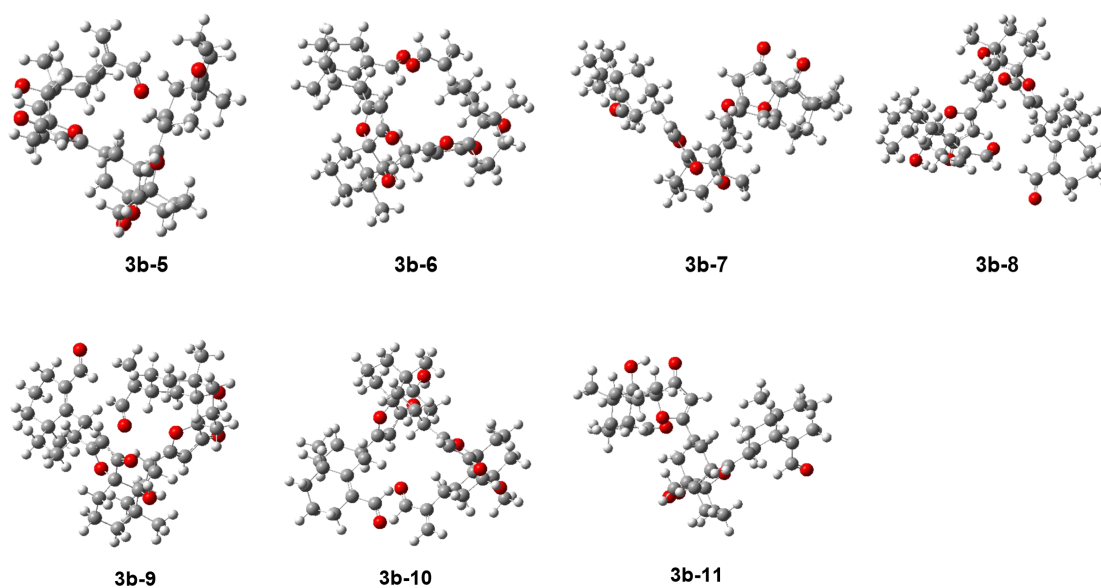


Figure S17. Optimized geometries of predominant conformers for **3b** at the B3LYP/6-31G (d,p) level

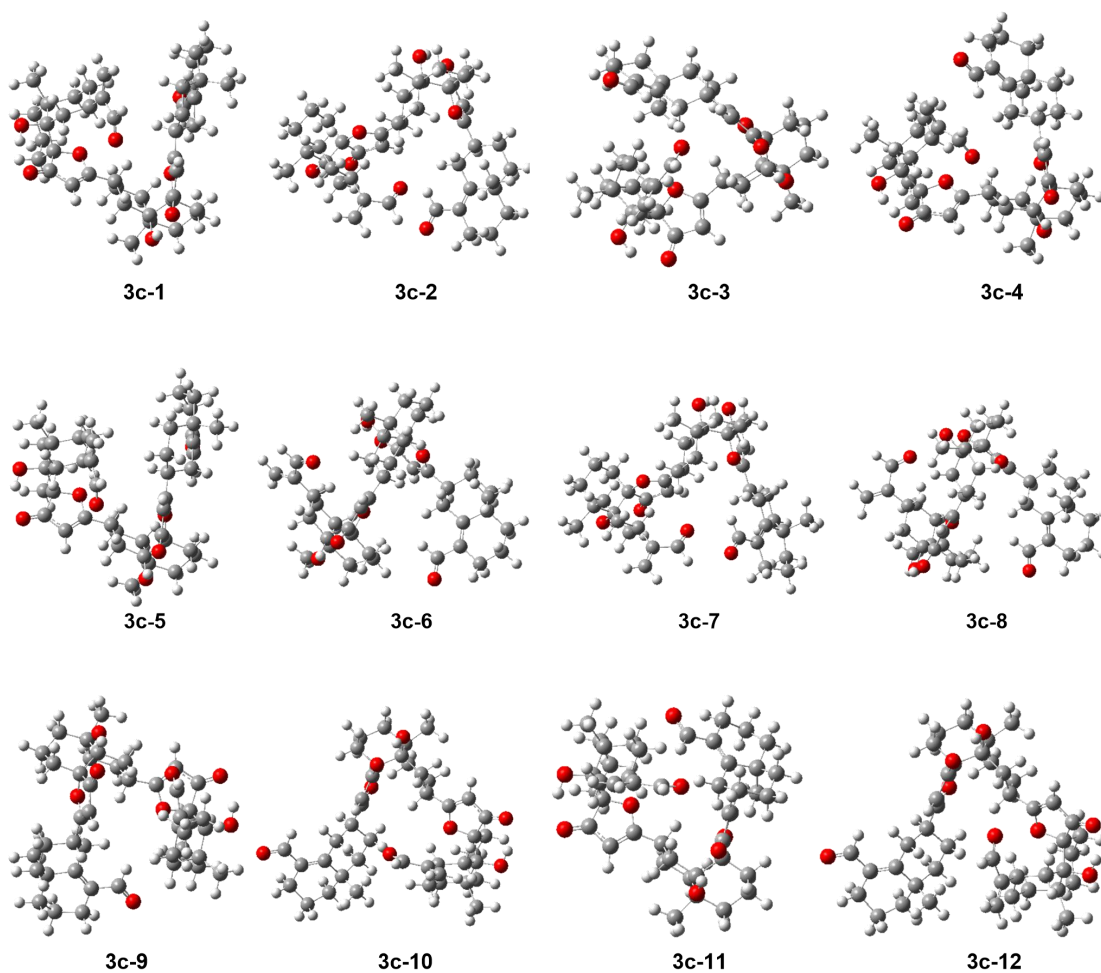


Figure S18. Optimized geometries of predominant conformers for **3c** at the S110

B3LYP/6-31G (d,p) level

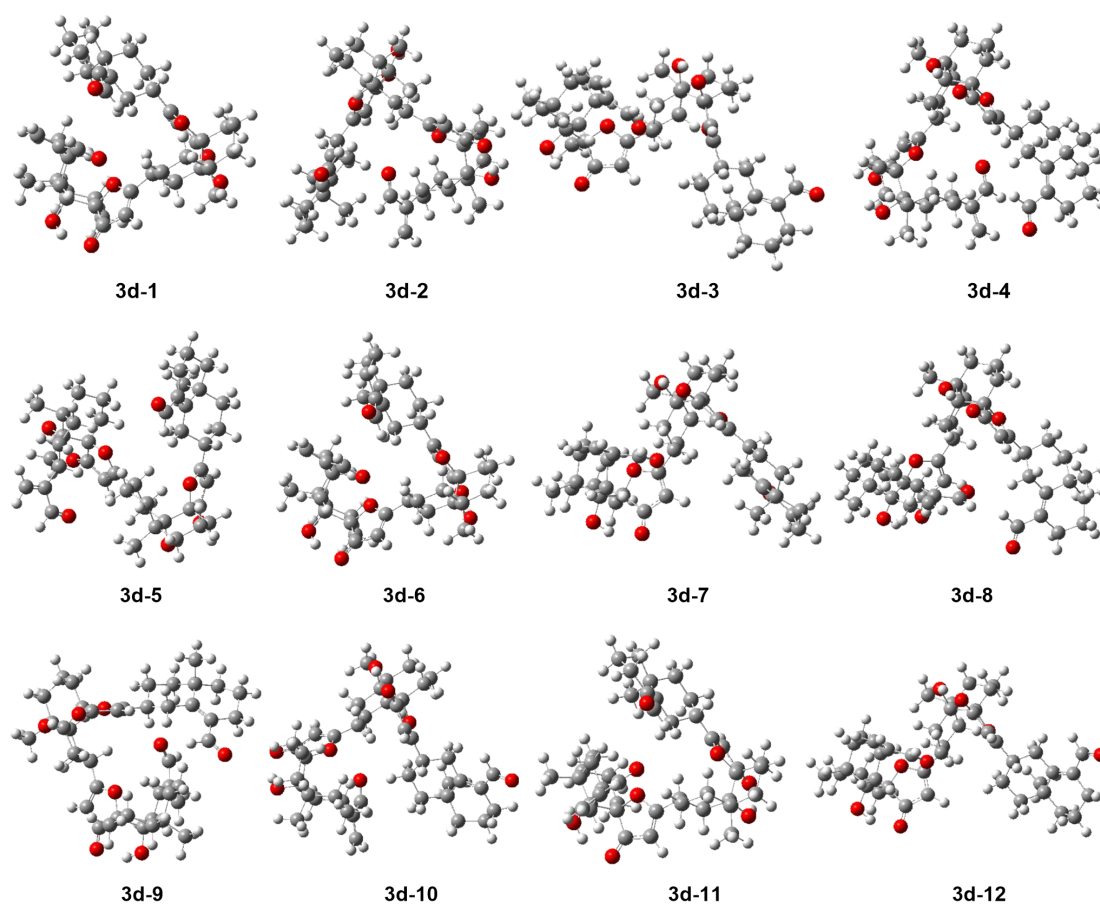


Figure S19. Optimized geometries of predominant conformers for **3d** at the B3LYP/6-31G (d,p) level

Table S6. Conformational analysis of the optimized **3a-3d** at the B3LYP/6-31G(d,p) level in the gas phase

	<i>Conformers</i>	G (Hartree)	ΔG (Kcal/mol)	Population
3a	3a-1	-2273.321998	1.23744972	4.53%
	3a-2	-2273.319115	3.04656105	0.21%
	3a-3	-2273.321414	1.60391556	2.44%
	3a-4	-2273.322442	0.95883528	7.25%
	3a-5	-2273.32397	0	36.58%
	3a-6	-2273.321728	1.40687742	3.40%
	3a-7	-2273.322682	0.80823288	9.34%
	3a-8	-2273.323849	0.07592871	32.18%
	3a-9	-2273.320317	2.29229403	0.76%
	3a-10	-2273.321497	1.55183223	2.66%

	3a-11	-2273.319892	2.55898578	0.49%
	3a-12	-2273.318919	3.16955301	0.17%
	<i>Conformers</i>	G (Hartree)	ΔG (Kcal/mol)	Population
3b	3b-1	-2273.325528	0.00439257	22.08%
	3b-2	-2273.325535	0	22.24%
	3b-3	-2273.325533	0.00125502	22.19%
	3b-4	-2273.324086	0.90926199	4.79%
	3b-5	-2273.323998	0.96448287	4.36%
	3b-6	-2273.320878	2.92231407	0.16%
	3b-7	-2273.325395	0.0878514	19.17%
	3b-8	-2273.323579	1.22740956	2.80%
	3b-9	-2273.319852	3.56613933	0.05%
	3b-10	-2273.318724	4.27397061	0.02%
	3b-11	-2273.323325	1.3867971	2.14%
	<i>Conformers</i>	G (Hartree)	ΔG (Kcal/mol)	Population
3c	3c-1	-2273.323715	0	35.43%
	3c-2	-2273.322943	0.48443772	15.63%
	3c-3	-2273.320363	2.10341352	1.02%
	3c-4	-2273.319772	2.47427193	0.54%
	3c-5	-2273.322755	0.6024096	12.81%
	3c-6	-2273.322371	0.84337344	8.53%
	3c-7	-2273.322552	0.72979413	10.33%
	3c-8	-2273.320667	1.91265048	1.40%
	3c-9	-2273.321005	1.7005521	2.01%
	3c-10	-2273.32244	0.80007525	9.18%
	3c-11	-2273.31965	2.55082815	0.48%
	3c-12	-2273.321268	1.53551697	2.65%
	<i>Conformers</i>	G (Hartree)	ΔG (Kcal/mol)	Population
3d	3d-1	-2273.321013	2.79179199	0.41%
	3d-2	-2273.321006	2.79618456	0.41%
	3d-3	-2273.323818	1.03162644	8.08%
	3d-4	-2273.323431	1.27447281	5.36%
	3d-5	-2273.323067	1.50288645	3.65%

3d-6	-2273.319479	3.75439233	0.08%
3d-7	-2273.323584	1.17846378	6.31%
3d-8	-2273.325462	0	46.15%
3d-9	-2273.324662	0.502008	19.77%
3d-10	-2273.323377	1.30835835	5.07%
3d-11	-2273.321147	2.70770565	0.48%
3d-12	-2273.323208	1.41440754	4.24%

Functional mPW1PW91		Solvent? PCM		Basis Set 6-311+G(d, p)			Type of Data Unscaled Shifts	
Nuclei	sp2?	DP4+	0.00%	0.00%	100.00%	0.00%	-	
		xperimenta	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	
C		18.5	22.00516	21.61972	21.85539	21.35694		
C		33.2	37.4723	37.585	37.50901	37.15228		
C		93.6	100.52166	100.58886	100.49547	100.16015		
C		74.4	80.56591	80.71014	80.72082	80.73122		
C		37.9	42.90397	43.01747	42.99306	42.8591		
C		36.3	38.28195	38.42252	38.34745	38.39945		
C		36.1	37.60372	39.47538	38.49826	37.62716		
C		38	42.48272	42.77595	42.33652	42.65059		
C		24.9	30.15873	27.13492	27.8934	29.17111		
C		32.4	34.97551	34.53289	34.59852	35.01451		
C		23.4	23.27989	23.35754	23.32334	23.34326		
C	x	210.3	220.0469	220.01784	220.00722	220.02076		
C	x	197.6	210.5433	209.49968	209.55278	208.99988		
C	x	102.3	107.04463	107.91173	107.76269	108.56628		
C		18.5	21.89665	21.60234	21.7993	22.06709		
C		33.1	36.91326	36.1583	36.90431	36.63697		
C		93.3	99.95709	100.18042	99.97775	99.96724		
C		74.9	81.07304	81.30202	81.04933	81.07785		
C		37.9	43.14715	43.06538	43.25677	43.08001		
C		36.5	38.49565	38.2375	38.59989	38.4872		
C		39.3	41.31081	39.80418	42.85913	41.95287		
C		33.1	36.58307	35.67565	36.42268	36.52298		
C		25.7	28.22105	31.11239	27.13623	27.56201		
C		32.9	35.52049	35.7212	35.42076	35.19318		
C	x	154.8	163.44246	163.39381	163.7239	163.59607		
C	x	194.8	205.44158	205.3088	205.66095	205.96902		
C	x	133.7	146.48014	146.27892	146.3739	146.98392		
C		23.6	23.72291	23.71101	23.63809	23.47961		
C	x	210.6	219.76518	219.83176	219.81448	219.52942		
C		24.7	27.57358	27.67442	27.44229	27.2944		
C	x	134.4	141.87903	141.85574	142.02757	142.26977		
C	x	159.8	178.40818	176.93504	178.40419	178.23444		
C		36.8	43.15785	43.35943	43.29841	43.21295		
C		39.7	41.54968	41.65013	41.5843	41.44618		
C		27.7	31.23513	31.12004	30.09693	29.60188		
C		41.6	47.0894	46.02673	46.71105	46.64381		
C		25.4	27.44143	26.88702	28.05394	29.77849		
C		40.8	43.74743	44.03922	43.82498	44.04707		
C	x	195.4	206.84814	207.84825	206.51673	207.93039		
C	x	103.7	109.7072	108.67766	109.27521	108.31101		
C		25.1	26.60394	26.25846	26.58522	26.4609		
C	x	190.9	198.86649	199.82868	198.91614	200.20932		
C		18.3	21.14086	21.30726	21.26424	21.16564		
H		1.92	1.98827	1.58018	2.0071	1.53915		
H		1.5	1.56413	2.03494	1.56342	1.96668		
H		2.35	2.21952	1.43634	2.2329	1.41511		
H		1.43	1.36112	2.18361	1.39782	2.16659		
H		1.31	2.03817	1.35078	2.07621	1.32298		
H		2.09	1.31158	2.03378	1.32643	2.03706		
H		2.23	1.8737	1.66356	1.9773	1.56277		
H		2.14	2.00691	1.80406	1.60323	2.05469		
H		3.11	2.89315	3.13874	3.14615	3.16987		
H		2.05	1.7274	1.50107	2.07561	1.74438		
H		1.93	2.0049	1.87628	1.8838	1.91905		

H		2.57	2.64957	1.22682	2.53369	1.24002	
H		1.29	1.28497	2.57928	1.21601	2.53624	
H		1.27	1.56972	1.42815	1.62643	1.39783	
H		1.27	0.41483	0.44166	0.42501	0.40865	
H		1.27	1.46386	1.57781	1.42338	1.59587	
H		5.77	5.55723	5.62367	5.53677	5.56618	
H	x	5.81	5.64904	5.62395	5.62446	5.64433	
H		1.85	1.90934	1.85468	1.9351	1.8842	
H		1.5	1.51164	1.48116	1.53052	1.49193	
H		2.3	2.15736	2.12188	2.12527	2.12026	
H		1.32	1.31054	1.28127	1.2946	1.27379	
H		2.03	1.96434	1.94981	1.97506	1.93721	
H		1.27	1.26226	1.22979	1.26666	1.2737	
H		1.65	1.46194	1.69227	1.32664	1.33751	
H		1.63	1.24492	1.10954	1.25915	1.30306	
H		2.9	2.6946	2.87372	2.88507	2.77878	
H		1.52	1.63698	1.41111	1.43902	1.72293	
H		1.63	1.42961	1.41983	1.72712	1.29571	
H		1.15	1.12866	1.10551	1.19062	1.17619	
H		2.38	2.34229	2.34838	2.39416	2.37775	
H	x	9.44	9.64885	9.45425	9.4758	9.65677	
H	x	5.85	6.50218	6.43751	6.42927	6.48445	
H	x	6.18	6.83034	6.77967	6.81935	6.82224	
H		1.17	1.52252	1.48265	1.54196	1.53763	
H		1.17	0.3664	0.33701	0.3736	0.35553	
H		1.17	1.38149	1.38384	1.33654	1.33012	
H		2.51	2.04294	2.0127	2.52299	2.57831	
H		2.17	2.59021	2.52312	2.07096	2.01855	
H		1.29	1.40797	1.28521	1.4623	1.42979	
H		1.5	1.64956	1.62175	1.65325	1.64141	
H		3.8	2.57449	2.35408	4.06136	2.4884	
H		2.44	3.71994	4.45273	2.78435	4.18248	
H		2.93	3.11337	3.3933	2.96625	3.10982	
H		1.13	2.06199	2.08613	1.91421	2.18376	
H		2.03	2.35801	1.99235	2.19137	1.99907	
H		1.5	1.7804	1.87974	1.67131	1.81481	
H		1.73	1.73467	1.54953	1.89897	1.91833	
H	x	5.98	5.59725	5.79804	5.7815	5.65936	
H		1.18	1.56437	1.32511	0.80821	1.90107	
H		1.18	1.08426	1.87058	1.95031	1.34854	
H		1.18	1.53077	0.80472	1.29953	0.80325	
H	x	10.41	10.5188	10.87848	10.53796	10.67221	
H		5.66	5.5446	5.44611	5.53321	5.52304	
H		1.5	1.64557	1.55985	1.63802	1.63786	
H		1.5	1.69762	1.64052	1.6767	1.69681	

Functional	Solvent?		Basis Set		Type of Data	
mPW1PW91	PCM		6-311+G(d,p)		Unscaled Shifts	
	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	0.00%	0.00%	100.00%	0.00%	–	–
sDP4+ (C data)	1.36%	4.26%	87.82%	6.56%	–	–
sDP4+ (all data)	0.00%	0.00%	100.00%	0.00%	–	–
uDP4+ (H data)	0.00%	0.00%	100.00%	0.00%	–	–
uDP4+ (C data)	18.50%	8.13%	61.03%	12.34%	–	–
uDP4+ (all data)	0.00%	0.00%	100.00%	0.00%	–	–
DP4+ (H data)	0.00%	0.00%	100.00%	0.00%	–	–
DP4+ (C data)	0.46%	0.63%	97.44%	1.47%	–	–
DP4+ (all data)	0.00%	0.00%	100.00%	0.00%	–	–

Figure S20. DP4+ analysis of experimental NMR data of **3** and unscaled shifts of **3a-3d** (Isomer 1-4)

Table S7. The Cartesian coordinates of the lowest energy conformers for **3a-3d** in the gas phase at the B3LYP/6-31G(d,p) level

3a-1	X axis(Å)	Y axis(Å)	Z axis(Å)	3a-2	X axis(Å)	Y axis(Å)	Z axis(Å)
C	2.9055	4.0582	2.425	C	5.7147	0.7164	-1.2828
C	3.2373	4.2135	0.9455	C	5.3437	0.8226	0.1907
C	2.3428	3.3094	0.0875	C	3.9654	0.2001	0.4593
C	0.8199	3.6206	0.3128	C	3.9117	-1.3033	0.0165
C	0.4283	3.5522	1.8364	C	4.3642	-1.488	-1.4814
C	1.4373	4.3622	2.701	C	5.6967	-0.7326	-1.7536
C	-0.1326	2.7297	-0.5227	C	2.5375	-1.9837	0.2459
C	-0.2629	1.282	-0.0288	C	1.4357	-1.5943	-0.7539
C	-0.56	1.2044	1.4757	C	1.9073	-1.6545	-2.2143
C	0.3687	2.0806	2.3194	C	3.2622	-0.9879	-2.4484
C	-0.9614	4.2023	2.0999	C	4.6582	-2.9805	-1.8115
C	2.7388	3.4359	-1.3655	C	3.6201	0.3792	1.9196
O	2.4769	4.3724	-2.1071	O	4.0625	-0.2809	2.8499
O	0.5776	4.9848	-0.1095	O	4.8653	-2.0413	0.8208
C	-1.2794	0.5425	-0.8651	C	0.1769	-2.4222	-0.6124
O	-2.6219	0.6967	-0.5251	O	-1.0276	-1.7218	-0.7146
C	-0.9948	-0.2553	-1.8924	C	0.0986	-3.7378	-0.4177
C	-5.1826	1.7526	-1.5309	C	-3.2643	-1.4826	-2.646
C	-4.1256	1.0358	-2.3634	C	-2.5513	-2.7711	-2.2562
C	-3.3967	-0.0153	-1.519	C	-2.0832	-2.7107	-0.7966
C	-4.3928	-1.0775	-0.9279	C	-3.2811	-2.4662	0.1866
C	-5.5762	-0.4047	-0.1359	C	-4.1361	-1.2059	-0.2155
C	-6.1929	0.7688	-0.9518	C	-4.4579	-1.2141	-1.738
C	-3.7024	-2.1553	-0.0532	C	-2.8568	-2.376	1.6757
C	-3.2616	-1.6756	1.3406	C	-2.1706	-1.0584	2.0896
C	-4.4256	-1.0009	2.0857	C	-3.0078	0.1524	1.6498
C	-5.092	0.0971	1.2492	C	-3.3947	0.0978	0.17
C	-2.5787	-2.8033	2.0961	C	-1.8407	-0.9658	3.5735
C	-1.1679	-3.1128	1.7088	C	-0.7742	-6.00E-04	3.9752
C	-3.0926	-3.5336	3.0989	C	-2.3805	-1.6844	4.5721
O	-0.5689	-2.492	0.8359	O	-0.1819	0.7105	3.1723
C	-6.7477	-1.4043	0.098	C	-5.5208	-1.2002	0.4977
C	-2.3113	-0.6747	-2.3413	C	-1.3337	-3.9779	-0.4518
O	-2.4821	-1.4662	-3.2586	O	-1.8312	-5.0708	-0.2181
C	3.7825	-4.5867	1.1007	C	-2.5219	4.2553	-2.3447
C	3.2381	-3.1859	0.9386	C	-1.5306	3.2251	-1.8542
C	3.5514	-2.3722	-0.101	C	-0.8873	3.3051	-0.6626
C	4.5373	-2.8197	-1.1981	C	-1.1169	4.4955	0.2916
C	5.3367	-4.0871	-0.7882	C	-1.8326	5.6802	-0.4141
C	2.9747	-0.9802	-0.325	C	0.0908	2.2643	-0.1311

C	4.0538	0.0952	-0.5641	C	1.42	2.8681	0.3571
C	4.9715	-0.3243	-1.7224	C	1.1609	3.97	1.3933
C	5.58	-1.7032	-1.4706	C	0.236	5.0425	0.8198
C	3.4255	1.4629	-0.7417	C	2.3561	1.7809	0.8355
C	3.4831	2.2646	-1.8038	C	2.6711	1.466	2.091
O	2.7138	1.937	0.3628	O	2.969	1.0357	-0.175
C	3.7489	-3.1312	-2.4925	C	-1.9903	4.0311	1.4805
C	2.294	-2.801	2.037	C	-1.353	2.0899	-2.8151
O	2.0179	-3.552	2.9688	O	-1.8871	2.0683	-3.9195
O	-5.0025	-1.7837	-2.0378	O	-4.1769	-3.6027	0.0901
C	4.4518	-5.1442	-0.149	C	-3.002	5.2201	-1.2684
H	3.1533	3.0464	2.7651	H	5.0335	1.3225	-1.8904
H	3.5321	4.742	3.0097	H	6.7172	1.1335	-1.4345
H	3.1255	5.2633	0.6468	H	6.1123	0.3344	0.8031
H	4.2954	3.9592	0.802	H	5.3508	1.884	0.4701
H	1.2832	5.4364	2.5294	H	6.5219	-1.2562	-1.2515
H	1.2352	4.1953	3.7669	H	5.9307	-0.7598	-2.8257
H	0.1815	2.7352	-1.5749	H	2.1865	-1.7872	1.2677
H	-1.1267	3.1981	-0.5506	H	2.6907	-3.0707	0.2319
H	0.6929	0.7807	-0.1909	H	1.1532	-0.5616	-0.5347
H	-1.5993	1.4879	1.6802	H	1.9585	-2.6966	-2.5548
H	-0.4592	0.1666	1.8157	H	1.162	-1.1708	-2.86
H	1.364	1.6269	2.3307	H	3.1356	0.0964	-2.3799
H	0.026	2.0446	3.3621	H	3.5655	-1.1754	-3.487
H	-1.7635	3.7388	1.5195	H	3.8006	-3.6328	-1.6268
H	-1.2354	4.1153	3.1582	H	4.9328	-3.0972	-2.8667
H	-0.9619	5.2706	1.8564	H	5.4936	-3.3697	-1.2189
H	0.8878	5.0861	-1.0338	H	4.6816	-1.8577	1.7668
H	-0.056	-0.5431	-2.3231	H	0.8595	-4.4864	-0.3085
H	-4.709	2.3262	-0.7262	H	-2.5667	-0.6397	-2.613
H	-5.7071	2.4801	-2.1615	H	-3.609	-1.5588	-3.6839
H	-4.5916	0.5734	-3.2423	H	-3.2167	-3.629	-2.4145
H	-3.4179	1.7848	-2.7416	H	-1.6971	-2.9093	-2.9316
H	-6.7738	0.3621	-1.7911	H	-5.2107	-1.9867	-1.9465
H	-6.9093	1.3208	-0.3298	H	-4.917	-0.2603	-2.0286
H	-4.3814	-3.0123	0.0603	H	-3.7556	-2.5327	2.2863
H	-2.8505	-2.5785	-0.5998	H	-2.2104	-3.2245	1.9345
H	-2.5046	-0.8986	1.2257	H	-1.2115	-1.0152	1.5636
H	-5.1832	-1.7371	2.3757	H	-3.9097	0.233	2.2687
H	-4.057	-0.5579	3.0198	H	-2.4504	1.0782	1.8243
H	-5.941	0.4992	1.8175	H	-4.0242	0.9681	-0.0574
H	-4.3933	0.9327	1.1427	H	-2.4916	0.227	-0.434
H	-0.6865	-3.9396	2.2589	H	-0.5414	0.0412	5.0529
H	-2.5271	-4.3157	3.5988	H	-2.0771	-1.566	5.6089
H	-4.1044	-3.3822	3.4598	H	-3.1576	-2.4217	4.3987
H	-6.4334	-2.312	0.6195	H	-5.4381	-1.2463	1.5866
H	-7.5391	-0.9405	0.6989	H	-6.0795	-0.2892	0.2519

H	-7.2071	-1.7192	-0.8457	H	-6.1409	-2.0483	0.1865
H	4.5082	-4.5796	1.9242	H	-2.0507	4.8266	-3.155
H	2.9813	-5.2797	1.3854	H	-3.4059	3.7645	-2.7702
H	6.1252	-3.8223	-0.0701	H	-1.1262	6.2174	-1.0621
H	5.8493	-4.5147	-1.6591	H	-2.1836	6.4108	0.3256
H	2.2944	-1.0207	-1.1854	H	-0.3944	1.7184	0.6857
H	2.3595	-0.6571	0.5149	H	0.3297	1.5136	-0.8842
H	4.6768	0.1547	0.3405	H	1.9106	3.3478	-0.503
H	4.4224	-0.3303	-2.6715	H	0.7237	3.5553	2.3088
H	5.7859	0.4023	-1.837	H	2.109	4.4392	1.685
H	6.2069	-1.9771	-2.329	H	0.0579	5.8062	1.5879
H	6.2593	-1.6162	-0.6112	H	0.7731	5.5477	0.005
H	3.9504	2.1454	-2.7624	H	2.3275	1.8612	3.0274
H	3.2314	-2.2532	-2.8913	H	-1.4951	3.2689	2.0893
H	4.4181	-3.494	-3.2812	H	-2.2241	4.8693	2.147
H	2.9851	-3.8988	-2.327	H	-2.9398	3.601	1.1437
H	1.8452	-1.8018	1.9887	H	-0.7212	1.2526	-2.4951
H	-4.2901	-2.1341	-2.6133	H	-3.6585	-4.424	0.2269
H	3.6923	-5.4906	-0.8591	H	-3.7666	4.7396	-0.6474
H	5.051	-6.0226	0.1175	H	-3.4837	6.0845	-1.7401
3a-3	X axis(Å)	Y axis(Å)	Z axis(Å)	3a-4	X axis(Å)	Y axis(Å)	Z axis(Å)
C	5.5885	0.2473	-1.6236	C	-5.1748	-2.3383	-1.484
C	5.411	0.4874	-0.1295	C	-4.6447	-2.7324	-0.1122
C	4.0451	-0.0273	0.3501	C	-3.6383	-1.701	0.4117
C	3.8678	-1.554	0.0492	C	-4.2439	-0.2549	0.473
C	4.1208	-1.8867	-1.4689	C	-4.8916	0.1704	-0.8997
C	5.4404	-1.2298	-1.9673	C	-5.8134	-0.9553	-1.4499
C	2.5058	-2.1353	0.5012	C	-3.2324	0.8261	0.9435
C	1.2962	-1.7708	-0.3796	C	-2.1739	1.2374	-0.0981
C	1.5842	-1.9821	-1.875	C	-2.8136	1.5757	-1.4541
C	2.9267	-1.4116	-2.333	C	-3.7961	0.5113	-1.9394
C	4.3071	-3.415	-1.6993	C	-5.8092	1.4174	-0.7377
C	3.8807	0.2924	1.8181	C	-3.1271	-2.1571	1.7574
O	4.4075	-0.3013	2.7488	O	-3.7563	-2.1516	2.8065
O	4.8812	-2.2739	0.7956	O	-5.3224	-0.258	1.4404
C	0.0288	-2.5222	-0.0183	C	-1.2867	2.388	0.3259
O	-1.1547	-1.995	-0.5474	O	-0.1575	2.5787	-0.4745
C	-0.0845	-3.6102	0.7423	C	-1.4389	3.2186	1.3559
C	-3.2478	-2.7169	-2.5321	C	0.7413	4.5583	-2.477
C	-2.5669	-3.6658	-1.5539	C	0.0593	4.8765	-1.1516
C	-2.2107	-2.9405	-0.2509	C	0.4327	3.8381	-0.0848
C	-3.474	-2.3053	0.4317	C	1.9817	3.7701	0.1377
C	-4.2988	-1.3988	-0.56	C	2.7611	3.5308	-1.2103
C	-4.5093	-2.1153	-1.9249	C	2.2561	4.4984	-2.3197
C	-3.1393	-1.5263	1.7309	C	2.4141	2.7297	1.1995
C	-2.5011	-0.1439	1.5136	C	2.377	1.2604	0.7439
C	-3.3215	0.7062	0.5323	C	3.0613	1.0473	-0.6171

C	-3.5911	-0.0376	-0.7773	C	2.6128	2.0585	-1.6749
C	-2.2536	0.5353	2.8487	C	2.9605	0.3757	1.8324
C	-0.8735	0.4719	3.4125	C	2.0299	-0.428	2.6717
C	-3.17	1.1959	3.5754	C	4.2676	0.2615	2.1231
O	0.0682	-0.0412	2.8192	O	0.8273	-0.5111	2.4497
C	-5.7305	-1.1161	-0.0156	C	4.2796	3.837	-1.0532
C	-1.5063	-3.8972	0.6834	C	-0.3169	4.1312	1.1947
O	-2.0323	-4.7943	1.3281	O	-0.0458	5.008	2.0035
C	-2.1818	4.3935	-2.3717	C	4.7482	-3.6262	-0.1894
C	-1.2571	3.3112	-1.8627	C	3.3867	-3.5703	0.4571
C	-0.5822	3.389	-0.6886	C	2.2175	-3.6139	-0.2273
C	-0.6927	4.633	0.2183	C	2.1957	-3.7796	-1.7582
C	-1.3402	5.8383	-0.5172	C	3.5846	-3.5	-2.3974
C	0.3213	2.2966	-0.1296	C	0.8404	-3.5069	0.4169
C	1.7114	2.8178	0.2725	C	-0.072	-2.4609	-0.26
C	1.577	3.9785	1.268	C	-0.1846	-2.7709	-1.7609
C	0.7152	5.0953	0.6804	C	1.1964	-2.7926	-2.4125
C	2.589	1.6873	0.757	C	-1.4319	-2.323	0.3975
C	3.0119	1.4453	1.997	C	-1.7448	-2.5941	1.6642
O	3.028	0.8141	-0.2408	O	-2.4452	-1.7845	-0.3981
C	-1.5573	4.2892	1.4546	C	1.7793	-5.2326	-2.089
C	-1.1869	2.1308	-2.7836	C	3.4438	-3.5034	1.9481
O	-1.7814	2.0944	-3.8562	O	4.4392	-3.1277	2.5577
O	-4.3654	-3.3813	0.8185	O	2.4158	5.0611	0.6337
C	-2.5622	5.4316	-1.324	C	4.7239	-4.1433	-1.6221
H	4.8666	0.8438	-2.1927	H	-4.3691	-2.3692	-2.2258
H	6.5832	0.5919	-1.9299	H	-5.9211	-3.0731	-1.8082
H	6.2232	0.0011	0.4251	H	-5.4818	-2.8428	0.5888
H	5.5076	1.5645	0.0581	H	-4.1741	-3.7206	-0.1961
H	6.2982	-1.7596	-1.5308	H	-6.7192	-1.0204	-0.8315
H	5.5324	-1.3518	-3.0543	H	-6.156	-0.6985	-2.4606
H	2.3007	-1.8459	1.5403	H	-2.7337	0.4944	1.8636
H	2.6117	-3.2272	0.5514	H	-3.8016	1.7112	1.2584
H	1.079	-0.7105	-0.2192	H	-1.4965	0.3925	-0.2486
H	1.5458	-3.0519	-2.1173	H	-3.3213	2.547	-1.3995
H	0.7888	-1.5169	-2.4725	H	-2.0313	1.6936	-2.2157
H	2.857	-0.3201	-2.3483	H	-3.2303	-0.3807	-2.2249
H	3.0867	-1.7023	-3.3798	H	-4.2616	0.8667	-2.8682
H	3.4515	-4.0036	-1.3582	H	-5.2843	2.2777	-0.3142
H	4.4449	-3.632	-2.7654	H	-6.2142	1.7296	-1.7078
H	5.1913	-3.7986	-1.1782	H	-6.6655	1.2089	-0.0867
H	4.8069	-2.0206	1.7404	H	-4.9919	-0.6405	2.2806
H	0.6456	-4.1923	1.2705	H	-2.1896	3.2772	2.12
H	-2.5564	-1.9237	-2.8379	H	0.3643	3.6119	-2.8808
H	-3.512	-3.2658	-3.4436	H	0.4842	5.3313	-3.2108
H	-3.2197	-4.5244	-1.3523	H	0.3354	5.8859	-0.8219
H	-1.6638	-4.0649	-2.0334	H	-1.0255	4.8889	-1.3184

H	-5.2375	-2.9286	-1.8014	H	2.6063	5.5167	-2.1015
H	-4.9545	-1.4198	-2.6481	H	2.7027	4.227	-3.285
H	-4.0605	-1.4134	2.3198	H	3.4286	2.9838	1.5379
H	-2.4938	-2.1354	2.3769	H	1.8071	2.8463	2.107
H	-1.5276	-0.2802	1.0363	H	1.33	0.9758	0.602
H	-4.2733	1.0184	0.9747	H	4.1518	1.0963	-0.5252
H	-2.7813	1.6313	0.3074	H	2.8421	0.0342	-0.9784
H	-4.2032	0.605	-1.4236	H	3.2061	1.8939	-2.5841
H	-2.6438	-0.17	-1.3089	H	1.5812	1.8347	-1.962
H	-0.7389	0.9302	4.407	H	2.4906	-0.9696	3.5158
H	-2.9378	1.6653	4.5271	H	4.6409	-0.3923	2.9079
H	-4.2016	1.2769	3.2455	H	5.0217	0.8223	1.5793
H	-5.7236	-0.672	0.9833	H	4.7507	3.2501	-0.2604
H	-6.2682	-0.4262	-0.6769	H	4.8174	3.6185	-1.9835
H	-6.3297	-2.0316	0.045	H	4.4584	4.8929	-0.8212
H	-1.6906	4.8966	-3.2146	H	5.178	-2.6162	-0.1757
H	-3.1106	3.9548	-2.7568	H	5.4222	-4.269	0.3901
H	-0.6153	6.2973	-1.2035	H	3.7704	-2.4176	-2.4373
H	-1.6178	6.6205	0.2005	H	3.6043	-3.8514	-3.4368
H	-0.1725	1.8519	0.7415	H	0.3632	-4.495	0.3891
H	0.4589	1.4768	-0.8349	H	0.9233	-3.2382	1.4714
H	2.1959	3.2226	-0.6287	H	0.4118	-1.4777	-0.1678
H	1.1444	3.6348	2.215	H	-0.7019	-3.7245	-1.9203
H	2.568	4.3855	1.5057	H	-0.7835	-2.0035	-2.2674
H	0.6221	5.9002	1.4209	H	1.0828	-3.0253	-3.4792
H	1.2599	5.5253	-0.1716	H	1.6015	-1.7723	-2.366
H	2.8182	1.9436	2.9265	H	-1.1523	-2.9537	2.4828
H	-2.5594	3.9521	1.1694	H	0.7721	-5.4694	-1.7312
H	-1.1174	3.4953	2.0653	H	1.7862	-5.4062	-3.1713
H	-1.6769	5.1638	2.1045	H	2.4564	-5.9631	-1.6329
H	-0.5781	1.2764	-2.4642	H	2.5406	-3.8128	2.4925
H	-3.8586	-4.0368	1.3435	H	1.8861	5.2808	1.4295
H	-3.3424	5.0323	-0.666	H	4.622	-5.2345	-1.6258
H	-2.9931	6.3099	-1.8186	H	5.6802	-3.9188	-2.1086
3a-5	X axis(Å)	Y axis(Å)	Z axis(Å)	3a-6	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-3.336	4.2121	-1.0331	C	3.6849	-4.3915	0.1404
C	-3.1423	3.8689	0.4389	C	3.4817	-3.5968	-1.1441
C	-1.8333	3.0972	0.6524	C	2.7315	-2.2891	-0.8623
C	-0.5914	3.91	0.1447	C	3.4886	-1.3998	0.1875
C	-0.7644	4.3646	-1.3534	C	3.824	-2.1902	1.5088
C	-2.16	5.0169	-1.5744	C	4.4465	-3.578	1.1802
C	0.7634	3.178	0.3266	C	2.7493	-0.0802	0.5236
C	1.0221	2.0273	-0.6596	C	1.5283	-0.24	1.4389
C	0.752	2.4321	-2.1165	C	1.8599	-1.0396	2.7056
C	-0.5776	3.162	-2.3127	C	2.5556	-2.3653	2.3836
C	0.2716	5.4587	-1.7444	C	4.895	-1.4465	2.3605
C	-1.7032	2.7197	2.1112	C	2.4938	-1.5506	-2.1613

O	-1.4012	3.4749	3.0251	O	3.3201	-0.9121	-2.7984
O	-0.5	5.1253	0.9292	O	4.7633	-1.028	-0.391
C	2.4128	1.439	-0.5626	C	0.8789	1.0924	1.7239
O	2.502	0.0656	-0.8047	O	-0.2216	1.4063	0.922
C	3.5476	2.0765	-0.279	C	1.2314	1.9821	2.6501
C	3.5407	-1.6744	-2.9642	C	-3.1517	1.7821	1.1656
C	4.2198	-0.4254	-2.4158	C	-2.1007	2.2488	2.1647
C	3.9089	-0.2508	-0.9232	C	-0.7958	2.6256	1.4501
C	4.3678	-1.496	-0.0877	C	-1.0248	3.7473	0.3742
C	3.7921	-2.8451	-0.6603	C	-2.1759	3.3763	-0.6359
C	3.9799	-2.9196	-2.2033	C	-3.4322	2.8527	0.1187
C	4.0599	-1.3825	1.4274	C	0.2622	4.1376	-0.3978
C	2.5843	-1.5932	1.8257	C	0.7271	3.118	-1.4554
C	2.0267	-2.8867	1.2091	C	-0.423	2.7475	-2.4074
C	2.295	-2.9939	-0.2944	C	-1.6863	2.3192	-1.6573
C	2.341	-1.577	3.3301	C	1.9905	3.6052	-2.1482
C	0.9523	-1.2876	3.7955	C	3.261	3.5139	-1.3672
C	3.2487	-1.7653	4.3029	C	2.1003	4.0787	-3.4002
O	0.0239	-1.0646	3.0282	O	3.3	3.0933	-0.217
C	4.551	-4.0811	-0.0927	C	-2.6628	4.6244	-1.4303
C	4.5425	1.0258	-0.4179	C	0.2385	3.0297	2.4777
O	5.7248	1.1879	-0.1493	O	0.2609	4.0838	3.0981
C	-5.595	-4.1433	-0.6093	C	-5.0916	-2.9372	1.297
C	-5.2803	-2.7418	-0.1382	C	-3.6316	-2.5912	1.1144
C	-4.1394	-2.0797	-0.4535	C	-3.062	-2.3287	-0.0885
C	-3.0423	-2.7426	-1.3155	C	-3.893	-2.3545	-1.3856
C	-3.2555	-4.2743	-1.4658	C	-5.2629	-3.0605	-1.1915
C	-3.8049	-0.655	-0.0246	C	-1.5959	-1.9685	-0.2906
C	-2.4249	-0.5513	0.6497	C	-0.8978	-2.7594	-1.4146
C	-1.3347	-1.1108	-0.2701	C	-1.7049	-2.6723	-2.7173
C	-1.6463	-2.5522	-0.6634	C	-3.1442	-3.1326	-2.4984
C	-2.1287	0.8709	1.053	C	0.5441	-2.3156	-1.557
C	-1.9756	1.3057	2.3019	C	1.1064	-1.6746	-2.5801
O	-1.983	1.8015	0.0267	O	1.3767	-2.6351	-0.4806
C	-3.0534	-2.1036	-2.7249	C	-4.1475	-0.8987	-1.8435
C	-6.3738	-2.1531	0.6981	C	-2.8841	-2.5332	2.4112
O	-7.3598	-2.7952	1.0451	O	-3.3745	-2.9011	3.4735
O	5.8104	-1.5984	-0.2003	O	-1.4679	4.9426	1.063
C	-4.7058	-4.6303	-1.7458	C	-5.9613	-2.6254	0.0863
H	-3.4725	3.2976	-1.6213	H	2.719	-4.7147	0.5446
H	-4.2573	4.7946	-1.1506	H	4.2468	-5.3055	-0.0853
H	-3.1524	4.7867	1.04	H	4.452	-3.3924	-1.6137
H	-4.0017	3.2706	0.7681	H	2.9186	-4.2214	-1.8495
H	-2.1816	6.0026	-1.0897	H	5.4701	-3.4387	0.8061
H	-2.3209	5.2036	-2.644	H	4.5398	-4.1731	2.0978
H	0.8545	2.8047	1.3551	H	2.4544	0.4216	-0.4054
H	1.5651	3.9242	0.2512	H	3.4616	0.6171	0.9853

H	0.3338	1.2196	-0.4016	H	0.7745	-0.8193	0.9044
H	1.5676	3.0643	-2.4901	H	2.4899	-0.4534	3.3843
H	0.7569	1.5376	-2.7536	H	0.936	-1.251	3.2595
H	-1.3927	2.4401	-2.2072	H	1.8345	-3.0317	1.8998
H	-0.6335	3.5052	-3.3543	H	2.8187	-2.8583	3.3286
H	1.3058	5.1334	-1.6042	H	4.5987	-0.4258	2.6163
H	0.1603	5.7385	-2.7989	H	5.0797	-1.978	3.3016
H	0.1376	6.3729	-1.1554	H	5.8556	-1.3809	1.8374
H	-0.5065	4.8837	1.8798	H	4.596	-0.5486	-1.2289
H	3.7494	3.1057	-0.0531	H	2.0357	1.9831	3.36
H	2.451	-1.5666	-2.9193	H	-2.8298	0.8546	0.682
H	3.7967	-1.7895	-4.024	H	-4.0797	1.5454	1.6994
H	5.3028	-0.4852	-2.5813	H	-2.4858	3.0998	2.7403
H	3.8637	0.4395	-2.9903	H	-1.927	1.4377	2.8838
H	5.0409	-3.0894	-2.4328	H	-3.9267	3.6911	0.6281
H	3.4425	-3.7886	-2.6044	H	-4.1648	2.4627	-0.5998
H	4.6915	-2.1146	1.9469	H	0.1054	5.1108	-0.8842
H	4.4084	-0.4146	1.8101	H	1.0664	4.34	0.32
H	2.0182	-0.7505	1.4152	H	1.0038	2.1864	-0.9551
H	2.4471	-3.7598	1.7232	H	-0.6704	3.5867	-3.0667
H	0.9434	-2.9464	1.369	H	-0.1073	1.926	-3.0635
H	1.9194	-3.9641	-0.6451	H	-2.4756	2.1179	-2.3932
H	1.6903	-2.2448	-0.8141	H	-1.4934	1.3616	-1.1672
H	0.8004	-1.282	4.8883	H	4.1745	3.8505	-1.8861
H	2.9927	-1.7246	5.3584	H	3.0506	4.3931	-3.8233
H	4.2914	-1.9758	4.0888	H	1.2418	4.1783	-4.0558
H	4.5364	-4.1241	0.9994	H	-1.8548	5.1269	-1.9682
H	4.1044	-5.0126	-0.4606	H	-3.4207	4.3415	-2.1706
H	5.6026	-4.0881	-0.4008	H	-3.1227	5.3701	-0.7721
H	-5.4936	-4.8247	0.2454	H	-5.1644	-4.0082	1.5262
H	-6.6357	-4.2088	-0.95	H	-5.5097	-2.3967	2.1553
H	-2.9493	-4.7916	-0.546	H	-5.1245	-4.1498	-1.1512
H	-2.6184	-4.6729	-2.2653	H	-5.9174	-2.8676	-2.0508
H	-3.8442	-0.0096	-0.9118	H	-1.5303	-0.8947	-0.5001
H	-4.5422	-0.2405	0.6658	H	-1.0202	-2.1346	0.6207
H	-2.4497	-1.1708	1.558	H	-0.8743	-3.8186	-1.1188
H	-1.2283	-0.4962	-1.1719	H	-1.6999	-1.6506	-3.1147
H	-0.3648	-1.0804	0.2388	H	-1.2445	-3.3076	-3.4846
H	-0.8629	-2.9144	-1.3415	H	-3.6913	-3.05	-3.4465
H	-1.5751	-3.1687	0.2434	H	-3.1215	-4.2028	-2.2501
H	-2.0097	0.7779	3.2355	H	0.7004	-1.3137	-3.5053
H	-2.8188	-1.0347	-2.7036	H	-4.6637	-0.3142	-1.0742
H	-2.313	-2.5806	-3.3774	H	-3.2204	-0.3656	-2.0728
H	-4.0322	-2.2026	-3.2067	H	-4.7653	-0.8741	-2.7485
H	-6.2669	-1.1041	0.9993	H	-1.8635	-2.1313	2.3853
H	6.2059	-0.7385	0.0571	H	-0.8206	5.1522	1.7699
H	-5.0336	-4.191	-2.6948	H	-6.1897	-1.554	0.0541

H	-4.8105	-5.7162	-1.8531	H	-6.9223	-3.1442	0.1824
3a-7	X axis(Å)	Y axis(Å)	Z axis(Å)	3a-8	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-4.9508	-2.7701	-1.2239	C	-3.1633	4.1574	-1.2685
C	-4.3615	-2.937	0.17	C	-3.0527	3.8907	0.2281
C	-3.4255	-1.7718	0.522	C	-1.7713	3.108	0.5483
C	-4.1485	-0.3844	0.4187	C	-0.4928	3.8764	0.0694
C	-4.8547	-0.1928	-0.978	C	-0.5752	4.2582	-1.456
C	-5.6955	-1.4472	-1.3508	C	-1.9468	4.9145	-1.7882
C	-3.2282	0.828	0.7184	C	0.837	3.1391	0.3615
C	-2.2267	1.1824	-0.3963	C	1.1432	1.935	-0.5476
C	-2.904	1.2807	-1.7712	C	0.959	2.2752	-2.035
C	-3.8094	0.0909	-2.0855	C	-0.3492	3.0071	-2.3417
C	-5.8649	0.9913	-0.9514	C	0.4956	5.3208	-1.8412
C	-2.8413	-2.0192	1.8929	C	-1.7288	2.7932	2.0273
O	-3.429	-1.9021	2.9594	O	-1.4846	3.5862	2.926
O	-5.2037	-0.354	1.4111	O	-0.429	5.1281	0.798
C	-1.4415	2.4523	-0.1513	C	2.5272	1.3502	-0.3427
O	-0.2088	2.5145	-0.8048	O	2.7022	0.0421	-0.8077
C	-1.773	3.4907	0.6137	C	3.5756	1.9272	0.243
C	1.1578	4.0168	-2.9511	C	4.2172	-1.4472	-2.8815
C	0.2191	4.6073	-1.9051	C	4.7346	-0.2763	-2.0556
C	0.3277	3.8379	-0.5837	C	4.1058	-0.2782	-0.6573
C	1.7935	3.8444	-0.0261	C	4.3847	-1.6203	0.1099
C	2.8359	3.3324	-1.0906	C	3.9856	-2.8895	-0.7368
C	2.6032	4.0224	-2.4662	C	4.5135	-2.7752	-2.196
C	1.9522	3.0622	1.301	C	3.7242	-1.6722	1.5134
C	1.9516	1.5302	1.1637	C	2.209	-1.9366	1.5079
C	2.9319	1.0454	0.084	C	1.8606	-3.1767	0.6709
C	2.7559	1.7908	-1.2424	C	2.448	-3.0886	-0.7399
C	2.1856	0.8982	2.5246	C	1.6766	-1.9796	2.9289
C	1.0052	0.3553	3.2529	C	1.1465	-0.7057	3.4976
C	3.3717	0.7966	3.1462	C	1.6264	-3.0594	3.7258
O	-0.1144	0.3014	2.7584	O	1.0779	0.3339	2.8526
C	4.2935	3.6992	-0.6835	C	4.6373	-4.1832	-0.1628
C	-0.6539	4.3985	0.4203	C	4.6085	0.9144	0.1234
O	-0.5447	5.4606	1.0177	O	5.7231	1.037	0.613
C	5.0258	-3.3749	-0.4546	C	-5.8815	-3.945	-0.5405
C	3.7565	-3.0769	0.3086	C	-5.4941	-2.5557	-0.0878
C	2.5193	-3.4566	-0.0976	C	-4.3238	-1.9549	-0.4173
C	2.3261	-4.2713	-1.392	C	-3.2698	-2.6784	-1.2834
C	3.5875	-4.2461	-2.2991	C	-3.5623	-4.1981	-1.4234
C	1.2252	-3.1563	0.6533	C	-3.9151	-0.5464	-0.0018
C	0.1049	-2.5746	-0.2381	C	-2.5241	-0.5027	0.6582
C	-0.1298	-3.482	-1.4548	C	-1.4715	-1.1306	-0.2605
C	1.1631	-3.6941	-2.236	C	-1.8627	-2.5561	-0.6402
C	-1.2008	-2.3237	0.4891	C	-2.1588	0.9116	1.0277
C	-1.4535	-2.4426	1.7918	C	-2.0439	1.3927	2.2636

O	-2.2514	-1.8733	-0.3145	O	-1.918	1.7892	-0.0265
C	2.0184	-5.7398	-1.0128	C	-3.2575	-2.0474	-2.6961
C	4.0082	-2.3505	1.5908	C	-6.553	-1.9019	0.7442
O	5.0897	-1.8417	1.8649	O	-7.5435	-2.504	1.1451
O	2.1543	5.218	0.2639	O	5.8147	-1.7244	0.3263
C	4.8711	-4.4576	-1.5139	C	-5.0319	-4.4816	-1.685
H	-4.1614	-2.8387	-1.9807	H	-3.2846	3.2149	-1.8144
H	-5.6435	-3.5957	-1.4251	H	-4.067	4.7462	-1.4652
H	-5.1713	-3.0148	0.9065	H	-3.0753	4.8391	0.7792
H	-3.8189	-3.8908	0.2007	H	-3.9399	3.326	0.5426
H	-6.5813	-1.4987	-0.703	H	-1.979	5.9258	-1.36
H	-6.0765	-1.3521	-2.3758	H	-2.0469	5.0439	-2.8737
H	-2.6884	0.6626	1.6595	H	0.8669	2.8228	1.4121
H	-3.8673	1.6945	0.9337	H	1.6491	3.8746	0.2891
H	-1.4833	0.3806	-0.4426	H	0.4378	1.1397	-0.2905
H	-3.4857	2.2088	-1.84	H	1.8031	2.8808	-2.389
H	-2.1395	1.3526	-2.5562	H	0.9882	1.3529	-2.6304
H	-3.1814	-0.7855	-2.271	H	-1.178	2.2994	-2.2468
H	-4.3197	0.2856	-3.0381	H	-0.3423	3.298	-3.4005
H	-5.4006	1.9386	-0.6653	H	1.5161	4.9921	-1.6284
H	-6.317	1.1375	-1.9398	H	0.4462	5.5497	-2.9126
H	-6.6855	0.8082	-0.2489	H	0.3417	6.2642	-1.3055
H	-4.8143	-0.5697	2.2851	H	-0.4586	4.9284	1.7579
H	-2.6362	3.6802	1.2218	H	3.6991	2.8922	0.6948
H	0.8483	2.9972	-3.2072	H	3.1411	-1.3423	-3.0599
H	1.0843	4.603	-3.8747	H	4.6972	-1.4344	-3.8671
H	0.4482	5.6696	-1.7548	H	5.8287	-0.3224	-1.9879
H	-0.8055	4.5605	-2.2962	H	4.4926	0.6533	-2.5866
H	2.9273	5.0705	-2.4068	H	5.6034	-2.9137	-2.2014
H	3.236	3.5546	-3.2313	H	4.1037	-3.5897	-2.8072
H	2.8837	3.3856	1.7869	H	4.2248	-2.4473	2.111
H	1.174	3.3695	2.0119	H	3.9392	-0.7456	2.0612
H	0.963	1.2136	0.8218	H	1.7114	-1.1015	1.0097
H	3.9708	1.1465	0.416	H	2.215	-4.0939	1.153
H	2.7771	-0.0261	-0.0927	H	0.772	-3.2805	0.5984
H	3.5299	1.4441	-1.9398	H	2.1905	-4.0076	-1.2823
H	1.8059	1.4877	-1.6931	H	1.9475	-2.2791	-1.2811
H	1.1975	-0.0172	4.2735	H	0.8052	-0.7512	4.5457
H	3.4909	0.3371	4.1232	H	1.2287	-3.0241	4.7362
H	4.2841	1.1731	2.691	H	2.0009	-4.0247	3.3992
H	4.5683	3.3121	0.3012	H	4.4044	-4.342	0.8933
H	5.0118	3.2926	-1.4055	H	4.2926	-5.0679	-0.7113
H	4.4467	4.7838	-0.6573	H	5.7295	-4.1603	-0.2495
H	5.3645	-2.4468	-0.933	H	-5.7999	-4.6229	0.3189
H	5.8216	-3.6905	0.2313	H	-6.9288	-3.964	-0.8661
H	3.6609	-3.28	-2.8174	H	-3.2722	-4.7263	-0.5046
H	3.5086	-5.0082	-3.0846	H	-2.9554	-4.6323	-2.2279

H	0.8836	-4.0865	1.1257	H	-3.934	0.0952	-0.8926
H	1.3891	-2.4444	1.4653	H	-4.6238	-0.0941	0.6952
H	0.4496	-1.5976	-0.6077	H	-2.568	-1.102	1.5793
H	-0.5513	-4.4448	-1.1416	H	-0.5025	-1.149	0.2485
H	-0.8662	-3.0307	-2.1319	H	-1.3306	-0.5312	-1.1678
H	0.9577	-4.3513	-3.0909	H	-1.8211	-3.1676	0.2719
H	1.4604	-2.7249	-2.6603	H	-1.1027	-2.9654	-1.3183
H	-0.8315	-2.7246	2.6183	H	-2.1569	0.9213	3.2201
H	1.0952	-5.838	-0.433	H	-2.5461	-2.5646	-3.3503
H	1.9038	-6.3605	-1.9089	H	-4.2431	-2.1001	-3.1714
H	2.8184	-6.1787	-0.4066	H	-2.9694	-0.9916	-2.6823
H	3.1754	-2.2971	2.3034	H	-6.4149	-0.842	0.9904
H	1.4684	5.6044	0.8486	H	6.1293	-0.8982	0.7516
H	4.8752	-5.4473	-1.0431	H	-5.3482	-4.0303	-2.6323
H	5.7324	-4.4328	-2.1915	H	-5.1926	-5.5613	-1.7853
3a-9	X axis(Å)	Y axis(Å)	Z axis(Å)	3a-10	X axis(Å)	Y axis(Å)	Z axis(Å)
C	5.3799	2.0132	-0.8764	C	2.865	4.0487	2.4255
C	4.9454	1.6989	0.5498	C	3.2017	4.1981	0.9467
C	3.6813	0.8278	0.5594	C	2.3023	3.3001	0.0868
C	3.8938	-0.5107	-0.2296	C	0.7808	3.6212	0.3088
C	4.4323	-0.2605	-1.6885	C	0.3864	3.5593	1.8322
C	5.6254	0.7379	-1.6737	C	1.3986	4.3653	2.6964
C	2.637	-1.4145	-0.2709	C	-0.1761	2.7333	-0.5255
C	1.5347	-0.9648	-1.2425	C	-0.3145	1.2878	-0.0274
C	2.0746	-0.6398	-2.6409	C	-0.6138	1.216	1.4769
C	3.3025	0.2716	-2.6067	C	0.3182	2.0896	2.3193
C	4.992	-1.5684	-2.3211	C	-0.9999	4.2179	2.0918
C	3.2474	0.5928	1.9902	C	2.7047	3.4261	-1.3645
O	3.7475	-0.1893	2.7863	O	2.4473	4.3629	-2.1073
O	4.9229	-1.265	0.4558	O	0.5471	4.9858	-0.1172
C	0.4024	-1.9626	-1.3257	C	-1.3299	0.5466	-0.8638
O	-0.8685	-1.4754	-1.0127	O	-2.6707	0.6732	-0.5063
C	0.5018	-3.2527	-1.6429	C	-1.0438	-0.2335	-1.9042
C	-3.5354	-1.0163	-2.2376	C	-5.2659	1.6884	-1.4689
C	-2.613	-2.199	-2.5049	C	-4.2048	1.0023	-2.3217
C	-1.8046	-2.5559	-1.2513	C	-3.4446	-0.0429	-1.498
C	-2.7371	-2.8841	-0.0286	C	-4.4114	-1.1314	-0.9058
C	-3.789	-1.7437	0.24	C	-5.5988	-0.4911	-0.0931
C	-4.4846	-1.3066	-1.0815	C	-6.2491	0.6778	-0.8893
C	-1.9585	-3.2148	1.2714	C	-3.6885	-2.2038	-0.0503
C	-1.3183	-2.0049	1.9803	C	-3.243	-1.7306	1.3443
C	-2.3566	-0.8894	2.1957	C	-4.4115	-1.0863	2.1089
C	-3.1093	-0.5263	0.9125	C	-5.1085	0.0068	1.2911
C	-0.5923	-2.4458	3.2439	C	-2.5315	-2.8527	2.0817
C	0.6922	-3.1876	3.0585	C	-1.1147	-3.1242	1.6878
C	-0.9586	-2.2149	4.5153	C	-3.0258	-3.6091	3.075
O	1.1467	-3.4543	1.9524	O	-0.5322	-2.4803	0.8205

C	-4.9383	-2.2309	1.1708	C	-6.7468	-1.5169	0.1441
C	-0.875	-3.7075	-1.5644	C	-2.3578	-0.6718	-2.3418
O	-1.2056	-4.8741	-1.7276	O	-2.5251	-1.4562	-3.2659
C	-3.287	4.3737	-1.7405	C	4.0928	-4.4227	1.147
C	-2.1507	3.4272	-1.4271	C	3.3249	-3.1471	0.902
C	-1.5766	3.317	-0.2029	C	3.5088	-2.3771	-0.1984
C	-2.055	4.1776	0.9837	C	4.4451	-2.8091	-1.3454
C	-2.943	5.3667	0.525	C	5.1063	-4.1971	-1.1132
C	-0.4445	2.3585	0.1398	C	2.8983	-1.0009	-0.413
C	0.7313	3.0256	0.8749	C	3.9948	0.0769	-0.5626
C	0.2314	3.7741	2.1178	C	5.0025	-0.3086	-1.6623
C	-0.8452	4.7897	1.7391	C	5.5506	-1.7292	-1.4739
C	1.8105	2.0057	1.1637	C	3.3787	1.4493	-0.7407
C	2.114	1.4397	2.3303	C	3.4499	2.2541	-1.7995
O	2.5852	1.6345	0.0624	O	2.6627	1.9245	0.3607
C	-2.8778	3.29	1.9472	C	3.6658	-2.9315	-2.6786
C	-1.7435	2.6022	-2.6099	C	2.3782	-2.8003	2.0086
O	-2.2008	2.7872	-3.733	O	2.1658	-3.5481	2.9593
O	-3.5085	-4.0665	-0.3556	O	-5.0202	-1.839	-2.0154
C	-3.975	4.9508	-0.5103	C	5.3912	-4.4794	0.3514
H	4.6269	2.6339	-1.3748	H	3.1039	3.0357	2.7683
H	6.3015	2.6066	-0.8511	H	3.4954	4.7288	3.0103
H	5.7618	1.199	1.086	H	3.099	5.2482	0.6459
H	4.7658	2.6482	1.0707	H	4.2581	3.9352	0.8066
H	6.5088	0.244	-1.2461	H	1.2529	5.4399	2.5203
H	5.8999	1.009	-2.7013	H	1.1924	4.204	3.7624
H	2.2149	-1.4967	0.7369	H	0.1401	2.7343	-1.5772
H	2.952	-2.4394	-0.5088	H	-1.1677	3.2066	-0.5562
H	1.1027	-0.0451	-0.8416	H	0.6397	0.7829	-0.1857
H	2.3229	-1.5611	-3.1818	H	-1.6519	1.505	1.6795
H	1.2892	-0.1512	-3.2327	H	-0.5177	0.1789	1.8204
H	2.9866	1.2743	-2.3033	H	1.311	1.6304	2.3328
H	3.6783	0.3856	-3.6321	H	-0.0258	2.0583	3.3616
H	4.2551	-2.3755	-2.3464	H	-1.8038	3.7574	1.5114
H	5.317	-1.3918	-3.3534	H	-1.2761	4.1354	3.1498
H	5.8626	-1.9442	-1.772	H	-0.994	5.2856	1.8454
H	4.6248	-1.4306	1.3749	H	0.8607	5.0834	-1.0408
H	1.3549	-3.8538	-1.8922	H	-0.1053	-0.5007	-2.3484
H	-2.9478	-0.1164	-2.0281	H	-4.7944	2.2626	-0.6634
H	-4.1194	-0.8012	-3.1401	H	-5.8126	2.4119	-2.0851
H	-3.2019	-3.0606	-2.8435	H	-4.6721	0.5402	-3.2001
H	-1.943	-1.9328	-3.3326	H	-3.517	1.7697	-2.6999
H	-5.1742	-2.0966	-1.4091	H	-6.831	0.2679	-1.7263
H	-5.1057	-0.4196	-0.9017	H	-6.9696	1.2082	-0.2534
H	-2.6353	-3.7226	1.9732	H	-4.3477	-3.0764	0.0604
H	-1.2028	-3.9789	1.0533	H	-2.8331	-2.6023	-0.6101
H	-0.5469	-1.5731	1.3355	H	-2.5028	-0.9378	1.2293

H	-3.0859	-1.1795	2.9603	H	-5.1516	-1.8396	2.3998
H	-1.8551	0.0082	2.5786	H	-4.0411	-0.6455	3.0434
H	-3.8623	0.2345	1.1548	H	-5.9584	0.3868	1.8731
H	-2.4172	-0.0402	0.2206	H	-4.4271	0.8566	1.185
H	1.2173	-3.4868	3.9815	H	-0.6119	-3.9447	2.2281
H	-0.3711	-2.5583	5.3627	H	-2.4414	-4.3851	3.5625
H	-1.869	-1.6804	4.7653	H	-4.0402	-3.4868	3.4398
H	-4.5752	-2.6201	2.1255	H	-6.4076	-2.4237	0.6515
H	-5.6297	-1.4099	1.3956	H	-7.5398	-1.0759	0.7599
H	-5.5293	-3.0264	0.7032	H	-7.2115	-1.8307	-0.7974
H	-2.8903	5.1964	-2.3495	H	4.3538	-4.5205	2.2077
H	-4.0518	3.8684	-2.3433	H	3.4547	-5.2772	0.8898
H	-2.3191	6.1578	0.0867	H	6.0348	-4.2813	-1.6918
H	-3.4498	5.82	1.3863	H	4.4482	-4.9953	-1.4845
H	-0.8489	1.5504	0.7597	H	2.2512	-1.0181	-1.2976
H	-0.042	1.878	-0.7518	H	2.2444	-0.7107	0.4095
H	1.1739	3.7758	0.2031	H	4.5583	0.1114	0.3821
H	-0.1651	3.077	2.865	H	4.5417	-0.2283	-2.6538
H	1.0656	4.303	2.5959	H	5.8439	0.3961	-1.6566
H	-1.1896	5.2985	2.6487	H	6.2104	-1.9635	-2.3191
H	-0.3737	5.5623	1.1161	H	6.1848	-1.7371	-0.5774
H	1.6805	1.5412	3.3062	H	3.9225	2.1353	-2.7554
H	-3.7331	2.8277	1.4429	H	3.2236	-1.9892	-3.0129
H	-2.2856	2.4751	2.3738	H	4.326	-3.2757	-3.4836
H	-3.2668	3.8779	2.7866	H	2.8465	-3.6548	-2.5882
H	-1.0132	1.8017	-2.4385	H	1.8535	-1.8399	1.9395
H	-2.891	-4.7745	-0.6386	H	-4.3082	-2.1678	-2.6039
H	-4.6685	4.2147	-0.0882	H	5.8455	-5.4709	0.4593
H	-4.5815	5.8161	-0.8022	H	6.1121	-3.7539	0.747
3a-11	X axis(Å)	Y axis(Å)	Z axis(Å)	3a-12	X axis(Å)	Y axis(Å)	Z axis(Å)
C	5.7284	0.4258	-1.1844	C	5.5669	-0.1795	-1.5696
C	5.3243	0.5203	0.2809	C	5.3864	0.0662	-0.077
C	3.909	-0.0343	0.5022	C	3.9811	-0.3518	0.3829
C	3.7851	-1.5219	0.0208	C	3.6978	-1.86	0.0701
C	4.2697	-1.6977	-1.4684	C	3.9482	-2.2026	-1.4465
C	5.6481	-1.0103	-1.6866	C	5.3188	-1.6409	-1.9224
C	2.3682	-2.1279	0.1958	C	2.2902	-2.3426	0.4988
C	1.3211	-1.6561	-0.8273	C	1.1245	-1.8854	-0.3978
C	1.8311	-1.7146	-2.2745	C	1.418	-2.1106	-1.8899
C	3.2253	-1.1162	-2.4536	C	2.8049	-1.6372	-2.3249
C	4.4918	-3.1964	-1.8253	C	4.0262	-3.7392	-1.6835
C	3.5422	0.1288	1.9593	C	3.8241	-0.0281	1.8509
O	3.9284	-0.5762	2.8818	O	4.2936	-0.6644	2.7842
O	4.6728	-2.3311	0.832	O	4.6451	-2.6557	0.8262
C	0.0143	-2.4126	-0.7346	C	-0.2009	-2.5415	-0.0608
O	-1.1467	-1.6369	-0.7808	O	-1.3341	-1.9131	-0.5893
C	-0.1403	-3.7319	-0.6325	C	-0.4062	-3.6312	0.6777

C	-3.3758	-1.1357	-2.6741	C	-3.4567	-2.4284	-2.6046
C	-2.7347	-2.4859	-2.3798	C	-2.8633	-3.4476	-1.6401
C	-2.259	-2.5544	-0.9231	C	-2.4636	-2.7782	-0.32
C	-3.4367	-2.3101	0.0845	C	-3.6794	-2.0584	0.3647
C	-4.223	-0.9806	-0.2248	C	-4.4197	-1.0697	-0.615
C	-4.5505	-0.8671	-1.7418	C	-4.6723	-1.7398	-1.9963
C	-2.9997	-2.3436	1.5725	C	-3.2972	-1.3346	1.6823
C	-2.2409	-1.0953	2.0674	C	-2.5495	-0.0031	1.4996
C	-3.0168	0.1844	1.7202	C	-3.2907	0.9293	0.5298
C	-3.4106	0.2519	0.2427	C	-3.6049	0.2358	-0.7976
C	-1.8934	-1.122	3.5499	C	-2.2615	0.6241	2.8519
C	-0.7827	-0.2328	4.0038	C	-0.9002	0.4256	3.4302
C	-2.4532	-1.8866	4.5022	C	-3.125	1.3488	3.5822
O	-0.1728	0.5109	3.2448	O	0.001	-0.1525	2.834
C	-5.6029	-0.9488	0.4972	C	-5.8303	-0.6857	-0.0771
C	-1.5841	-3.8847	-0.6728	C	-1.8454	-3.805	0.6009
O	-2.1443	-4.9602	-0.512	O	-2.4465	-4.6706	1.2227
C	-1.9436	4.6818	-2.319	C	-1.4844	4.7718	-2.4009
C	-1.2672	3.4447	-1.7807	C	-0.9101	3.5031	-1.8186
C	-0.7636	3.3682	-0.5248	C	-0.3622	3.444	-0.5803
C	-0.9579	4.5059	0.5003	C	-0.3964	4.65	0.3832
C	-1.797	5.6933	-0.051	C	-1.1373	5.8847	-0.2032
C	0.109	2.2349	-0.0052	C	0.4115	2.256	-0.0273
C	1.498	2.7561	0.4153	C	1.8637	2.6562	0.2965
C	1.3774	3.9124	1.4239	C	1.9083	3.8703	1.2417
C	0.4472	5.0191	0.9111	C	1.0703	5.0382	0.706
C	2.3748	1.6179	0.8843	C	2.6511	1.4633	0.7841
C	2.6493	1.2609	2.1379	C	3.0439	1.1871	2.0266
O	2.9715	0.8672	-0.1319	O	3.0332	0.5634	-0.2134
C	-1.7183	3.9988	1.7499	C	-1.1441	4.2936	1.692
C	-1.1686	2.3343	-2.779	C	-0.9676	2.3372	-2.7561
O	-1.5889	2.4343	-3.927	O	-1.4489	2.4165	-3.8816
O	-4.3952	-3.386	-0.0799	O	-4.657	-3.0679	0.7215
C	-1.5752	5.9347	-1.5337	C	-0.9593	6.0217	-1.705
H	5.0961	1.0794	-1.7956	H	4.8973	0.4693	-2.1453
H	6.755	0.7927	-1.3011	H	6.5878	0.0945	-1.8607
H	6.0503	-0.0205	0.9011	H	6.1545	-0.4792	0.4856
H	5.3795	1.5738	0.5841	H	5.5572	1.1329	0.1174
H	6.4291	-1.5876	-1.173	H	6.1298	-2.2325	-1.4758
H	5.9115	-1.0284	-2.7521	H	5.4181	-1.7652	-3.0085
H	1.9984	-1.9315	1.2109	H	2.0914	-2.0438	1.5364
H	2.459	-3.2216	0.1627	H	2.315	-3.4394	0.5441
H	1.0929	-0.6128	-0.5969	H	0.9845	-0.8127	-0.2347
H	1.8377	-2.7508	-2.6355	H	1.3055	-3.1737	-2.1388
H	1.132	-1.1791	-2.9309	H	0.6674	-1.586	-2.4963
H	3.154	-0.0286	-2.3608	H	2.815	-0.5434	-2.334
H	3.5489	-1.2951	-3.4876	H	2.9589	-1.9332	-3.3711

H	3.5961	-3.8052	-1.6763	H	3.1253	-4.2657	-1.3577
H	4.7868	-3.3051	-2.8759	H	4.1629	-3.9604	-2.7488
H	5.2898	-3.6428	-1.2214	H	4.8727	-4.1887	-1.1525
H	4.4755	-2.1571	1.777	H	4.5757	-2.4027	1.7714
H	0.5771	-4.5283	-0.581	H	0.2712	-4.2786	1.2
H	-2.6328	-0.3363	-2.5869	H	-2.7013	-1.687	-2.8884
H	-3.727	-1.12	-3.7125	H	-3.7544	-2.9365	-3.5294
H	-3.4479	-3.2922	-2.5925	H	-3.5843	-4.2551	-1.4614
H	-1.892	-2.6241	-3.0694	H	-1.9901	-3.908	-2.12
H	-5.3443	-1.5824	-1.9973	H	-5.4643	-2.4947	-1.8959
H	-4.9587	0.1276	-1.9631	H	-5.0532	-0.9968	-2.7088
H	-3.902	-2.4924	2.1801	H	-4.2126	-1.1607	2.2656
H	-2.3987	-3.2411	1.7674	H	-2.7088	-2.006	2.3212
H	-1.285	-1.066	1.5346	H	-1.5852	-0.2056	1.027
H	-3.9113	0.2662	2.3497	H	-4.2197	1.3057	0.971
H	-2.4137	1.0673	1.9552	H	-2.678	1.8141	0.3286
H	-3.993	1.1682	0.0795	H	-4.1585	0.9376	-1.435
H	-2.504	0.3731	-0.3578	H	-2.6657	0.0407	-1.3245
H	-0.5343	-0.2794	5.0778	H	-0.7398	0.8454	4.4378
H	-2.1347	-1.8545	5.5407	H	-2.8645	1.7758	4.5465
H	-3.2622	-2.5772	4.2872	H	-4.1408	1.5288	3.2425
H	-5.5191	-1.0762	1.5796	H	-5.7986	-0.2638	0.9309
H	-6.1112	0.0066	0.3201	H	-6.3051	0.0576	-0.7285
H	-6.2703	-1.7375	0.132	H	-6.5004	-1.5521	-0.0408
H	-1.6611	4.8561	-3.3641	H	-1.2329	4.8601	-3.4646
H	-3.0299	4.5298	-2.2979	H	-2.5783	4.7318	-2.3284
H	-1.5765	6.6111	0.5084	H	-0.802	6.8043	0.2927
H	-2.8685	5.5003	0.0991	H	-2.2149	5.8098	-3.00E-04
H	-0.3899	1.7404	0.8338	H	-0.0901	1.876	0.8676
H	0.2543	1.454	-0.7511	H	0.4334	1.4146	-0.7206
H	1.9827	3.1762	-0.4791	H	2.3393	2.9782	-0.6426
H	1.0108	3.5509	2.3914	H	1.5537	3.5978	2.2425
H	2.369	4.343	1.6131	H	2.9457	4.207	1.364
H	0.3558	5.7873	1.6897	H	1.0926	5.8514	1.4428
H	0.931	5.5061	0.054	H	1.5598	5.4276	-0.1965
H	2.3048	1.6497	3.0766	H	2.8792	1.6947	2.9567
H	-1.1848	3.2149	2.2935	H	-0.6733	3.4828	2.2538
H	-1.8891	4.8172	2.4596	H	-1.188	5.1605	2.3621
H	-2.6975	3.5899	1.4734	H	-2.1751	3.9847	1.4837
H	-0.7177	1.3934	-2.44	H	-0.5783	1.3786	-2.3912
H	-3.9233	-4.2425	-0.0035	H	-4.209	-3.7715	1.2378
H	-2.1924	6.775	-1.8719	H	-1.5048	6.9005	-2.0672
H	-0.5309	6.2098	-1.7241	H	0.0975	6.1789	-1.9518
3b-1	X axis(Å)	Y axis(Å)	Z axis(Å)	3b-2	X axis(Å)	Y axis(Å)	Z axis(Å)
C	4.2017	-3.2755	0.8694	C	5.1977	1.7467	0.7946
C	3.8672	-3.1801	-0.6127	C	4.8954	1.4378	-0.6649
C	2.3945	-2.8102	-0.824	C	3.7291	0.4514	-0.7929

C	1.4183	-3.8207	-0.1222	C	3.9806	-0.8819	-0.0035
C	1.787	-4.054	1.3943	C	4.4173	-0.6228	1.49
C	3.3134	-4.2989	1.5651	C	5.5178	0.4734	1.5669
C	-0.0767	-3.423	-0.2607	C	2.7697	-1.8526	-0.0522
C	-0.5294	-2.2763	0.6575	C	1.592	-1.4795	0.8682
C	-0.1416	-2.5259	2.1203	C	2.0607	-1.2259	2.3061
C	1.346	-2.8485	2.2634	C	3.2022	-0.2101	2.3585
C	1.0963	-5.332	1.956	C	5.0534	-1.8953	2.1239
C	2.123	-2.7066	-2.3072	C	3.4656	0.1956	-2.2594
O	2.0228	-3.6405	-3.0911	O	4.1548	-0.4783	-3.0123
O	1.5651	-5.1099	-0.768	O	5.0935	-1.5689	-0.6265
C	-1.9998	-1.988	0.4689	C	0.4978	-2.512	0.7414
O	-2.288	-0.9747	-0.4461	O	-0.377	-2.3129	-0.3297
C	-3.0259	-2.5266	1.1244	C	0.2481	-3.5422	1.5475
C	-3.7822	-0.261	-2.9019	C	-1.2687	-3.5648	-2.8487
C	-4.2497	-1.2181	-1.8121	C	-0.9514	-4.2981	-1.5509
C	-3.7198	-0.7836	-0.4425	C	-1.2986	-3.4268	-0.3384
C	-4.1596	0.6808	-0.076	C	-2.8115	-3.0048	-0.3357
C	-3.7988	1.7116	-1.2141	C	-3.2464	-2.338	-1.6964
C	-4.2245	1.1679	-2.6087	C	-2.7386	-3.1678	-2.9111
C	-3.6071	1.1795	1.2887	C	-3.1965	-2.0946	0.8604
C	-2.1102	1.5483	1.2859	C	-2.7327	-0.6305	0.7473
C	-1.7752	2.5247	0.1519	C	-3.1585	-0.0196	-0.5973
C	-2.2823	2.0344	-1.2067	C	-2.7225	-0.881	-1.7859
C	-1.5826	2.0765	2.6083	C	-3.1787	0.1583	1.9672
C	-0.173	1.7252	2.9585	C	-2.3538	0.0037	3.2037
C	-2.2585	2.8103	3.5068	C	-4.217	1.0054	2.0505
O	0.5314	1.0265	2.2372	O	-1.3747	-0.7329	3.2496
C	-4.5733	3.0514	-1.0383	C	-4.7971	-2.3021	-1.8421
C	-4.1594	-1.7751	0.6113	C	-0.9198	-4.151	0.934
O	-5.2987	-1.9195	1.0328	O	-1.5033	-5.1137	1.4134
C	2.7588	4.9543	1.2611	C	-2.7749	4.6751	1.3736
C	2.8769	3.4657	1.029	C	-1.4928	3.8965	1.1859
C	2.843	2.8904	-0.1989	C	-0.8261	3.8203	0.0074
C	2.6369	3.7367	-1.471	C	-1.3749	4.4935	-1.2661
C	2.1902	5.191	-1.1524	C	-2.8405	4.9828	-1.0964
C	2.9903	1.3962	-0.4703	C	0.4928	3.0872	-0.208
C	1.8365	0.8206	-1.3175	C	0.4323	2.0625	-1.3612
C	1.6836	1.6242	-2.62	C	-0.0597	2.7448	-2.6493
C	1.5212	3.1173	-2.3508	C	-1.381	3.4798	-2.4384
C	2.0138	-0.6674	-1.5502	C	1.7505	1.3351	-1.5481
C	1.9592	-1.3207	-2.7098	C	2.2359	0.8403	-2.6858
O	2.2101	-1.4397	-0.4021	O	2.5153	1.1313	-0.3965
C	3.9637	3.7934	-2.2638	C	-0.4903	5.7106	-1.6238
C	3.0454	2.6964	2.3033	C	-1.0321	3.2318	2.4459
O	2.9245	3.2216	3.4072	O	-1.7406	3.1612	3.4461
O	-5.6044	0.6994	0.0369	O	-3.6096	-4.2081	-0.2085

C	2.9666	5.7917	0.0066	C	-3.0705	5.6549	0.2461
H	5.2513	-3.5703	0.9848	H	6.055	2.4279	0.8499
H	4.1019	-2.2942	1.3465	H	4.3543	2.2731	1.2552
H	4.5227	-2.425	-1.0655	H	4.6595	2.3808	-1.1746
H	4.0988	-4.1325	-1.1061	H	5.7935	1.0352	-1.1503
H	3.5715	-4.3261	2.6316	H	5.7147	0.7339	2.6148
H	3.5716	-5.2898	1.1669	H	6.4618	0.0724	1.1731
H	-0.3013	-3.1734	-1.306	H	2.4168	-1.954	-1.087
H	-0.698	-4.3088	-0.0668	H	3.1182	-2.864	0.2015
H	-0.013	-1.3587	0.3606	H	1.1447	-0.5422	0.5241
H	-0.3714	-1.6368	2.721	H	1.2268	-0.8441	2.9062
H	-0.7349	-3.3399	2.5515	H	2.377	-2.158	2.7873
H	1.5583	-3.0521	3.3211	H	3.5135	-0.0897	3.4044
H	1.9246	-1.9527	2.016	H	2.8151	0.7677	2.054
H	1.4631	-6.2405	1.465	H	5.9945	-2.1664	1.6321
H	1.2998	-5.4446	3.0275	H	5.2839	-1.7284	3.1828
H	0.0105	-5.3162	1.8298	H	4.3987	-2.7689	2.0658
H	1.4653	-4.9932	-1.7363	H	4.919	-1.6545	-1.5873
H	-3.0625	-3.2821	1.8853	H	0.74	-3.882	2.4381
H	-2.6925	-0.3074	-3.0078	H	-0.6315	-2.6793	-2.9524
H	-4.1999	-0.578	-3.8647	H	-1.0339	-4.2162	-3.6987
H	-5.3457	-1.2676	-1.8052	H	-1.4984	-5.2484	-1.5151
H	-3.8915	-2.2255	-2.0607	H	0.1167	-4.5511	-1.5507
H	-5.3194	1.1996	-2.6931	H	-3.3264	-4.0926	-2.9915
H	-3.8423	1.8264	-3.3995	H	-2.918	-2.6155	-3.8427
H	-4.2049	2.0454	1.6006	H	-4.2887	-2.1152	0.9839
H	-3.8018	0.4318	2.0683	H	-2.827	-2.539	1.7931
H	-1.562	0.6258	1.0914	H	-1.639	-0.5962	0.7489
H	-0.6893	2.6658	0.0924	H	-2.7201	0.9798	-0.7001
H	-2.1908	3.5163	0.3685	H	-4.2437	0.1223	-0.6395
H	-2.0615	2.8038	-1.958	H	-3.0859	-0.4092	-2.7083
H	-1.6941	1.1611	-1.5056	H	-1.6308	-0.8585	-1.8587
H	0.2046	2.1298	3.9133	H	-2.6756	0.591	4.0806
H	-1.8118	3.1466	4.4387	H	-4.4482	1.5489	2.9637
H	-3.2859	3.1168	3.3385	H	-4.8775	1.1936	1.2114
H	-4.3961	3.5191	-0.0664	H	-5.2904	-1.8003	-1.0056
H	-4.2756	3.775	-1.8066	H	-5.0887	-1.7744	-2.758
H	-5.6556	2.9103	-1.1357	H	-5.2221	-3.3102	-1.9059
H	1.7632	5.1616	1.6743	H	-3.6054	3.9635	1.4588
H	3.4919	5.2852	2.0071	H	-2.7423	5.2444	2.3107
H	1.1225	5.2123	-0.893	H	-3.5358	4.1355	-1.1757
H	2.2997	5.8287	-2.0386	H	-3.1106	5.6733	-1.9052
H	3.947	1.2266	-0.9814	H	1.2792	3.8268	-0.4065
H	3.0546	0.8187	0.4532	H	0.8121	2.5638	0.6946
H	0.9073	0.9369	-0.7426	H	-0.3032	1.2967	-1.0786
H	2.5481	1.4622	-3.2755	H	0.6986	3.4434	-3.024
H	0.8018	1.2765	-3.1734	H	-0.2131	1.9985	-3.4387

H	1.4641	3.6465	-3.311	H	-1.6565	3.9883	-3.3715
H	0.5472	3.2642	-1.8674	H	-2.1572	2.7221	-2.2668
H	1.7923	-0.9794	-3.7132	H	1.8441	0.8323	-3.6846
H	4.779	4.2044	-1.6584	H	-0.4424	6.431	-0.7997
H	4.2898	2.8069	-2.608	H	0.5403	5.4269	-1.8585
H	3.862	4.4243	-3.1544	H	-0.8833	6.2368	-2.5015
H	3.2779	1.6274	2.2206	H	-0.0279	2.79	2.4462
H	-5.8847	-0.0201	0.641	H	-3.2982	-4.7074	0.5764
H	4.034	5.8517	-0.2347	H	-2.4395	6.5456	0.3446
H	2.6297	6.8184	0.1911	H	-4.1091	5.9973	0.3208
3b-3	X axis(Å)	Y axis(Å)	Z axis(Å)	3b-4	X axis(Å)	Y axis(Å)	Z axis(Å)
C	2.391	4.8437	-0.2829	C	2.4428	5.0172	-0.6471
C	1.909	4.432	1.1016	C	2.2089	4.486	0.7607
C	0.7845	3.3929	1.0077	C	1.4066	3.1785	0.7318
C	-0.4299	3.9102	0.1607	C	0.0329	3.3466	-0.0109
C	0.0193	4.4489	-1.2509	C	0.193	4.0023	-1.4354
C	1.2451	5.3976	-1.1201	C	1.1229	5.2472	-1.3725
C	-1.5602	2.8599	0.0019	C	-0.7718	2.0251	-0.1136
C	-1.2704	1.7274	-1	C	-0.2678	1.0346	-1.1787
C	-0.7905	2.2761	-2.3519	C	-0.0925	1.7046	-2.5451
C	0.3579	3.2746	-2.2041	C	0.7493	2.9776	-2.4552
C	-1.0988	5.3054	-1.9148	C	-1.1699	4.5271	-1.9763
C	0.3748	2.9834	2.4034	C	1.2199	2.6851	2.152
O	-0.3008	3.642	3.1819	O	0.4389	3.1336	2.9803
O	-1.0105	5.041	0.856	O	-0.7786	4.2689	0.759
C	-2.4699	0.8101	-1.0975	C	-1.1356	-0.1933	-1.3099
O	-2.6959	0.0124	0.0276	O	-2.5109	-0.0301	-1.1617
C	-3.2882	0.6403	-2.1344	C	-0.6848	-1.4258	-1.5352
C	-4.7065	-0.573	2.1399	C	-5.0699	-0.2811	-2.617
C	-4.9985	-0.2442	0.6814	C	-3.8726	-1.2153	-2.746
C	-3.8846	-0.7683	-0.231	C	-3.1212	-1.3183	-1.4141
C	-3.6687	-2.316	-0.0736	C	-4.0525	-1.8299	-0.2565
C	-3.4702	-2.7408	1.4321	C	-5.3665	-0.9704	-0.1301
C	-4.5416	-2.0743	2.3425	C	-6.0229	-0.7516	-1.5244
C	-2.5099	-2.8688	-0.9472	C	-3.3373	-1.9294	1.1166
C	-1.0937	-2.5698	-0.4201	C	-3.0872	-0.584	1.8192
C	-0.9397	-2.9645	1.0552	C	-4.376	0.2513	1.9025
C	-2.0484	-2.3722	1.9274	C	-5.0654	0.394	0.5419
C	-0.0349	-3.2042	-1.3043	C	-2.3826	-0.804	3.1472
C	0.8353	-2.3049	-2.1158	C	-0.9034	-1.0136	3.1068
C	0.1848	-4.524	-1.4249	C	-2.9459	-0.8021	4.3664
O	0.7955	-1.0828	-2.0294	O	-0.2512	-1.0068	2.068
C	-3.662	-4.2749	1.6205	C	-6.4455	-1.7003	0.7237
C	-4.1911	-0.3951	-1.6634	C	-1.9082	-2.2067	-1.579
O	-5.0539	-0.8984	-2.3698	O	-1.9172	-3.4221	-1.7162
C	5.0878	-2.904	-1.4778	C	4.642	-4.4778	-0.1101
C	4.3518	-1.6164	-1.1842	C	3.6785	-3.3503	0.1806

C	4.0454	-1.1964	0.0682	C	3.9273	-2.0542	-0.1291
C	4.3765	-2.0561	1.3035	C	5.2612	-1.6193	-0.7745
C	4.8132	-3.4991	0.9248	C	6.3286	-2.7482	-0.7347
C	3.3566	0.1208	0.407	C	2.9689	-0.8993	0.1178
C	2.0902	-0.0646	1.2702	C	3.6213	0.2184	0.9454
C	2.4278	-0.8756	2.5331	C	4.8807	0.7374	0.2418
C	3.1162	-2.1965	2.1947	C	5.8648	-0.406	-0.0113
C	1.4259	1.2647	1.5735	C	2.6412	1.3246	1.2363
C	0.8821	1.6591	2.724	C	2.0969	1.5621	2.4275
O	1.3533	2.1627	0.5064	O	2.2561	2.1441	0.1745
C	5.5216	-1.3916	2.1024	C	5.0086	-1.234	-2.2514
C	4.001	-0.8575	-2.4281	C	2.4162	-3.8191	0.8384
O	4.1986	-1.3187	-3.5487	O	2.2766	-4.9679	1.2461
O	-4.8743	-2.9858	-0.5191	O	-4.4833	-3.1732	-0.59
C	5.7635	-3.5195	-0.2598	C	5.7463	-4.106	-1.0918
H	3.1685	5.61	-0.1822	H	2.9927	5.9639	-0.5894
H	2.8593	3.9934	-0.7912	H	3.0759	4.3259	-1.2144
H	2.7647	4.026	1.6565	H	3.1861	4.3289	1.2354
H	1.5694	5.317	1.6544	H	1.6882	5.2434	1.3603
H	1.6264	5.6565	-2.1163	H	1.3339	5.6091	-2.3871
H	0.9267	6.3448	-0.6634	H	0.6008	6.068	-0.8621
H	-1.8084	2.4354	0.9837	H	-0.791	1.5339	0.8657
H	-2.4843	3.3758	-0.2956	H	-1.8247	2.2728	-0.3059
H	-0.4606	1.1039	-0.6091	H	0.7159	0.6812	-0.8648
H	-0.4563	1.4468	-2.9886	H	0.3993	1.0104	-3.2391
H	-1.6151	2.7567	-2.8908	H	-1.0695	1.9294	-2.9901
H	0.6104	3.6634	-3.1994	H	0.8005	3.4324	-3.4531
H	1.2499	2.7366	-1.8686	H	1.7788	2.6987	-2.208
H	-1.3048	6.2169	-1.3425	H	-1.5636	5.3437	-1.3607
H	-0.7998	5.6212	-2.9214	H	-1.0585	4.9202	-2.9939
H	-2.045	4.7664	-2.0104	H	-1.939	3.7507	-2.0093
H	-1.2138	4.7727	1.7767	H	-0.8325	3.9446	1.6826
H	-3.3102	1.0955	-3.1056	H	0.3122	-1.7987	-1.665
H	-3.8096	-0.0419	2.4778	H	-4.7345	0.742	-2.4127
H	-5.5327	-0.2128	2.764	H	-5.6055	-0.2457	-3.573
H	-5.9673	-0.6699	0.3915	H	-4.2058	-2.2054	-3.0812
H	-5.0934	0.8452	0.586	H	-3.213	-0.8241	-3.5313
H	-5.5182	-2.5431	2.1598	H	-6.4758	-1.6929	-1.865
H	-4.308	-2.2663	3.3977	H	-6.8488	-0.0334	-1.4404
H	-2.6414	-3.9547	-1.0518	H	-3.9282	-2.5769	1.7798
H	-2.6062	-2.4976	-1.9758	H	-2.3934	-2.4773	1.0009
H	-0.9419	-1.4895	-0.4552	H	-2.4015	0.0068	1.2115
H	0.0265	-2.6109	1.4312	H	-4.1405	1.2524	2.2859
H	-0.9237	-4.0539	1.1725	H	-5.0837	-0.1878	2.6137
H	-1.9074	-2.7268	2.9569	H	-5.9992	0.9541	0.6831
H	-1.9165	-1.2865	1.9736	H	-4.4452	1.0233	-0.1038
H	1.5387	-2.8067	-2.8025	H	-0.415	-1.1762	4.0827

H	0.9541	-4.9338	-2.0735	H	-2.3727	-0.9547	5.2766
H	-0.4132	-5.2456	-0.8755	H	-4.0121	-0.6551	4.505
H	-3.0025	-4.8657	0.9794	H	-6.0873	-1.9685	1.721
H	-3.4577	-4.5673	2.6574	H	-7.3308	-1.0666	0.8544
H	-4.689	-4.5858	1.3983	H	-6.7839	-2.626	0.2448
H	4.3721	-3.6235	-1.8964	H	5.0935	-4.8002	0.837
H	5.8604	-2.7385	-2.2386	H	4.1063	-5.3421	-0.5218
H	3.9352	-4.1072	0.6663	H	6.7672	-2.8205	0.2701
H	5.2834	-3.9954	1.783	H	7.1593	-2.5144	-1.4124
H	4.0728	0.7659	0.9326	H	2.6436	-0.5115	-0.8549
H	3.0839	0.6766	-0.4911	H	2.0556	-1.2108	0.6255
H	1.3685	-0.6447	0.6799	H	3.9348	-0.217	1.9061
H	3.0651	-0.2888	3.206	H	4.6259	1.2254	-0.7067
H	1.5105	-1.1021	3.0912	H	5.3696	1.5	0.8611
H	3.3731	-2.7121	3.1291	H	6.734	-0.0147	-0.5555
H	2.3808	-2.8351	1.6873	H	6.2412	-0.7392	0.9659
H	0.7792	1.1648	3.6705	H	2.214	1.0589	3.3674
H	6.4163	-1.253	1.4855	H	4.5478	-2.0557	-2.8105
H	5.2473	-0.406	2.4908	H	4.3454	-0.3691	-2.3522
H	5.8056	-2.0056	2.9649	H	5.9471	-0.9756	-2.7554
H	3.5403	0.1306	-2.3072	H	1.6055	-3.0886	0.9531
H	-5.1099	-2.6534	-1.4112	H	-3.6907	-3.7195	-0.7771
H	6.685	-2.975	-0.0239	H	5.3539	-4.0988	-2.1151
H	6.0584	-4.5507	-0.4861	H	6.5326	-4.8692	-1.0643
3b-5	X axis(Å)	Y axis(Å)	Z axis(Å)	3b-6	X axis(Å)	Y axis(Å)	Z axis(Å)
C	5.3856	0.9977	0.7753	C	-3.1338	4.7011	-0.0668
C	5.0071	0.7755	-0.6823	C	-2.5117	4.1733	-1.3554
C	3.7123	-0.0369	-0.8006	C	-1.4637	3.0958	-1.0478
C	3.7999	-1.4152	-0.0551	C	-0.3267	3.6508	-0.1224
C	4.3048	-1.2629	1.4314	C	-0.9043	4.2735	1.2
C	5.5464	-0.3293	1.5058	C	-2.0739	5.2506	0.8822
C	2.4683	-2.2118	-0.0955	C	0.7711	2.6147	0.2113
C	1.3744	-1.7107	0.8664	C	0.3741	1.5149	1.2149
C	1.9085	-1.5649	2.2967	C	-0.2984	2.1136	2.4649
C	3.1788	-0.7152	2.3442	C	-1.3791	3.1552	2.1612
C	4.7766	-2.6285	2.013	C	0.1612	5.1292	1.9451
C	3.3761	-0.2091	-2.2645	C	-0.9193	2.5185	-2.3364
O	3.9386	-0.9547	-3.0542	O	-0.1269	3.0663	-3.0903
O	4.7934	-2.2265	-0.7286	O	0.3361	4.7285	-0.8283
C	0.149	-2.5845	0.7426	C	1.577	0.6485	1.5514
O	-0.6871	-2.2744	-0.333	O	2.4814	0.4248	0.5078
C	-0.2429	-3.5642	1.555	C	1.8811	0.0966	2.7256
C	-1.7519	-3.4072	-2.8429	C	5.1889	1.5168	-0.0968
C	-1.5388	-4.1674	-1.5394	C	4.6952	1.0299	1.2588
C	-1.7572	-3.2464	-0.3338	C	3.6853	-0.1172	1.0974
C	-3.1944	-2.6131	-0.3331	C	4.2972	-1.3209	0.3044
C	-3.5339	-1.9038	-1.6998	C	4.9228	-0.8709	-1.07

C	-3.1513	-2.8078	-2.9074	C	5.8269	0.3816	-0.887
C	-3.4415	-1.6458	0.855	C	3.3081	-2.493	0.0801
C	-2.7757	-0.2634	0.7252	C	2.2309	-2.2618	-1.0008
C	-3.1183	0.3887	-0.6234	C	2.8495	-1.7482	-2.3109
C	-2.8098	-0.5362	-1.8039	C	3.8081	-0.5749	-2.1035
C	-3.0978	0.5923	1.9387	C	1.3633	-3.4809	-1.2837
C	-2.283	0.3467	3.1673	C	0.029	-3.2409	-1.9077
C	-4.0176	1.5668	2.022	C	1.6453	-4.7638	-1.0017
O	-1.4093	-0.5123	3.2125	O	-0.4127	-2.117	-2.1201
C	-5.0644	-1.6507	-1.844	C	5.8537	-1.9689	-1.6637
C	-1.484	-4.0079	0.9438	C	3.1732	-0.519	2.4613
O	-2.1971	-4.8754	1.4296	O	3.7409	-1.2472	3.2632
C	-2.1727	4.9271	1.3507	C	-4.0371	-4.4945	1.0798
C	-0.8889	4.1402	1.2342	C	-3.1445	-3.3125	0.792
C	-0.1799	4.0519	0.082	C	-3.601	-2.0847	0.4461
C	-0.5975	4.8196	-1.1879	C	-5.1116	-1.7986	0.3234
C	-1.8213	5.7518	-0.9679	C	-5.9606	-3.1011	0.3145
C	1.012	3.1334	-0.1461	C	-2.7121	-0.8859	0.1359
C	0.692	2.0751	-1.2276	C	-3.0546	-0.2279	-1.2133
C	0.1667	2.741	-2.5174	C	-4.5374	0.1603	-1.2631
C	-0.9483	3.7615	-2.2631	C	-5.4231	-1.0559	-1.0033
C	1.8697	1.1522	-1.4751	C	-2.1956	0.9803	-1.4838
C	2.2476	0.6251	-2.6388	C	-1.4672	1.1925	-2.5779
O	2.6158	0.7925	-0.3495	O	-2.1658	1.9589	-0.4946
C	0.5445	5.7336	-1.6948	C	-5.554	-0.9308	1.5254
C	-0.5096	3.4274	2.4945	C	-1.6924	-3.6196	0.9513
O	-1.2453	3.3856	3.4761	O	-1.2562	-4.766	0.9326
O	-4.1559	-3.6888	-0.1932	O	5.3923	-1.8562	1.0892
C	-2.836	5.1728	0.0021	C	-5.4869	-4.1114	1.3471
H	6.3297	1.553	0.8231	H	-3.8489	5.4959	-0.3095
H	4.6346	1.621	1.2732	H	-3.709	3.9101	0.4279
H	4.8916	1.7564	-1.161	H	-3.3145	3.7647	-1.9825
H	5.8282	0.2672	-1.2036	H	-2.064	4.9997	-1.9212
H	5.8021	-0.1286	2.5542	H	-2.5615	5.566	1.8137
H	6.4169	-0.8435	1.0759	H	-1.6689	6.1661	0.4293
H	2.0806	-2.234	-1.1225	H	1.127	2.1565	-0.7209
H	2.6822	-3.268	0.122	H	1.6572	3.1451	0.5887
H	1.0489	-0.7126	0.5579	H	-0.3438	0.8488	0.7292
H	1.149	-1.0926	2.9305	H	-0.7552	1.3094	3.0564
H	2.1072	-2.5452	2.7438	H	0.4587	2.5709	3.1145
H	3.5288	-0.6701	3.3838	H	-1.707	3.5983	3.1111
H	2.9216	0.3148	2.0771	H	-2.2626	2.6425	1.7707
H	5.6591	-3.0101	1.4873	H	0.4859	5.9859	1.344
H	5.0542	-2.5261	3.0689	H	-0.2489	5.5309	2.8794
H	4.0075	-3.4029	1.9511	H	1.0572	4.5593	2.2048
H	4.5809	-2.2622	-1.6849	H	0.6394	4.3876	-1.6965
H	0.194	-3.9618	2.4502	H	1.371	0.0999	3.6693

H	-0.9964	-2.6212	-2.9543	H	4.3643	1.9616	-0.665
H	-1.6127	-4.0921	-3.6877	H	5.9273	2.3135	0.0516
H	-2.2145	-5.0306	-1.4954	H	5.5467	0.7086	1.8719
H	-0.5171	-4.5687	-1.5378	H	4.2393	1.8806	1.7817
H	-3.8637	-3.6413	-2.9784	H	6.7502	0.092	-0.3667
H	-3.2535	-2.2443	-3.8438	H	6.1406	0.7641	-1.8669
H	-4.5251	-1.5105	0.9818	H	3.9029	-3.3801	-0.1721
H	-3.1342	-2.1284	1.7913	H	2.823	-2.7605	1.0279
H	-1.6883	-0.3843	0.7209	H	1.5581	-1.487	-0.6174
H	-2.5452	1.3157	-0.7373	H	2.0583	-1.4246	-2.999
H	-4.1731	0.6804	-0.6642	H	3.3723	-2.564	-2.8255
H	-3.1049	-0.0268	-2.7306	H	4.2571	-0.319	-3.0723
H	-1.7257	-0.6679	-1.877	H	3.2257	0.3053	-1.8143
H	-2.5133	0.982	4.0395	H	-0.5584	-4.1415	-2.1563
H	-4.1657	2.1454	2.9308	H	0.9491	-5.5732	-1.2081
H	-4.6601	1.8268	1.1882	H	2.5766	-5.0659	-0.5351
H	-5.4801	-1.0784	-1.0106	H	5.3449	-2.9258	-1.8059
H	-5.2808	-1.094	-2.7636	H	6.243	-1.6599	-2.6412
H	-5.6274	-2.5893	-1.8996	H	6.7202	-2.1571	-1.0199
H	-2.9003	4.4058	1.9823	H	-3.9939	-5.1787	0.2227
H	-1.9535	5.8845	1.8398	H	-3.6687	-5.0487	1.9519
H	-2.3115	5.9722	-1.9246	H	-5.9109	-3.5783	-0.674
H	-1.4893	6.7205	-0.5687	H	-7.0192	-2.8689	0.4866
H	1.8903	3.7248	-0.4304	H	-2.818	-0.1623	0.9544
H	1.3084	2.6159	0.768	H	-1.6527	-1.1492	0.1123
H	-0.114	1.4419	-0.8307	H	-2.8765	-0.9677	-2.0066
H	0.9905	3.2329	-3.0495	H	-4.7598	0.9494	-0.5344
H	-0.2242	1.9741	-3.1985	H	-4.7835	0.5743	-2.2493
H	-1.1915	4.2557	-3.2127	H	-6.4746	-0.7413	-1.02
H	-1.8515	3.2138	-1.9676	H	-5.2971	-1.7458	-1.8494
H	1.84	0.7134	-3.6274	H	-1.3154	0.5831	-3.4482
H	0.8528	6.443	-0.9175	H	-5.3365	-1.4214	2.4805
H	1.4381	5.183	-2.001	H	-5.0521	0.0417	1.5475
H	0.2185	6.3154	-2.5654	H	-6.632	-0.7347	1.492
H	0.4711	2.9354	2.5172	H	-1.0147	-2.7655	1.0865
H	-3.9157	-4.2218	0.5945	H	5.0551	-2.0763	1.9835
H	-3.6735	5.8688	0.1259	H	-5.5881	-3.7026	2.359
H	-3.255	4.2388	-0.3909	H	-6.1158	-5.0084	1.3084
3b-7	X axis(Å)	Y axis(Å)	Z axis(Å)	3b-8	X axis(Å)	Y axis(Å)	Z axis(Å)
C	2.3291	4.4843	-0.6622	C	2.4298	5.0047	-0.5014
C	2.0657	3.9916	0.756	C	2.2094	4.4157	0.8854
C	1.2158	2.7172	0.7401	C	1.3979	3.1157	0.8104
C	-0.1488	2.9319	-0.0054	C	0.016	3.3248	0.0937
C	0.0408	3.5414	-1.4457	C	0.163	4.0392	-1.3038
C	1.0259	4.7453	-1.4094	C	1.1029	5.2739	-1.2002
C	-1.0113	1.6484	-0.078	C	-0.8006	2.0149	-0.0542
C	-0.5391	0.6008	-1.0999	C	-0.3174	1.0666	-1.1661

C	-0.3433	1.2186	-2.4881	C	-0.1539	1.7924	-2.5053
C	0.5467	2.4645	-2.4408	C	0.6986	3.0547	-2.373
C	-1.2966	4.1136	-2.0022	C	-1.2027	4.596	-1.8044
C	1.0054	2.2241	2.1557	C	1.2248	2.5621	2.2099
O	0.2874	2.7388	3.0026	O	0.4583	2.9804	3.0671
O	-0.9164	3.9061	0.7451	O	-0.7785	4.2195	0.9125
C	-1.4611	-0.5916	-1.1618	C	-1.1944	-0.1498	-1.338
O	-2.8287	-0.3414	-1.2558	O	-2.5647	0.0098	-1.1458
C	-1.0719	-1.8633	-1.0965	C	-0.755	-1.3708	-1.6366
C	-5.1474	-0.7425	-3.044	C	-5.161	-0.1579	-2.5442
C	-4.0157	-1.736	-2.8103	C	-3.9722	-1.0888	-2.752
C	-3.486	-1.6258	-1.3759	C	-3.187	-1.262	-1.4473
C	-4.6191	-1.8754	-0.3151	C	-4.0904	-1.829	-0.2934
C	-5.8709	-0.9507	-0.5583	C	-5.3963	-0.9722	-0.0886
C	-6.2881	-0.963	-2.0577	C	-6.0876	-0.6796	-1.4521
C	-4.1349	-1.7539	1.1543	C	-3.3404	-2.0018	1.0535
C	-3.8977	-0.3153	1.6454	C	-3.0648	-0.6953	1.8172
C	-5.1181	0.5783	1.3645	C	-4.3465	0.1395	1.9773
C	-5.5769	0.499	-0.0947	C	-5.0708	0.3547	0.6445
C	-3.426	-0.3121	3.0906	C	-2.3266	-0.9868	3.1128
C	-1.9878	-0.6363	3.3396	C	-0.8502	-1.2003	3.0219
C	-4.1577	-0.0119	4.1762	C	-2.8576	-1.0463	4.345
O	-1.2014	-0.9309	2.446	O	-0.2255	-1.1381	1.9681
C	-7.1188	-1.4628	0.2207	C	-6.4564	-1.7409	0.7547
C	-2.33	-2.5832	-1.1859	C	-1.9825	-2.1448	-1.688
O	-2.4095	-3.8012	-1.1007	O	-2.0002	-3.3519	-1.8854
C	7.1245	-2.2464	-1.5388	C	4.8891	-4.3399	-0.0626
C	6.2237	-1.1082	-1.1152	C	3.7845	-3.3179	0.0572
C	5.4839	-1.1171	0.0217	C	3.9262	-2.0312	-0.3433
C	5.4826	-2.3388	0.9655	C	5.2016	-1.5296	-1.0541
C	6.1287	-3.5913	0.3109	C	6.2332	-2.661	-1.3205
C	4.5982	0.0279	0.4994	C	2.9371	-0.916	-0.05
C	3.1584	-0.4259	0.8063	C	3.5922	0.1341	0.866
C	3.1687	-1.5701	1.8302	C	4.887	0.6853	0.2473
C	4.0277	-2.7333	1.337	C	5.8491	-0.4424	-0.1532
C	2.3081	0.7571	1.2092	C	2.6247	1.2332	1.2179
C	1.757	1.0037	2.396	C	2.0948	1.4205	2.4244
O	2.0252	1.6571	0.1792	O	2.234	2.1017	0.198
C	6.276	-1.9897	2.247	C	4.865	-0.9285	-2.4412
C	6.25	0.0382	-2.0788	C	2.545	-3.8455	0.7121
O	6.8703	-0.0016	-3.1364	O	2.4828	-4.9693	1.1999
O	-5.09	-3.2374	-0.4762	O	-4.5366	-3.1518	-0.6841
C	7.4093	-3.2561	-0.4347	C	6.2653	-3.7026	-0.2151
H	2.9127	5.4114	-0.6198	H	2.987	5.9446	-0.4104
H	2.9415	3.7586	-1.2092	H	3.0511	4.3342	-1.1054
H	3.0323	3.8034	1.2409	H	3.191	4.2322	1.3409
H	1.571	4.7792	1.3378	H	1.7012	5.1501	1.5231

H	1.2614	5.0671	-2.432	H	1.3042	5.6767	-2.2012
H	0.5352	5.6029	-0.9289	H	0.5931	6.0761	-0.6493
H	-1.0704	1.1942	0.9162	H	-0.8118	1.483	0.9038
H	-2.0484	1.9377	-0.2965	H	-1.8537	2.2782	-0.2228
H	0.4334	0.2176	-0.7809	H	0.6673	0.6939	-0.8794
H	0.1182	0.4827	-3.1593	H	0.3242	1.1247	-3.2341
H	-1.3122	1.4673	-2.9379	H	-1.1346	2.0423	-2.928
H	0.605	2.8883	-3.4519	H	0.7403	3.5508	-3.3514
H	1.568	2.1557	-2.1959	H	1.729	2.7585	-2.1513
H	-1.6589	4.9557	-1.4019	H	-1.5826	5.3882	-1.1496
H	-1.1638	4.4852	-3.0252	H	-1.101	5.0315	-2.8056
H	-2.097	3.3693	-2.0278	H	-1.9778	3.8271	-1.8607
H	-0.9804	3.6055	1.6756	H	-0.823	3.8567	1.8221
H	-0.096	-2.2962	-0.9932	H	0.2369	-1.7397	-1.8098
H	-4.7739	0.285	-2.9686	H	-4.8151	0.8522	-2.2972
H	-5.5259	-0.8595	-4.0663	H	-5.7211	-0.0719	-3.4828
H	-4.3648	-2.7553	-3.0177	H	-4.3189	-2.0593	-3.1281
H	-3.2173	-1.5253	-3.5335	H	-3.3313	-0.6607	-3.5335
H	-6.7503	-1.9301	-2.2989	H	-6.5544	-1.6004	-1.8282
H	-7.063	-0.2064	-2.2366	H	-6.907	0.0367	-1.3099
H	-4.8676	-2.2416	1.8128	H	-3.9174	-2.6801	1.6979
H	-3.2285	-2.3568	1.2918	H	-2.4029	-2.547	0.8851
H	-3.0831	0.1204	1.067	H	-2.392	-0.0768	1.2227
H	-4.8715	1.6216	1.6003	H	-4.0958	1.1187	2.4052
H	-5.9581	0.31	2.0142	H	-5.0375	-0.3328	2.6836
H	-6.4772	1.1168	-0.2095	H	-5.9976	0.9101	0.839
H	-4.8196	0.9703	-0.7288	H	-4.4646	1.0141	0.0158
H	-1.662	-0.5976	4.393	H	-0.3373	-1.4189	3.9741
H	-3.7432	-0.0155	5.1806	H	-2.2613	-1.2485	5.2305
H	-5.2094	0.2459	4.1064	H	-3.9189	-0.9023	4.5194
H	-6.939	-1.5583	1.2946	H	-6.0739	-2.0611	1.7274
H	-7.9649	-0.7775	0.0913	H	-7.3348	-1.1115	0.9407
H	-7.4461	-2.4451	-0.1382	H	-6.8117	-2.6397	0.2382
H	6.6532	-2.7616	-2.3858	H	4.9241	-4.9834	0.8244
H	8.0883	-1.861	-1.8935	H	4.6786	-4.9871	-0.9232
H	5.4296	-4.0498	-0.4021	H	7.2368	-2.239	-1.4574
H	6.3346	-4.3567	1.0696	H	5.9919	-3.1771	-2.2604
H	5.0505	0.4681	1.3978	H	2.6071	-0.467	-0.9926
H	4.5505	0.8438	-0.2238	H	2.0253	-1.2719	0.4311
H	2.7222	-0.8253	-0.1213	H	3.8751	-0.3763	1.7994
H	3.5404	-1.2227	2.8014	H	4.6632	1.3057	-0.6289
H	2.1464	-1.9327	1.9972	H	5.391	1.3442	0.9659
H	4.0359	-3.5196	2.1029	H	6.7167	-2.00E-04	-0.6595
H	3.5283	-3.1668	0.4592	H	6.2332	-0.9035	0.7664
H	1.7831	0.457	3.3187	H	2.2184	0.8749	3.3395
H	7.3021	-1.6826	2.0169	H	4.3424	-1.66	-3.0692
H	5.8207	-1.1713	2.8133	H	4.2306	-0.0395	-2.3868

H	6.3317	-2.8524	2.9209	H	5.7799	-0.6317	-2.9679
H	5.6837	0.9372	-1.8077	H	1.6684	-3.1849	0.7315
H	-4.3178	-3.8408	-0.4396	H	-3.7517	-3.6905	-0.9198
H	8.1629	-2.8579	0.2542	H	7.0037	-4.4768	-0.4532
H	7.8369	-4.1659	-0.8718	H	6.5784	-3.2461	0.7314
3b-9	X axis(Å)	Y axis(Å)	Z axis(Å)	3b-10	X axis(Å)	Y axis(Å)	Z axis(Å)
C	3.3347	4.7228	-0.0916	C	-3.095	4.7	-0.1636
C	2.8451	4.2025	1.253	C	-2.5015	4.1105	-1.4389
C	1.6563	3.2432	1.0754	C	-1.4573	3.0378	-1.1034
C	0.4676	3.929	0.3225	C	-0.2985	3.6221	-0.2241
C	0.9284	4.569	-1.0401	C	-0.8462	4.307	1.0801
C	2.2142	5.4231	-0.8488	C	-2.013	5.2804	0.7411
C	-0.7477	2.9976	0.0941	C	0.7964	2.5913	0.1347
C	-0.5971	1.9486	-1.0255	C	0.4081	1.5395	1.1917
C	-0.0382	2.5668	-2.3195	C	-0.2366	2.1977	2.4265
C	1.1775	3.4652	-2.0977	C	-1.3129	3.2362	2.0976
C	-0.1413	5.5518	-1.5998	C	0.2402	5.1841	1.768
C	1.2627	2.6963	2.4301	C	-0.9417	2.3996	-2.375
O	0.5741	3.2607	3.2681	O	-0.16	2.9074	-3.1671
O	-0.0045	5.0232	1.1466	O	0.3601	4.6618	-0.9884
C	-1.9274	1.2443	-1.2268	C	1.6077	0.6757	1.5466
O	-2.4418	0.5946	-0.0994	O	2.5145	0.4297	0.5104
C	-2.6526	1.1736	-2.3426	C	1.9055	0.1436	2.7316
C	-4.7108	0.872	1.7967	C	5.2315	1.49	-0.1064
C	-4.7649	1.0936	0.2905	C	4.731	1.0303	1.2563
C	-3.783	0.1633	-0.4326	C	3.7125	-0.1113	1.1124
C	-4.0682	-1.347	-0.1186	C	4.3161	-1.3332	0.3413
C	-4.1352	-1.6313	1.4295	C	4.9469	-0.9115	-1.0397
C	-5.0234	-0.5769	2.1508	C	5.8612	0.3364	-0.8763
C	-3.0686	-2.3124	-0.8055	C	3.3185	-2.5015	0.1352
C	-1.6737	-2.3782	-0.1592	C	2.2444	-2.2802	-0.9506
C	-1.7724	-2.6314	1.3538	C	2.8673	-1.7917	-2.2683
C	-2.7137	-1.6425	2.046	C	3.8359	-0.6234	-2.0793
C	-0.8074	-3.3707	-0.9152	C	1.3695	-3.4979	-1.2164
C	-0.0907	-2.86	-2.121	C	0.0354	-3.2586	-1.8416
C	-0.6061	-4.6616	-0.6063	C	1.6454	-4.7789	-0.9203
O	-0.1512	-1.6907	-2.4834	O	-0.4087	-2.1348	-2.0493
C	-4.8014	-3.0072	1.7276	C	5.8693	-2.0268	-1.6139
C	-3.8295	0.4376	-1.9177	C	3.1939	-0.4854	2.4816
O	-4.7192	0.0986	-2.6862	O	3.7539	-1.2041	3.2975
C	3.6091	-4.9463	0.1531	C	-4.2118	-4.4685	0.8961
C	2.8654	-3.7211	0.6299	C	-3.2508	-3.31	0.8098
C	3.0789	-2.474	0.1449	C	-3.6453	-2.0269	0.6328
C	4.2237	-2.188	-0.8494	C	-5.1339	-1.6267	0.6485
C	5.1758	-3.405	-1.0222	C	-6.0815	-2.8223	0.9486
C	2.2661	-1.2351	0.5057	C	-2.7122	-0.8746	0.2858
C	3.1559	-0.1208	1.0742	C	-3.0759	-0.2763	-1.0898

C	4.2886	0.2231	0.0904	C	-4.5612	0.117	-1.1628
C	5.0883	-1.0179	-0.305	C	-5.4812	-1.0334	-0.7409
C	2.3461	1.0997	1.4347	C	-2.2132	0.9112	-1.4314
C	1.8413	1.3757	2.6357	C	-1.5037	1.0687	-2.5468
O	2.1408	2.0431	0.429	O	-2.1587	1.933	-0.4879
C	3.6439	-1.8244	-2.2357	C	-5.408	-0.5782	1.7545
C	1.875	-4.0189	1.7091	C	-1.8131	-3.7009	0.8887
O	1.5611	-5.1614	2.025	O	-1.4259	-4.8532	0.7265
O	-5.3802	-1.6743	-0.6407	O	5.4059	-1.8635	1.137
C	4.4157	-4.7176	-1.1189	C	-5.5916	-4.1282	0.3449
H	4.1578	5.4286	0.071	H	-3.8075	5.4903	-0.428
H	3.7454	3.9021	-0.6902	H	-3.6679	3.937	0.3756
H	3.6839	3.6972	1.7488	H	-3.3193	3.6823	-2.0327
H	2.5652	5.0447	1.8985	H	-2.0574	4.9072	-2.0485
H	2.5958	5.7502	-1.8246	H	-2.4805	5.6407	1.6666
H	1.9642	6.3412	-0.2995	H	-1.6084	6.1714	0.2413
H	-1.0041	2.4967	1.0371	H	1.1313	2.0899	-0.7828
H	-1.6314	3.6187	-0.1126	H	1.6935	3.1295	0.4732
H	0.1111	1.1806	-0.6945	H	-0.3239	0.8601	0.7473
H	0.24	1.7648	-3.0159	H	-0.6907	1.4244	3.0597
H	-0.8109	3.1531	-2.8308	H	0.5365	2.6742	3.0426
H	1.4472	3.9253	-3.0577	H	-1.6188	3.7232	3.0332
H	2.0341	2.84	-1.83	H	-2.2084	2.716	1.7462
H	-0.2863	6.4123	-0.937	H	0.5618	6.0102	1.1241
H	0.1678	5.9471	-2.5748	H	-0.1494	5.6304	2.6907
H	-1.1195	5.083	-1.735	H	1.1354	4.6172	2.0368
H	-0.2413	4.666	2.0286	H	0.6443	4.2804	-1.8461
H	-2.4823	1.5564	-3.3301	H	1.3915	0.1657	3.6729
H	-3.7276	1.1561	2.1884	H	4.4117	1.9322	-0.6836
H	-5.44	1.5288	2.2853	H	5.9763	2.2829	0.0301
H	-5.7877	0.9337	-0.0731	H	5.5787	0.7129	1.8766
H	-4.5217	2.1447	0.0885	H	4.2809	1.8934	1.7635
H	-6.0783	-0.758	1.9028	H	6.7812	0.048	-0.3496
H	-4.9441	-0.7016	3.2385	H	6.1796	0.6997	-1.862
H	-3.506	-3.3209	-0.8219	H	3.9069	-3.3971	-0.1011
H	-2.9781	-2.0562	-1.8689	H	2.8303	-2.7495	1.0868
H	-1.1839	-1.4049	-0.2569	H	1.5764	-1.495	-0.5802
H	-0.7793	-2.5397	1.8068	H	2.0784	-1.4725	-2.9611
H	-2.1086	-3.652	1.5643	H	3.3835	-2.6196	-2.7702
H	-2.7705	-1.9038	3.1108	H	4.288	-0.3878	-3.0518
H	-2.2623	-0.6458	2.0152	H	3.2607	0.2666	-1.8059
H	0.5118	-3.6004	-2.674	H	-0.55	-4.1596	-2.0938
H	0.039	-5.312	-1.1905	H	0.9434	-5.5863	-1.1163
H	-1.079	-5.1285	0.2525	H	2.5766	-5.0813	-0.4538
H	-4.3045	-3.8376	1.2192	H	5.3525	-2.9815	-1.7417
H	-4.7817	-3.2232	2.8025	H	6.2629	-1.737	-2.5955
H	-5.8525	-3.0245	1.4182	H	6.733	-2.212	-0.9655

H	4.2833	-5.2761	0.9541	H	-3.8353	-5.3309	0.3335
H	2.9093	-5.769	-0.038	H	-4.2954	-4.779	1.945
H	5.8663	-3.4734	-0.1702	H	-7.095	-2.6074	0.587
H	5.8052	-3.2769	-1.9118	H	-6.1731	-2.9679	2.0341
H	1.7471	-0.8787	-0.3928	H	-2.765	-0.1173	1.0768
H	1.4648	-1.4506	1.2158	H	-1.6637	-1.1785	0.2487
H	3.6234	-0.4996	1.9952	H	-2.9099	-1.0566	-1.8464
H	3.8893	0.6951	-0.8157	H	-4.7594	0.9963	-0.5376
H	4.9667	0.9562	0.5458	H	-4.8154	0.4137	-2.1887
H	5.845	-0.733	-1.0473	H	-6.5182	-0.674	-0.7497
H	5.6417	-1.352	0.5838	H	-5.4215	-1.8174	-1.5072
H	1.8589	0.8251	3.5561	H	-1.3715	0.4193	-3.391
H	3.012	-2.6268	-2.6306	H	-5.1241	-0.965	2.7407
H	3.033	-0.9169	-2.2152	H	-4.8618	0.358	1.6095
H	4.4466	-1.6487	-2.9614	H	-6.4737	-0.3229	1.792
H	1.4453	-3.1593	2.2384	H	-1.0962	-2.8981	1.1126
H	-5.4145	-1.4135	-1.5857	H	5.066	-2.0641	2.0347
H	3.7514	-4.7145	-1.9908	H	-6.292	-4.9365	0.5843
H	5.1171	-5.5475	-1.2624	H	-5.555	-4.0539	-0.7484
3b-11	X axis(Å)	Y axis(Å)	Z axis(Å)				
C	1.6862	5.0159	-0.9717				
C	1.7585	4.3706	0.4076				
C	1.0591	3.0058	0.4057				
C	-0.4423	3.1268	-0.0372				
C	-0.6059	3.8785	-1.4111				
C	0.2422	5.1828	-1.431				
C	-1.1812	1.7683	-0.0787				
C	-0.833	0.8742	-1.2784				
C	-0.9639	1.6281	-2.6058				
C	-0.2048	2.9582	-2.5925				
C	-2.0772	4.3355	-1.6396				
C	1.1871	2.3644	1.7701				
O	0.568	2.6745	2.7792				
O	-1.1302	3.9387	0.9483				
C	-1.6431	-0.3989	-1.3025				
O	-3.0111	-0.2944	-1.0571				
C	-1.1474	-1.618	-1.5048				
C	-5.6502	-0.7492	-2.3118				
C	-4.4159	-1.6271	-2.4791				
C	-3.5699	-1.6221	-1.2006				
C	-4.3915	-2.1173	0.045				
C	-5.7391	-1.3205	0.22				
C	-6.4996	-1.2104	-1.1334				
C	-3.5816	-2.107	1.369				
C	-3.3587	-0.7149	1.985				
C	-4.6828	0.0574	2.1138				
C	-5.4677	0.0916	0.799				

C	-2.5549	-0.8184	3.2709
C	-1.0745	-0.9806	3.1393
C	-3.0298	-0.7427	4.525
O	-0.5015	-1.0703	2.0588
C	-6.7167	-2.0573	1.1832
C	-2.3274	-2.4589	-1.4112
O	-2.2835	-3.6797	-1.4824
C	7.7141	-2.3574	-0.2534
C	6.7458	-1.3973	0.4001
C	5.4133	-1.3837	0.1467
C	4.7852	-2.3493	-0.8804
C	5.8543	-3.0527	-1.7618
C	4.3997	-0.4663	0.8198
C	3.523	0.3088	-0.187
C	2.8393	-0.6659	-1.1545
C	3.856	-1.5705	-1.847
C	2.5013	1.2226	0.4586
C	2.1631	1.2878	1.7454
O	1.855	2.1096	-0.4086
C	3.9746	-3.434	-0.1319
C	7.4141	-0.4769	1.3741
O	8.6293	-0.4566	1.5391
O	-4.7703	-3.4973	-0.1892
C	7.044	-3.5347	-0.9494
H	2.1696	5.9993	-0.9361
H	2.2491	4.4211	-1.6997
H	2.8156	4.2628	0.6823
H	1.3077	5.0357	1.1547
H	0.2381	5.6167	-2.4392
H	-0.2272	5.9322	-0.7788
H	-0.9927	1.2249	0.8526
H	-2.263	1.9584	-0.058
H	0.2114	0.5729	-1.1798
H	-0.5717	1.0091	-3.4233
H	-2.0201	1.8032	-2.8443
H	-0.3874	3.4722	-3.5453
H	0.8694	2.7482	-2.5769
H	-2.3941	5.0722	-0.8929
H	-2.188	4.8094	-2.6223
H	-2.7896	3.5074	-1.596
H	-0.9864	3.5419	1.833
H	-0.1436	-1.9494	-1.684
H	-5.3576	0.2988	-2.1816
H	-6.2505	-0.791	-3.2282
H	-4.7174	-2.649	-2.7408
H	-3.8339	-1.2452	-3.3278
H	-6.9216	-2.1906	-1.3946

H	-7.3565	-0.5327	-1.027				
H	-4.0906	-2.7472	2.1035				
H	-2.6199	-2.6121	1.2141				
H	-2.7488	-0.1254	1.3009				
H	-4.4774	1.0886	2.4289				
H	-5.3168	-0.3783	2.8934				
H	-6.4186	0.6111	0.9759				
H	-4.926	0.715	0.081				
H	-0.5097	-1.0188	4.0864				
H	-2.3876	-0.8088	5.3989				
H	-4.0876	-0.6168	4.7315				
H	-6.2778	-2.2534	2.1649				
H	-7.624	-1.4629	1.3443				
H	-7.0362	-3.0232	0.776				
H	8.3128	-1.7987	-0.9843				
H	8.4116	-2.7639	0.4893				
H	6.2253	-2.3625	-2.5321				
H	5.4101	-3.8989	-2.301				
H	3.7692	-1.082	1.4741				
H	4.8748	0.2644	1.4769				
H	4.1949	0.9539	-0.7723				
H	2.0949	-1.2712	-0.6237				
H	2.2959	-0.1107	-1.9288				
H	3.3204	-2.2721	-2.4996				
H	4.4631	-0.939	-2.5107				
H	2.4876	0.7236	2.5979				
H	4.5973	-3.9828	0.583				
H	3.1356	-3.0168	0.4335				
H	3.5544	-4.1635	-0.8339				
H	6.7705	0.1982	1.9507				
H	-3.9639	-4.0092	-0.4113				
H	6.7286	-4.2796	-0.2099				
H	7.7677	-4.0331	-1.6047				
3c-1	X axis(Å)	Y axis(Å)	Z axis(Å)	3c-2	X axis(Å)	Y axis(Å)	Z axis(Å)
C	5.4049	0.625	-1.5761	C	-3.4328	-3.8749	1.9801
C	5.2581	0.6858	-0.0617	C	-3.6352	-3.9581	0.4714
C	3.9604	0.0105	0.3973	C	-2.5658	-3.1428	-0.2665
C	3.8617	-1.4795	-0.0851	C	-1.1177	-3.6344	0.0881
C	4.101	-1.614	-1.6378	C	-0.8679	-3.6458	1.6424
C	5.3612	-0.8139	-2.0755	C	-2.0413	-4.3509	2.3828
C	2.5322	-2.178	0.3097	C	0.0032	-2.8405	-0.6259
C	1.2969	-1.7589	-0.5119	C	0.2443	-1.4263	-0.0785
C	1.5675	-1.8265	-2.0219	C	0.4112	-1.4198	1.4486
C	2.8625	-1.1244	-2.4294	C	-0.6848	-2.2023	2.1775
C	4.3825	-3.0894	-2.0474	C	0.4064	-4.4603	2.0113
C	3.8494	0.1329	1.8993	C	-2.8303	-3.1807	-1.7559
O	4.5284	-0.4635	2.7235	O	-2.6084	-4.1218	-2.5047

O	4.9263	-2.2278	0.5511	O	-0.9925	-5.0072	-0.3564
C	0.0382	-2.5362	-0.1949	C	1.4008	-0.789	-0.8121
O	-1.1457	-1.9466	-0.6477	O	2.67	-0.9126	-0.2511
C	-0.0764	-3.6761	0.484	C	1.2973	-0.1052	-1.9501
C	-3.3282	-2.447	-2.5907	C	5.3551	-2.0481	-0.7139
C	-2.6545	-3.4908	-1.7086	C	4.4502	-1.4328	-1.7751
C	-2.2189	-2.8756	-0.3736	C	3.6044	-0.3051	-1.1746
C	-3.4273	-2.2409	0.4021	C	4.4987	0.8217	-0.5423
C	-4.2437	-1.2294	-0.4899	C	5.5375	0.2457	0.4926
C	-4.5368	-1.8355	-1.8927	C	6.2682	-0.9993	-0.0895
C	-3.0148	-1.5716	1.7394	C	3.6805	1.9734	0.0971
C	-2.3204	-0.2048	1.6026	C	3.029	1.6348	1.449
C	-3.1289	0.7486	0.7087	C	4.0582	1.0559	2.4333
C	-3.4802	0.1119	-0.638	C	4.838	-0.1166	1.8284
C	-1.9944	0.3479	2.9803	C	2.2452	2.8291	1.9655
C	-0.7135	-0.1003	3.6022	C	0.8762	3.03	1.4004
C	-2.7322	1.2131	3.6949	C	2.643	3.7132	2.8945
O	0.0981	-0.8073	3.0164	O	0.3729	2.2635	0.586
C	-5.6402	-0.9242	0.1285	C	6.6631	1.2764	0.8043
C	-1.5087	-3.9205	0.4572	C	2.6757	0.258	-2.2275
O	-2.0387	-4.8504	1.0502	O	3.0033	0.9435	-3.1862
C	-2.4834	4.0942	-2.0848	C	-3.1269	5.1473	-0.4868
C	-1.2366	3.2761	-1.8375	C	-2.6327	3.7425	-0.7477
C	-0.3514	3.5393	-0.844	C	-3.2414	2.6291	-0.2686
C	-0.5874	4.6867	0.1586	C	-4.5211	2.7246	0.5879
C	-2.0288	5.2615	0.0704	C	-5.1721	4.1336	0.5202
C	0.9346	2.7639	-0.5898	C	-2.7449	1.2024	-0.4761
C	1.0209	2.2237	0.8535	C	-3.8434	0.2504	-0.9886
C	0.8828	3.3834	1.8519	C	-5.0751	0.2908	-0.0762
C	-0.4033	4.1734	1.6114	C	-5.5891	1.7189	0.0832
C	2.2572	1.38	1.0877	C	-3.3461	-1.1684	-1.1164
C	2.7892	1.0572	2.2657	C	-3.3855	-1.9164	-2.2165
O	2.852	0.8244	-0.0453	O	-2.802	-1.7457	0.0287
C	0.416	5.8284	-0.1264	C	-4.1639	2.417	2.0621
C	-1.084	2.1479	-2.8116	C	-1.3773	3.7159	-1.5653
O	-1.947	1.8706	-3.6384	O	-0.8871	4.7327	-2.0474
O	-4.3491	-3.3056	0.7459	O	5.2829	1.4192	-1.6051
C	-2.4922	5.4368	-1.3658	C	-4.1473	5.2487	0.6391
H	4.6217	1.2207	-2.0581	H	-3.5975	-2.849	2.3288
H	6.36	1.0791	-1.8653	H	-4.1858	-4.495	2.4806
H	6.1267	0.2119	0.4127	H	-3.6133	-5.0065	0.149
H	5.2711	1.7402	0.2431	H	-4.6391	-3.5805	0.2379
H	6.2627	-1.3227	-1.7074	H	-1.9936	-5.432	2.1929
H	5.442	-0.8114	-3.1702	H	-1.9257	-4.2303	3.4677
H	2.6795	-3.2631	0.2244	H	0.9384	-3.4161	-0.5739
H	2.3342	-2.0238	1.3783	H	-0.2066	-2.7924	-1.7026
H	1.0608	-0.721	-0.2627	H	-0.6319	-0.8138	-0.3027

H	1.5946	-2.8718	-2.3541	H	1.3885	-1.8275	1.7329
H	0.7365	-1.3626	-2.5698	H	0.3981	-0.3863	1.8149
H	2.7236	-0.0449	-2.3173	H	-1.6191	-1.6364	2.1169
H	3.0201	-1.2846	-3.5041	H	-0.4369	-2.2306	3.2469
H	3.5794	-3.7709	-1.7553	H	1.3082	-4.0804	1.524
H	4.5011	-3.1743	-3.1343	H	0.5856	-4.4307	3.0927
H	5.3067	-3.4664	-1.5953	H	0.3081	-5.5153	1.7324
H	4.8813	-2.0793	1.5192	H	-1.222	-5.0497	-1.3085
H	0.6571	-4.3016	0.9545	H	0.4435	0.1348	-2.5527
H	-2.6135	-1.6645	-2.8696	H	4.7548	-2.5376	0.0612
H	-3.6514	-2.9185	-3.5262	H	5.9676	-2.8334	-1.1724
H	-3.3363	-4.334	-1.5414	H	5.0546	-1.0616	-2.6121
H	-1.7879	-3.8915	-2.2503	H	3.8059	-2.2237	-2.1801
H	-5.2973	-2.6227	-1.7979	H	6.9763	-0.6758	-0.8648
H	-4.975	-1.0706	-2.5468	H	6.8744	-1.4762	0.6914
H	-3.9094	-1.459	2.3684	H	2.9208	2.3238	-0.6131
H	-2.3813	-2.2578	2.3161	H	4.3345	2.848	0.2223
H	-1.365	-0.3418	1.0886	H	2.2978	0.8391	1.301
H	-2.5505	1.6626	0.5301	H	3.5455	0.7093	3.3397
H	-4.052	1.0689	1.2027	H	4.7664	1.825	2.7597
H	-4.085	0.8251	-1.2131	H	5.5837	-0.4523	2.5608
H	-2.5604	-0.0226	-1.2149	H	4.1571	-0.9637	1.6985
H	-0.5248	0.2564	4.6289	H	0.3295	3.9167	1.7639
H	-2.4304	1.5691	4.676	H	2.0186	4.5413	3.2183
H	-3.6826	1.5903	3.3308	H	3.6203	3.6512	3.3621
H	-5.5772	-0.5514	1.1541	H	6.2749	2.2312	1.1682
H	-6.1695	-0.1675	-0.4628	H	7.3441	0.8874	1.5707
H	-6.2776	-1.8153	0.1502	H	7.2708	1.4939	-0.0813
H	-2.6071	4.2897	-3.1571	H	-2.2891	5.8088	-0.2345
H	-3.3522	3.5057	-1.7625	H	-3.5724	5.5325	-1.4131
H	-2.7371	4.5906	0.5761	H	-5.7042	4.2597	-0.4328
H	-2.0915	6.2218	0.5974	H	-5.928	4.2442	1.3078
H	1.0402	1.9254	-1.2789	H	-1.9136	1.1486	-1.1818
H	1.7916	3.4174	-0.7977	H	-2.3445	0.8418	0.4801
H	0.1644	1.5512	0.9939	H	-4.1507	0.6019	-1.9844
H	0.8577	3.0037	2.8806	H	-5.8752	-0.3291	-0.501
H	1.7522	4.0489	1.7864	H	-4.8473	-0.1366	0.9079
H	-1.245	3.5196	1.8777	H	-5.972	2.0474	-0.8931
H	-0.4397	5.0159	2.3142	H	-6.4506	1.7131	0.7633
H	2.4983	1.3039	3.268	H	-3.7428	-1.701	-3.2051
H	0.238	6.682	0.5379	H	-5.0441	2.517	2.7077
H	1.4555	5.5205	0.0236	H	-3.7808	1.4008	2.1986
H	0.3357	6.1889	-1.1577	H	-3.3944	3.0974	2.443
H	-0.1625	1.5559	-2.7589	H	-0.9004	2.7416	-1.7263
H	-3.8502	-4.0173	1.2005	H	4.676	1.7032	-2.3211
H	-1.8493	6.151	-1.8929	H	-3.6412	5.2045	1.6102
H	-3.505	5.8555	-1.384	H	-4.6474	6.2231	0.5934

3c-3	X axis(Å)	Y axis(Å)	Z axis(Å)	3c-4	X axis(Å)	Y axis(Å)	Z axis(Å)
C	5.8014	1.4048	-0.8226	C	5.7	0.811	-1.3189
C	5.1993	1.5411	0.569	C	5.342	1.1727	0.1163
C	3.8737	0.7739	0.6807	C	4.0157	0.5204	0.5385
C	4.0391	-0.7431	0.3245	C	4.0616	-1.0368	0.3905
C	4.737	-0.9428	-1.0747	C	4.5111	-1.4761	-1.0542
C	6.0115	-0.0588	-1.1892	C	5.7827	-0.6992	-1.5003
C	2.715	-1.5503	0.3815	C	2.7391	-1.7464	0.7748
C	1.7559	-1.3407	-0.805	C	1.5944	-1.6366	-0.2513
C	2.4623	-1.4134	-2.1674	C	2.0656	-1.9471	-1.682
C	3.7575	-0.6072	-2.2268	C	3.3663	-1.2473	-2.0711
C	5.2278	-2.4077	-1.2641	C	4.9076	-2.9807	-1.0992
C	3.3092	0.9827	2.0676	C	3.6818	0.9637	1.9453
O	3.7002	0.4391	3.0915	O	4.1817	0.5338	2.9754
O	4.9228	-1.3414	1.3046	O	5.0727	-1.5404	1.2987
C	0.6017	-2.3205	-0.7934	C	0.4061	-2.5276	0.058
O	-0.6776	-1.7714	-0.9005	O	-0.7722	-2.2122	-0.6268
C	0.689	-3.648	-0.7172	C	0.358	-3.5682	0.8888
C	-2.8576	-1.6516	-2.9119	C	-2.4471	-3.3492	-2.7884
C	-1.9925	-2.8651	-2.5963	C	-1.7775	-4.134	-1.6666
C	-1.5914	-2.8754	-1.1155	C	-1.7042	-3.2928	-0.3864
C	-2.8468	-2.876	-0.1743	C	-3.1257	-2.8273	0.086
C	-3.8485	-1.7085	-0.5126	C	-3.927	-2.1	-1.0594
C	-4.1101	-1.6254	-2.0443	C	-3.8491	-2.9045	-2.3892
C	-2.4921	-2.8609	1.3355	C	-3.0895	-1.9521	1.3642
C	-1.9998	-1.5062	1.8834	C	-2.6293	-0.5009	1.1483
C	-2.9745	-0.3806	1.5053	C	-3.4092	0.1753	0.0101
C	-3.3038	-0.358	0.0111	C	-3.3943	-0.6599	-1.2728
C	-1.7301	-1.4969	3.3822	C	-2.6834	0.2518	2.4655
C	-0.8289	-0.4259	3.9034	C	-1.4192	0.3696	3.2483
C	-2.1869	-2.3697	4.2956	C	-3.7726	0.8288	2.9985
O	-0.334	0.4339	3.1836	O	-0.331	0.0079	2.8153
C	-5.246	-1.9453	0.1328	C	-5.4447	-2.0064	-0.7211
C	-0.6964	-4.0638	-0.8433	C	-0.991	-4.0706	0.6954
O	-1.0546	-5.2281	-0.7315	O	-1.457	-4.9985	1.3425
C	-3.7528	4.4643	-0.3006	C	-3.1929	4.933	-0.3279
C	-2.6318	3.6955	0.3608	C	-2.1376	4.0632	0.3135
C	-1.5329	3.2538	-0.3001	C	-1.1103	3.4998	-0.3684
C	-1.3076	3.5803	-1.7898	C	-0.8748	3.8062	-1.8614
C	-2.2913	4.6638	-2.3119	C	-1.7597	4.9788	-2.3691
C	-0.4254	2.4043	0.3097	C	-0.0949	2.5256	0.2163
C	0.975	3.0098	0.1074	C	1.3462	3.0185	0.0239
C	1.2292	3.2794	-1.3849	C	1.6293	3.2776	-1.4659
C	0.1249	4.1431	-1.9921	C	0.6033	4.2353	-2.0724
C	2.0376	2.1306	0.7278	C	2.3346	2.0578	0.6379
C	2.2104	1.933	2.034	C	2.6787	2.0171	1.9242
O	2.8913	1.448	-0.1368	O	2.9512	1.1443	-0.2149

C	-1.4991	2.2979	-2.6332	C	-1.1923	2.5521	-2.7095
C	-2.8694	3.4664	1.8223	C	-2.3386	3.8824	1.7839
O	-3.8884	3.8428	2.3931	O	-3.3375	4.2777	2.3753
O	-3.5781	-4.1065	-0.4077	O	-3.8947	-4.0096	0.4215
C	-3.7114	4.4331	-1.823	C	-3.1858	4.8872	-1.8509
H	5.161	1.8964	-1.5633	H	4.9679	1.2394	-2.0125
H	6.7649	1.9271	-0.8528	H	6.667	1.2596	-1.575
H	5.9153	1.18	1.3182	H	6.1524	0.8654	0.7894
H	5.0463	2.6087	0.773	H	5.277	2.2661	0.1869
H	6.7947	-0.4596	-0.5312	H	6.6489	-1.0572	-0.9271
H	6.4161	-0.1143	-2.2081	H	6.0062	-0.9181	-2.5525
H	2.9703	-2.6147	0.4715	H	2.9728	-2.8034	0.9583
H	2.1842	-1.335	1.3184	H	2.3889	-1.384	1.7503
H	1.3228	-0.3392	-0.7115	H	1.2228	-0.6063	-0.2287
H	2.6808	-2.4552	-2.4331	H	2.1876	-3.0303	-1.8113
H	1.7837	-1.0477	-2.9497	H	1.2869	-1.6524	-2.3982
H	3.5072	0.4575	-2.2399	H	3.1629	-0.1813	-2.2083
H	4.241	-0.7995	-3.1938	H	3.6712	-1.6099	-3.0617
H	4.4234	-3.1408	-1.1616	H	4.1013	-3.6423	-0.772
H	5.6668	-2.5439	-2.2597	H	5.1784	-3.2797	-2.1189
H	6.0013	-2.6733	-0.5348	H	5.7752	-3.1901	-0.4636
H	4.586	-1.1271	2.2006	H	4.8709	-1.2102	2.2001
H	1.5393	-4.2973	-0.6328	H	1.0987	-4.0071	1.5287
H	-2.2817	-0.7302	-2.7756	H	-1.8371	-2.4812	-3.0628
H	-3.1501	-1.6802	-3.9681	H	-2.509	-3.9793	-3.6834
H	-2.5301	-3.785	-2.8582	H	-2.3244	-5.0677	-1.4858
H	-1.103	-2.8296	-3.2383	H	-0.7716	-4.4202	-1.9999
H	-4.7422	-2.4698	-2.3517	H	-4.4701	-3.807	-2.3057
H	-4.6839	-0.7191	-2.2773	H	-4.2819	-2.3162	-3.2086
H	-3.3834	-3.1825	1.8901	H	-4.0908	-1.9527	1.8179
H	-1.7493	-3.6387	1.5546	H	-2.4622	-2.4304	2.1278
H	-1.0382	-1.2945	1.4051	H	-1.5858	-0.5078	0.8222
H	-2.5476	0.5903	1.7749	H	-2.9706	1.1556	-0.2038
H	-3.8984	-0.4684	2.0899	H	-4.4471	0.3709	0.2994
H	-4.037	0.4385	-0.1718	H	-4.0004	-0.1452	-2.0298
H	-2.4082	-0.0604	-0.5416	H	-2.3762	-0.6716	-1.6747
H	-0.6287	-0.4469	4.9882	H	-1.5127	0.8287	4.2473
H	-1.9349	-2.2981	5.3503	H	-3.7527	1.3676	3.9422
H	-2.8424	-3.193	4.0307	H	-4.7388	0.7872	2.5045
H	-5.1969	-2.0717	1.2174	H	-5.6358	-1.5143	0.2361
H	-5.9133	-1.0982	-0.0662	H	-5.9801	-1.4402	-1.4926
H	-5.7344	-2.8382	-0.2733	H	-5.9111	-2.9968	-0.6711
H	-4.7264	4.0686	0.0134	H	-4.1928	4.6352	0.0106
H	-3.7039	5.5066	0.04	H	-3.0358	5.9677	0.0029
H	-1.9726	5.6602	-1.9759	H	-1.3403	5.9409	-2.0441
H	-2.28	4.6952	-3.4086	H	-1.7673	5.0067	-3.466
H	-0.5769	2.245	1.3761	H	-0.2625	2.3369	1.277

H	-0.4653	1.4025	-0.1359	H	-0.2261	1.5474	-0.2637
H	1.0073	3.9789	0.6266	H	1.449	3.9797	0.5491
H	2.1916	3.7915	-1.5122	H	2.6328	3.7056	-1.5855
H	1.3031	2.3382	-1.9434	H	1.6242	2.3384	-2.0325
H	0.1957	5.1416	-1.5385	H	0.7667	5.2242	-1.6218
H	0.327	4.2781	-3.0625	H	0.8117	4.3492	-3.144
H	1.668	2.3083	2.8807	H	2.3425	2.5911	2.7655
H	-1.3786	2.5099	-3.7018	H	-1.0704	2.7616	-3.7785
H	-0.7776	1.5145	-2.381	H	-0.5382	1.7064	-2.4763
H	-2.4965	1.8676	-2.4917	H	-2.2215	2.2105	-2.5549
H	-2.0827	2.9507	2.3863	H	-1.5325	3.388	2.3394
H	-2.962	-4.8626	-0.3049	H	-3.3811	-4.5448	1.0635
H	-4.0941	3.4739	-2.1902	H	-3.6641	3.9656	-2.2019
H	-4.3758	5.2076	-2.2234	H	-3.7819	5.7183	-2.2451
3c-5	X axis(Å)	Y axis(Å)	Z axis(Å)	3c-6	X axis(Å)	Y axis(Å)	Z axis(Å)
C	5.3915	0.2841	-1.6008	C	2.0679	5.0719	0.1197
C	5.2368	0.4243	-0.0928	C	1.6224	4.4563	-1.2012
C	3.9117	-0.1796	0.3894	C	0.9173	3.1139	-0.9668
C	3.7591	-1.6858	-0.0226	C	-0.3233	3.2672	-0.0197
C	4.0054	-1.9042	-1.5649	C	0.0457	3.9862	1.3306
C	5.2987	-1.1751	-2.0287	C	0.8878	5.2671	1.0642
C	2.3999	-2.3114	0.3924	C	-1.0493	1.9299	0.2653
C	1.1902	-1.8834	-0.4616	C	-0.3401	0.9831	1.2493
C	1.47	-2.0375	-1.9634	C	0.0681	1.7163	2.5371
C	2.7937	-1.4056	-2.3911	C	0.8181	3.0229	2.2671
C	4.2327	-3.4073	-1.9003	C	-1.2271	4.4751	2.0829
C	3.8034	0.0199	1.8832	C	0.541	2.501	-2.2993
O	4.4439	-0.5746	2.7391	O	-0.3944	2.8365	-3.0124
O	4.7887	-2.4435	0.6585	O	-1.2839	4.1245	-0.6859
C	-0.1031	-2.5897	-0.1204	C	-1.1665	-0.2671	1.4849
O	-1.2525	-1.9818	-0.6318	O	-1.4498	-1.0208	0.3413
C	-0.2774	-3.6779	0.6272	C	-1.6392	-0.7309	2.641
C	-3.4432	-2.4923	-2.5575	C	-0.8787	-3.6264	-0.9041
C	-2.8322	-3.5119	-1.6041	C	-1.138	-3.3884	0.5792
C	-2.3715	-2.8362	-0.3076	C	-2.1219	-2.2287	0.775
C	-3.548	-2.0899	0.4149	C	-3.4915	-2.5112	0.057
C	-4.2986	-1.0916	-0.5469	C	-3.2981	-2.8625	-1.466
C	-4.6183	-1.7689	-1.9108	C	-2.1731	-3.9219	-1.6525
C	-3.1092	-1.3625	1.7125	C	-4.5285	-1.3714	0.2182
C	-2.3341	-0.0502	1.4993	C	-4.2474	-0.1154	-0.6241
C	-3.0744	0.8897	0.5351	C	-4.0232	-0.479	-2.1024
C	-3.4579	0.192	-0.7722	C	-2.9773	-1.5846	-2.2834
C	-1.9898	0.5683	2.8443	C	-5.3096	0.9437	-0.3774
C	-0.7504	0.0764	3.5154	C	-5.2304	1.6838	0.9195
C	-2.6762	1.5255	3.4894	C	-6.2931	1.3155	-1.2129
O	0.0206	-0.7171	2.9887	O	-4.3816	1.4432	1.7704
C	-5.6785	-0.6675	0.0377	C	-4.5784	-3.5118	-2.0703

C	-1.7192	-3.8597	0.5942	C	-2.3078	-1.9614	2.2505
O	-2.2985	-4.7263	1.2351	O	-2.9284	-2.6649	3.0359
C	-2.2858	4.2088	-1.9764	C	5.4078	-3.769	0.4087
C	-0.985	3.4461	-1.8877	C	4.226	-2.8661	0.1395
C	-0.033	3.7143	-0.9605	C	4.3146	-1.5163	0.0434
C	-0.1711	4.8843	0.0327	C	5.674	-0.794	0.1674
C	-1.4282	5.76	-0.2266	C	6.8748	-1.7775	0.0897
C	1.196	2.8577	-0.6951	C	3.1387	-0.5721	-0.1794
C	1.1123	2.2282	0.7151	C	3.3662	0.3787	-1.3673
C	0.9031	3.317	1.7877	C	4.6721	1.1644	-1.1933
C	-0.2545	4.2673	1.4522	C	5.8547	0.2188	-0.9955
C	2.2849	1.3138	1.0058	C	2.2067	1.3231	-1.5543
C	2.8041	1.027	2.1988	C	1.4491	1.4185	-2.6445
O	2.8356	0.6547	-0.0946	O	1.9097	2.1733	-0.4903
C	1.0382	5.8468	-0.0559	C	5.7331	-0.0528	1.5243
C	-0.8838	2.3289	-2.8799	C	2.9393	-3.6182	0.0094
O	-1.7925	2.0476	-3.6543	O	2.8821	-4.843	0.022
O	-4.5297	-3.079	0.8138	O	-4.0822	-3.6848	0.6693
C	-2.6269	4.9513	-0.6904	C	6.6444	-3.0351	0.9105
H	4.6341	0.8836	-2.1179	H	2.8331	4.4457	0.592
H	6.3646	0.6884	-1.9037	H	2.5397	6.0423	-0.0746
H	6.0842	-0.0577	0.4111	H	0.9614	5.1522	-1.7328
H	5.2878	1.4912	0.1602	H	2.5091	4.3227	-1.8342
H	6.1772	-1.6981	-1.6266	H	0.2424	6.0438	0.6315
H	5.3887	-1.2302	-3.1213	H	1.2569	5.6767	2.0134
H	2.5034	-3.4045	0.3616	H	-2.0544	2.1537	0.6444
H	2.1996	-2.0964	1.45	H	-1.2366	1.4108	-0.6831
H	0.9962	-0.8251	-0.2665	H	0.582	0.6264	0.7825
H	1.4598	-3.0985	-2.2427	H	-0.8141	1.9299	3.1524
H	0.6623	-1.5705	-2.5427	H	0.7104	1.0648	3.1438
H	2.6954	-0.3175	-2.3306	H	1.8055	2.7837	1.8606
H	2.9538	-1.6224	-3.4555	H	1.013	3.5156	3.2288
H	3.4022	-4.0428	-1.5819	H	-1.9353	3.668	2.2878
H	4.3548	-3.5496	-2.9808	H	-0.9591	4.9256	3.046
H	5.1389	-3.7968	-1.423	H	-1.7669	5.2391	1.5121
H	4.7395	-2.2494	1.6183	H	-1.484	3.7422	-1.566
H	0.4212	-4.3011	1.1509	H	-1.5789	-0.3454	3.6403
H	-2.6845	-1.771	-2.8814	H	-0.3753	-2.7596	-1.3469
H	-3.7886	-3.0053	-3.4627	H	-0.1935	-4.4743	-1.0199
H	-3.5597	-4.3047	-1.3895	H	-1.52	-4.3057	1.0441
H	-1.9854	-3.9926	-2.1108	H	-0.1807	-3.1672	1.0678
H	-5.4234	-2.5036	-1.7728	H	-2.5352	-4.9007	-1.309
H	-5.0082	-1.0239	-2.6164	H	-1.9463	-4.0428	-2.7197
H	-4.0013	-1.1583	2.3218	H	-5.527	-1.7561	-0.0333
H	-2.523	-2.0468	2.3394	H	-4.6185	-1.1117	1.28
H	-1.3825	-0.2738	1.0096	H	-3.3098	0.3283	-0.2882
H	-3.9782	1.3008	0.9966	H	-3.6936	0.4108	-2.6541

H	-2.4356	1.7496	0.3034	H	-4.9604	-0.7986	-2.571
H	-4.0192	0.9023	-1.3934	H	-2.9149	-1.8315	-3.3514
H	-2.5458	-0.0281	-1.3353	H	-1.9925	-1.1853	-2.0217
H	-0.5525	0.4834	4.5215	H	-5.9897	2.4689	1.0746
H	-2.3632	1.9233	4.4508	H	-7.0058	2.0969	-0.964
H	-3.5938	1.9416	3.0858	H	-6.4302	0.8486	-2.1826
H	-5.5993	-0.23	1.0363	H	-5.4663	-2.8843	-1.9589
H	-6.1614	0.076	-0.6076	H	-4.4472	-3.7027	-3.1421
H	-6.3654	-1.518	0.1137	H	-4.8052	-4.4753	-1.6
H	-2.221	4.9179	-2.8111	H	5.1471	-4.5301	1.1544
H	-3.1209	3.5316	-2.192	H	5.6546	-4.3001	-0.5197
H	-1.6933	6.3245	0.6762	H	7.0517	-2.0787	-0.9521
H	-1.2104	6.5104	-0.9996	H	7.7962	-1.2841	0.4238
H	1.3038	2.0605	-1.432	H	2.1988	-1.0999	-0.3522
H	2.1066	3.4588	-0.7995	H	2.9825	0.0013	0.7433
H	0.2214	1.5852	0.7216	H	3.4623	-0.2358	-2.2744
H	0.6884	2.8532	2.7585	H	4.8564	1.7844	-2.08
H	1.8258	3.8948	1.9216	H	4.6025	1.856	-0.3448
H	-1.1929	3.7085	1.5601	H	6.0055	-0.3265	-1.9376
H	-0.2848	5.0624	2.2081	H	6.7638	0.8135	-0.8378
H	2.5416	1.353	3.1862	H	1.4721	0.8784	-3.5712
H	0.8992	6.7068	0.6102	H	6.7056	0.4334	1.6634
H	1.986	5.3808	0.2269	H	4.9712	0.7282	1.6104
H	1.1587	6.2319	-1.0755	H	5.5816	-0.7374	2.366
H	0.0538	1.7601	-2.9025	H	2.0244	-3.0268	-0.1049
H	-4.0739	-3.7872	1.3164	H	-4.129	-3.5391	1.6381
H	-3.4803	5.6162	-0.8664	H	6.53	-2.7864	1.9717
H	-2.9347	4.2428	0.0873	H	7.5168	-3.6949	0.8373
3c-7	X axis(Å)	Y axis(Å)	Z axis(Å)	3c-8	X axis(Å)	Y axis(Å)	Z axis(Å)
C	2.9038	3.7723	2.4549	C	2.0743	5.002	0.3869
C	3.1621	4.0548	0.9809	C	1.4998	4.4882	-0.9277
C	2.1763	3.2925	0.0882	C	0.7986	3.1377	-0.729
C	0.6809	3.6189	0.4387	C	-0.344	3.2263	0.3401
C	0.381	3.4249	1.974	C	0.1561	3.8484	1.6988
C	1.4706	4.1186	2.8407	C	0.9887	5.1384	1.4472
C	-0.3421	2.816	-0.4078	C	-1.0442	1.872	0.5995
C	-0.4844	1.3325	-0.0242	C	-0.2828	0.8622	1.4704
C	-0.7108	1.1479	1.4829	C	0.2435	1.5089	2.7597
C	0.2984	1.9197	2.3341	C	0.9929	2.8184	2.5009
C	-0.9648	4.0924	2.381	C	-1.04	4.2957	2.5913
C	2.5024	3.576	-1.3601	C	0.3288	2.6173	-2.0748
O	2.2842	4.6201	-1.9584	O	-0.5818	3.0512	-2.7635
O	0.449	5.0191	0.1543	O	-1.3484	4.1355	-0.1649
C	-1.5477	0.676	-0.872	C	-1.1493	-0.363	1.6917
O	-2.8534	0.6748	-0.3868	O	-1.4331	-1.1059	0.541
C	-1.3244	0.0679	-2.0355	C	-1.6759	-0.8017	2.8336
C	-5.5887	1.6226	-0.9529	C	-0.8942	-3.7852	-0.6166

C	-4.5794	1.1391	-1.988	C	-1.217	-3.4852	0.8418
C	-3.6809	0.0482	-1.3958	C	-2.1651	-2.2844	0.955
C	-4.5174	-1.1787	-0.8797	C	-3.5027	-2.5269	0.167
C	-5.6539	-0.7433	0.1201	C	-3.2413	-2.9417	-1.3305
C	-6.448	0.4734	-0.4386	C	-2.1614	-4.0584	-1.4167
C	-3.6499	-2.3028	-0.2552	C	-4.4991	-1.3385	0.2225
C	-3.0992	-1.9948	1.1478	C	-4.1323	-0.128	-0.6593
C	-4.2221	-1.5472	2.0986	C	-3.8034	-0.5523	-2.0986
C	-5.0587	-0.4052	1.5114	C	-2.808	-1.7126	-2.1676
C	-2.2544	-3.1528	1.6509	C	-5.1642	0.991	-0.6656
C	-0.8581	-3.2519	1.1236	C	-4.6752	2.3696	-0.9759
C	-2.615	-4.0857	2.547	C	-6.4756	0.8816	-0.3957
O	-0.3802	-2.4334	0.3441	O	-3.4956	2.6281	-1.1849
C	-6.7099	-1.8724	0.3105	C	-4.5151	-3.5487	-1.9896
C	-2.6513	-0.3816	-2.4175	C	-2.414	-1.9827	2.4148
O	-2.8681	-1.0347	-3.4292	O	-3.1427	-2.613	3.1683
C	3.9383	-4.4785	0.8159	C	5.3377	-3.7708	0.1988
C	3.5816	-3.0115	0.8823	C	4.1493	-2.8454	0.076
C	4.1412	-2.0676	0.0853	C	4.2507	-1.5058	-0.1087
C	5.1326	-2.4446	-1.0331	C	5.6282	-0.8181	-0.2221
C	5.1877	-3.9779	-1.2826	C	6.7802	-1.8378	-0.4406
C	3.8692	-0.5718	0.1732	C	3.0718	-0.5439	-0.2073
C	3.362	0.0084	-1.1634	C	3.1472	0.369	-1.4442
C	4.3793	-0.2948	-2.2769	C	4.4817	1.1227	-1.4862
C	4.6854	-1.7907	-2.368	C	5.6564	0.1492	-1.4354
C	3.0091	1.4791	-1.0488	C	1.9998	1.3453	-1.4942
C	3.0912	2.4089	-1.9991	C	1.1564	1.501	-2.5109
O	2.4818	1.8833	0.1783	O	1.8219	2.1662	-0.384
C	6.5512	-1.9592	-0.655	C	5.9065	-0.0321	1.0815
C	2.5405	-2.712	1.9173	C	2.8413	-3.5582	0.2107
O	2.0627	-3.5779	2.6456	O	2.7531	-4.7798	0.2699
O	-5.1916	-1.7707	-2.019	O	-4.1826	-3.6508	0.7811
C	5.2004	-4.7703	0.0139	C	6.6552	-3.0537	0.462
H	3.1175	2.7221	2.6829	H	2.8697	4.3365	0.741
H	3.5954	4.3667	3.0635	H	2.5413	5.9797	0.2197
H	3.093	5.134	0.7944	H	0.8035	5.2264	-1.3448
H	4.1948	3.7626	0.7505	H	2.3229	4.3932	-1.6477
H	1.358	5.2088	2.7649	H	0.3182	5.9493	1.1311
H	1.3197	3.8726	3.8997	H	1.4484	5.4764	2.3849
H	-1.3242	3.3047	-0.3384	H	-2.0249	2.0652	1.0566
H	-0.0872	2.9023	-1.4724	H	-1.2812	1.4079	-0.3653
H	0.4472	0.8134	-0.2628	H	0.5899	0.5076	0.9159
H	-1.7261	1.4515	1.7638	H	-0.5774	1.7006	3.4604
H	-0.6306	0.085	1.7392	H	0.9195	0.811	3.2705
H	1.2754	1.4363	2.2395	H	1.9351	2.5919	1.993
H	0.0215	1.8039	3.3903	H	1.2825	3.2481	3.4689
H	-1.8154	3.714	1.8078	H	-1.7461	3.4852	2.7904

H	-1.182	3.9129	3.4408	H	-0.6843	4.6653	3.5604
H	-0.9374	5.1787	2.2403	H	-1.6092	5.11	2.1288
H	0.7274	5.2063	-0.7665	H	-1.8997	3.6588	-0.8295
H	-0.4173	-0.084	-2.587	H	-1.6304	-0.4168	3.8341
H	-5.0739	2.1131	-0.119	H	-0.336	-2.9542	-1.0622
H	-6.2356	2.3826	-1.4066	H	-0.2384	-4.6621	-0.669
H	-5.1041	0.77	-2.8779	H	-1.6574	-4.3716	1.3153
H	-3.9787	1.9988	-2.3122	H	-0.2766	-3.2853	1.3707
H	-7.0847	0.1411	-1.2701	H	-2.5856	-5.0043	-1.0528
H	-7.1321	0.8577	0.329	H	-1.8877	-4.2348	-2.465
H	-2.8298	-2.556	-0.9389	H	-5.4886	-1.7191	-0.0608
H	-4.2412	-3.2285	-0.2137	H	-4.6306	-1.0092	1.2615
H	-2.4236	-1.1419	1.0813	H	-3.2287	0.2981	-0.2234
H	-3.7874	-1.2133	3.0495	H	-3.3799	0.2952	-2.6526
H	-4.8847	-2.3841	2.344	H	-4.7237	-0.8236	-2.6305
H	-5.8674	-0.1698	2.2156	H	-2.6864	-2.0025	-3.2196
H	-4.4415	0.4975	1.4666	H	-1.8247	-1.349	-1.8535
H	-0.2717	-4.1168	1.4774	H	-5.4444	3.1602	-1.0005
H	-1.9402	-4.8747	2.8691	H	-7.1483	1.735	-0.411
H	-3.6027	-4.1005	2.9953	H	-6.9373	-0.0707	-0.1564
H	-6.2686	-2.8135	0.6487	H	-5.3726	-2.8715	-1.96
H	-7.4616	-1.5792	1.0531	H	-4.3286	-3.7901	-3.0429
H	-7.2476	-2.0864	-0.6201	H	-4.8218	-4.4789	-1.4984
H	4.0837	-4.8834	1.8249	H	5.1819	-4.4901	1.0122
H	3.0937	-5.0198	0.3704	H	5.4206	-4.3498	-0.73
H	4.3163	-4.3	-1.8692	H	6.7847	-2.1865	-1.4826
H	6.0691	-4.2379	-1.8822	H	7.7529	-1.3572	-0.2765
H	3.1527	-0.3371	0.9611	H	2.1111	-1.0613	-0.2449
H	4.7916	-0.0592	0.4756	H	3.0475	0.0574	0.7106
H	2.4246	-0.5112	-1.4115	H	3.0953	-0.2728	-2.336
H	3.9875	0.0303	-3.2486	H	4.5493	1.7128	-2.4092
H	5.3065	0.2669	-2.1099	H	4.5524	1.8391	-0.6586
H	3.7763	-2.2892	-2.7329	H	5.6495	-0.431	-2.3687
H	5.4505	-1.9508	-3.1387	H	6.5932	0.7212	-1.4381
H	3.419	2.3566	-3.0196	H	1.0907	1.001	-3.458
H	7.2846	-2.2655	-1.41	H	6.8966	0.4373	1.0525
H	6.616	-0.8698	-0.5751	H	5.1785	0.767	1.2536
H	6.875	-2.3703	0.3075	H	5.8745	-0.6833	1.9618
H	2.1928	-1.6747	1.9972	H	1.939	-2.9387	0.2622
H	-4.5249	-1.9602	-2.7126	H	-4.2655	-3.4807	1.7433
H	6.089	-4.5239	0.6064	H	6.719	-2.7587	1.5156
H	5.2566	-5.8432	-0.2031	H	7.4892	-3.7416	0.2806
3c-9	X axis(Å)	Y axis(Å)	Z axis(Å)	3c-10	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-2.7716	4.9107	-0.1837	C	-2.2119	5.1543	-1.1113
C	-2.167	4.4021	1.1194	C	-2.3095	4.5542	0.2855
C	-1.184	3.2529	0.8538	C	-1.2451	3.4669	0.4936
C	-0.0336	3.6897	-0.1156	C	0.2035	4.0227	0.2671

C	-0.587	4.3163	-1.4509	C	0.3464	4.7302	-1.1332
C	-1.6891	5.373	-1.1516	C	-0.824	5.7274	-1.3707
C	0.9689	2.5538	-0.4309	C	1.3222	2.9651	0.4481
C	0.4643	1.4886	-1.4146	C	1.4683	1.9599	-0.7062
C	-0.1258	2.1106	-2.6885	C	1.4907	2.636	-2.0851
C	-1.1446	3.2122	-2.3861	C	0.3904	3.6802	-2.2713
C	0.5259	5.0848	-2.2227	C	1.644	5.5862	-1.2131
C	-0.6611	2.721	2.1723	C	-1.4148	2.8655	1.8693
O	0.2143	3.2209	2.865	O	-1.0633	3.3731	2.9256
O	0.7168	4.739	0.542	O	0.4519	5.0458	1.2635
C	1.5511	0.4791	-1.7045	C	2.688	1.0752	-0.5698
O	1.4713	-0.7174	-0.9888	O	2.4899	-0.2826	-0.8304
C	2.5683	0.6138	-2.5543	C	3.9219	1.4568	-0.2427
C	0.9864	-3.5948	-1.4678	C	3.239	-2.2439	-2.9278
C	1.8151	-2.6714	-2.3506	C	4.1375	-1.1564	-2.3523
C	2.5045	-1.5898	-1.5082	C	3.7999	-0.8968	-0.8785
C	3.432	-2.2153	-0.4057	C	3.9387	-2.1967	-0.0114
C	2.666	-3.2649	0.485	C	3.1273	-3.4068	-0.6103
C	1.8479	-4.2525	-0.3968	C	3.3742	-3.5414	-2.1406
C	4.1328	-1.1604	0.4891	C	3.5732	-1.9893	1.4822
C	3.2285	-0.4808	1.5351	C	2.0644	-1.8821	1.7879
C	2.4637	-1.5255	2.366	C	1.3016	-3.0594	1.1612
C	1.7321	-2.5458	1.491	C	1.6149	-3.2405	-0.3254
C	4.0231	0.5221	2.358	C	1.7333	-1.7604	3.2698
C	4.3783	1.8094	1.6879	C	0.3851	-1.2245	3.6258
C	4.4152	0.396	3.6364	C	2.5353	-2.0502	4.3081
O	4.0764	2.0546	0.5259	O	-0.45	-0.9068	2.7874
C	3.6536	-4.1563	1.2945	C	3.5856	-4.7639	0.0018
C	3.2633	-0.6556	-2.4237	C	4.6733	0.2186	-0.3489
O	4.3161	-0.9054	-2.9946	O	5.8519	0.1261	-0.0347
C	-4.2647	-4.5247	0.0629	C	-6.2461	-3.2262	-1.0498
C	-3.276	-3.4173	0.3472	C	-5.6785	-2.035	-0.3118
C	-3.5394	-2.1023	0.1478	C	-4.3502	-1.7984	-0.1747
C	-4.9383	-1.628	-0.3024	C	-3.3006	-2.7354	-0.8092
C	-6.0003	-2.761	-0.2312	C	-3.9295	-3.7232	-1.8309
C	-2.5424	-0.9623	0.3297	C	-3.7381	-0.6349	0.5976
C	-3.0668	0.111	1.2972	C	-2.7369	0.1749	-0.2508
C	-4.4332	0.641	0.8352	C	-1.6408	-0.7442	-0.8029
C	-5.4337	-0.4964	0.6389	C	-2.2392	-1.9112	-1.5856
C	-2.083	1.2424	1.4569	C	-2.1282	1.3567	0.4711
C	-1.3508	1.4928	2.54	C	-2.0691	1.5711	1.7845
O	-1.9503	2.1184	0.3805	O	-1.5857	2.3451	-0.3542
C	-4.8681	-1.1154	-1.76	C	-2.6159	-3.5563	0.3078
C	-1.9726	-3.925	0.8754	C	-6.7404	-1.1541	0.2694
O	-1.73	-5.1189	1.0138	O	-7.9368	-1.3433	0.0747
O	4.4875	-2.9494	-1.0741	O	5.331	-2.6025	-0.0366
C	-5.4671	-4.0815	-0.7603	C	-5.2295	-4.3262	-1.3259

H	-3.3876	4.1314	-0.6465	H	-2.4593	4.4001	-1.8666
H	-3.4447	5.7486	0.0327	H	-2.9575	5.9514	-1.2155
H	-1.6658	5.2247	1.6447	H	-2.2038	5.3458	1.038
H	-2.9862	4.0704	1.7703	H	-3.3176	4.1384	0.4103
H	-1.2251	6.2725	-0.7241	H	-0.697	6.6009	-0.7164
H	-2.1636	5.6949	-2.0875	H	-0.7858	6.1123	-2.3979
H	1.8931	3.0016	-0.821	H	2.2699	3.4965	0.606
H	1.2841	2.0731	0.5028	H	1.1752	2.4187	1.3892
H	-0.3464	0.9298	-0.9374	H	0.5987	1.2984	-0.672
H	0.6653	2.52	-3.3271	H	2.4651	3.1087	-2.2621
H	-0.6157	1.3294	-3.2841	H	1.3875	1.8733	-2.8684
H	-2.0435	2.7535	-1.963	H	-0.5688	3.1644	-2.3731
H	-1.467	3.657	-3.3367	H	0.549	4.1823	-3.2349
H	1.3917	4.4584	-2.453	H	2.5493	5.0028	-1.0255
H	0.1416	5.4719	-3.1739	H	1.7496	6.0382	-2.2066
H	0.894	5.9455	-1.653	H	1.633	6.4075	-0.4879
H	1.0805	4.3796	1.3779	H	0.2615	4.6696	2.1492
H	2.8594	1.4315	-3.1849	H	4.3256	2.421	-3.00E-04
H	0.1645	-3.0368	-1.0072	H	2.195	-1.9111	-2.9365
H	0.5239	-4.3717	-2.0878	H	3.5149	-2.4252	-3.9733
H	2.5549	-3.2557	-2.912	H	5.1904	-1.4447	-2.4629
H	1.1475	-2.2158	-3.0934	H	3.9989	-0.245	-2.9479
H	2.5362	-4.9419	-0.9049	H	4.3879	-3.9284	-2.3132
H	1.2089	-4.8795	0.238	H	2.6907	-4.2876	-2.566
H	4.9798	-1.6356	1.004	H	4.0053	-2.8248	2.0484
H	4.6138	-0.4088	-0.1486	H	4.0922	-1.1059	1.876
H	2.4612	0.101	1.0178	H	1.7031	-0.9589	1.3231
H	1.7296	-1.0199	3.0065	H	0.2227	-2.9091	1.2657
H	3.1408	-2.0601	3.0412	H	1.5221	-3.9854	1.7061
H	1.2507	-3.2836	2.1461	H	1.0662	-4.1182	-0.6916
H	0.914	-2.0376	0.9729	H	1.2035	-2.3898	-0.8775
H	4.9357	2.5375	2.3012	H	0.1736	-1.1276	4.7044
H	4.9706	1.1725	4.1554	H	2.2246	-1.9208	5.3415
H	4.2026	-0.494	4.2191	H	3.5403	-2.4362	4.1722
H	4.3342	-3.5746	1.9215	H	3.5153	-4.7831	1.0924
H	3.1067	-4.8404	1.9543	H	2.971	-5.5883	-0.3789
H	4.2737	-4.7752	0.6363	H	4.625	-4.9953	-0.257
H	-3.776	-5.3455	-0.4763	H	-7.0716	-3.672	-0.4813
H	-4.6133	-4.9314	1.021	H	-6.6648	-2.8742	-2.0015
H	-6.3228	-2.9159	0.8077	H	-4.1397	-3.2072	-2.7778
H	-6.9017	-2.4776	-0.789	H	-3.2214	-4.5258	-2.0728
H	-1.5681	-1.3032	0.685	H	-4.4925	0.0583	0.9741
H	-2.3406	-0.5195	-0.654	H	-3.2436	-1.0395	1.4895
H	-3.2085	-0.3635	2.2794	H	-3.299	0.5845	-1.1033
H	-4.8314	1.3427	1.5793	H	-1.0096	-1.1195	0.0102
H	-4.338	1.2073	-0.0993	H	-0.9802	-0.1841	-1.4754
H	-5.6583	-0.9148	1.63	H	-2.6928	-1.4973	-2.497

H	-6.3768	-0.0803	0.2618	H	-1.4261	-2.5676	-1.9219
H	-1.2723	0.9754	3.4765	H	-2.3858	0.9719	2.6163
H	-5.8604	-0.8191	-2.1193	H	-1.873	-4.2457	-0.1097
H	-4.218	-0.242	-1.8697	H	-2.0956	-2.9224	1.0312
H	-4.4853	-1.8844	-2.4399	H	-3.3392	-4.1522	0.8749
H	-1.2266	-3.1765	1.1631	H	-6.4112	-0.3114	0.8889
H	4.9277	-2.3488	-1.7127	H	5.8861	-1.839	0.23
H	-5.1878	-3.9887	-1.8161	H	-5.0543	-4.9134	-0.4173
H	-6.2486	-4.8485	-0.71	H	-5.6344	-5.0202	-2.0716
3c-11	X axis(Å)	Y axis(Å)	Z axis(Å)	3c-12	X axis(Å)	Y axis(Å)	Z axis(Å)
C	4.6198	-3.1791	-0.7886	C	-2.1428	4.9962	-1.5178
C	4.0349	-3.1056	0.6161	C	-2.3973	4.553	-0.082
C	2.6114	-2.528	0.5897	C	-1.3602	3.5089	0.3582
C	1.6602	-3.3748	-0.3219	C	0.0982	4.0676	0.2457
C	2.2497	-3.558	-1.7706	C	0.4058	4.6227	-1.1947
C	3.7369	-4.0112	-1.7104	C	-0.7366	5.5602	-1.6823
C	0.2099	-2.835	-0.3965	C	1.1955	3.065	0.6763
C	-0.0041	-1.6027	-1.2935	C	1.4996	1.9339	-0.3229
C	0.6932	-1.7197	-2.659	C	1.685	2.4639	-1.7544
C	2.1271	-2.2409	-2.5768	C	0.6052	3.4548	-2.192
C	1.5055	-4.679	-2.5533	C	1.6936	5.4976	-1.2114
C	2.0961	-2.4163	2.0075	C	-1.6836	3.0373	1.7566
O	1.6927	-3.3436	2.6965	O	-1.4751	3.6541	2.7923
O	1.5648	-4.7051	0.2469	O	0.2106	5.1982	1.1473
C	-1.4818	-1.3265	-1.4903	C	2.714	1.1047	0.0532
O	-1.9625	-0.1	-1.0261	O	2.8496	-0.1067	-0.633
C	-2.3614	-2.1484	-2.0621	C	3.6486	1.3899	0.9592
C	-3.1504	2.426	-2.095	C	4.645	-1.3912	-2.6199
C	-3.413	1.0147	-2.6018	C	5.0747	-0.4943	-1.4657
C	-3.346	-5.00E-04	-1.454	C	4.1343	-0.6627	-0.2665
C	-4.3626	0.3441	-0.3062	C	4.0738	-2.1517	0.2261
C	-4.2254	1.8318	0.1914	C	3.7396	-3.1534	-0.9438
C	-4.1464	2.8169	-1.0104	C	4.6124	-2.855	-2.1969
C	-4.2942	-0.634	0.8973	C	3.1038	-2.3649	1.4174
C	-3.0821	-0.4449	1.8336	C	1.6108	-2.3715	1.0486
C	-2.96	1.0219	2.2764	C	1.318	-3.3331	-0.1133
C	-2.9774	1.9877	1.0911	C	2.2358	-3.0851	-1.3123
C	-3.0658	-1.3738	3.0392	C	0.7674	-2.6412	2.2823
C	-1.7509	-1.5621	3.7223	C	0.113	-1.4764	2.9459
C	-4.0947	-2.0768	3.5403	C	0.5549	-3.8457	2.838
O	-0.7355	-0.9734	3.3706	O	0.1808	-0.3328	2.5113
C	-5.4698	2.2809	1.013	C	4.0723	-4.6226	-0.5478
C	-3.5942	-1.3867	-2.0058	C	4.5614	0.2667	0.8455
O	-4.6739	-1.8461	-2.3515	O	5.5299	0.1168	1.5779
C	1.9468	5.694	-0.3544	C	-6.3263	-3.2581	-0.9666
C	1.5674	4.2432	-0.1715	C	-5.7626	-2.0503	-0.252
C	2.465	3.2329	-0.0588	C	-4.4354	-1.7932	-0.1408

C	3.9825	3.51	-0.1066	C	-3.3849	-2.7213	-0.7862
C	4.3136	5.0199	0.0539	C	-4.0189	-3.7192	-1.7944
C	2.1082	1.7573	0.1041	C	-3.8275	-0.6138	0.6092
C	2.8505	1.0853	1.2747	C	-2.8462	0.1982	-0.2601
C	4.3654	1.291	1.1553	C	-1.7436	-0.7157	-0.807
C	4.7072	2.7739	1.0502	C	-2.3432	-1.889	-1.5813
C	2.5497	-0.3887	1.3681	C	-2.2564	1.4065	0.4315
C	2.1637	-1.0372	2.4649	C	-2.3207	1.7301	1.7224
O	2.708	-1.1378	0.2037	O	-1.6003	2.3078	-0.4106
C	4.538	3.0257	-1.4673	C	-2.6789	-3.5303	0.3267
C	0.0887	4.0257	-0.1633	C	-6.8288	-1.1774	0.3347
O	-0.7197	4.9473	-0.1392	O	-8.0251	-1.4031	0.1848
O	-5.7041	0.2324	-0.8463	O	5.3923	-2.5221	0.7014
C	3.3958	5.9049	-0.7725	C	-5.2978	-4.3422	-1.2611
H	4.7537	-2.1713	-1.1976	H	-2.2981	4.1587	-2.2072
H	5.6188	-3.6284	-0.7417	H	-2.875	5.7638	-1.7948
H	4.0378	-4.1032	1.073	H	-2.3783	5.423	0.5862
H	4.6959	-2.4802	1.23	H	-3.4125	4.1396	-0.0257
H	3.7867	-5.0535	-1.3667	H	-0.6928	6.5066	-1.1259
H	4.1717	-4.0053	-2.7183	H	-0.5811	5.8234	-2.7365
H	-0.4393	-3.6557	-0.7319	H	2.11	3.64	0.8737
H	-0.1626	-2.6159	0.6131	H	0.9455	2.6312	1.6534
H	0.4249	-0.7355	-0.7793	H	0.646	1.2481	-0.3196
H	0.1229	-2.3717	-3.3319	H	2.6705	2.9366	-1.8551
H	0.7026	-0.7356	-3.1461	H	1.6892	1.623	-2.4607
H	2.7642	-1.456	-2.1596	H	-0.3283	2.9082	-2.3544
H	2.4976	-2.3954	-3.5989	H	0.8795	3.8515	-3.1785
H	0.4296	-4.5006	-2.6294	H	2.5768	4.9607	-0.8558
H	1.8943	-4.7619	-3.5752	H	1.913	5.8443	-2.2283
H	1.6369	-5.6588	-2.0806	H	1.5851	6.3905	-0.5856
H	1.3102	-4.6199	1.1907	H	-0.0578	4.905	2.0441
H	-2.2423	-3.1305	-2.4784	H	3.7704	2.2248	1.6218
H	-2.1255	2.5074	-1.7195	H	3.6637	-1.0824	-2.9973
H	-3.2305	3.1316	-2.9303	H	5.3483	-1.2712	-3.4523
H	-4.3917	0.9744	-3.0964	H	6.1092	-0.7234	-1.1811
H	-2.6646	0.7796	-3.3694	H	5.0697	0.5455	-1.8175
H	-5.1355	2.8954	-1.4823	H	5.648	-3.1662	-2.0023
H	-3.9026	3.8255	-0.6523	H	4.27	-3.462	-3.0449
H	-5.2236	-0.5242	1.4715	H	3.3613	-3.3112	1.9137
H	-4.3248	-1.6708	0.5381	H	3.2903	-1.6097	2.1921
H	-2.1869	-0.6959	1.2562	H	1.3396	-1.3787	0.6813
H	-2.0246	1.1803	2.8263	H	1.4103	-4.3779	0.2018
H	-3.763	1.2733	2.9798	H	0.2787	-3.2108	-0.4362
H	-2.9157	3.0144	1.4747	H	2.0062	-3.8296	-2.0858
H	-2.064	1.8329	0.5116	H	1.9821	-2.1173	-1.7561
H	-1.7412	-2.2651	4.5724	H	-0.4554	-1.7036	3.8638
H	-3.9901	-2.7317	4.4012	H	-0.0583	-3.9841	3.7238

H	-5.0915	-2.0232	3.1147	H	1.007	-4.7444	2.4285
H	-5.6724	1.6292	1.8668	H	3.5661	-4.9395	0.3678
H	-5.3307	3.296	1.4038	H	3.7738	-5.316	-1.3431
H	-6.3772	2.2975	0.3988	H	5.1466	-4.7661	-0.3865
H	1.3095	6.1653	-1.1128	H	-7.1291	-3.7142	-0.3743
H	1.7628	6.22	0.5912	H	-6.7749	-2.9212	-1.9101
H	4.2171	5.3189	1.1068	H	-4.2568	-3.2068	-2.7368
H	5.3576	5.2141	-0.2229	H	-3.3036	-4.5108	-2.051
H	1.0402	1.5987	0.2678	H	-4.5872	0.0723	0.9879
H	2.3404	1.2477	-0.8399	H	-3.3136	-1.001	1.4986
H	2.5159	1.5689	2.204	H	-3.4202	0.5845	-1.1158
H	4.8702	0.8729	2.0358	H	-1.0826	-0.1563	-1.4807
H	4.766	0.751	0.2885	H	-1.1135	-1.0832	0.0096
H	4.447	3.2458	2.0078	H	-2.8156	-1.4797	-2.4854
H	5.7942	2.8818	0.9416	H	-1.5317	-2.5387	-1.9324
H	1.9573	-0.6864	3.4578	H	-2.7464	1.2239	2.5663
H	5.6101	3.2381	-1.5511	H	-1.9697	-4.2491	-0.099
H	4.4126	1.9482	-1.6127	H	-2.1162	-2.8915	1.0133
H	4.0365	3.5178	-2.3078	H	-3.3949	-4.0944	0.9345
H	-0.2581	2.9876	-0.1919	H	-6.5029	-0.3068	0.916
H	-5.8009	-0.6428	-1.2778	H	5.69	-1.8532	1.3543
H	3.5142	5.6907	-1.8408	H	-5.0938	-4.9237	-0.3549
H	3.6674	6.9579	-0.6344	H	-5.7068	-5.045	-1.9963
3d-1	X axis(Å)	Y axis(Å)	Z axis(Å)	3d-2	X axis(Å)	Y axis(Å)	Z axis(Å)
C	5.5594	1.3904	0.9978	C	-2.6912	5.0272	0.2562
C	5.2394	1.2256	-0.4824	C	-2.1723	4.5989	-1.1114
C	3.9399	0.4312	-0.6769	C	-1.1199	3.4894	-0.9705
C	4.0165	-0.9815	-0.0024	C	0.0884	3.9531	-0.0883
C	4.441	-0.8924	1.5115	C	-0.3811	4.4922	1.3134
C	5.6753	0.0378	1.6893	C	-1.5555	5.5009	1.1551
C	2.7174	-1.8117	-0.1509	C	1.1821	2.8736	0.0893
C	1.5564	-1.4054	0.7732	C	0.8473	1.7329	1.0672
C	2.0031	-1.2417	2.2338	C	0.2976	2.2664	2.4011
C	3.2613	-0.3843	2.3781	C	-0.8024	3.3164	2.2311
C	4.8858	-2.2797	2.0615	C	0.7512	5.286	2.0289
C	3.6269	0.341	-2.1533	C	-0.6859	3.0251	-2.3421
O	4.1557	-0.4091	-2.9616	O	0.0955	3.5993	-3.0874
O	5.0607	-1.7341	-0.6689	O	0.7244	5.0682	-0.7612
C	0.4214	-2.3901	0.5924	C	2.0715	0.8506	1.2176
O	-0.492	-2.0817	-0.4202	O	2.4689	0.1788	0.0566
C	0.2016	-3.5037	1.2902	C	2.8016	0.6425	2.3125
C	-1.3615	-3.0976	-3.0588	C	4.7012	0.2087	-1.8933
C	-1.005	-3.9475	-1.8453	C	4.8265	0.3689	-0.3831
C	-1.3782	-3.2207	-0.5474	C	3.7447	-0.442	0.3404
C	-2.9076	-2.8661	-0.4975	C	3.8131	-1.9657	-0.0275
C	-3.3821	-2.0846	-1.7812	C	3.7996	-2.2058	-1.5849
C	-2.8475	-2.7612	-3.0765	C	4.8023	-1.2561	-2.3019

C	-3.3188	-2.1022	0.7885	C	2.7105	-2.8096	0.6606
C	-2.912	-0.6186	0.8219	C	1.3048	-2.667	0.0527
C	-3.3865	0.1053	-0.447	C	1.3257	-2.8869	-1.4677
C	-2.9239	-0.6053	-1.7214	C	2.3731	-2.0093	-2.1592
C	-3.363	0.0239	2.1226	C	0.3333	-3.5549	0.8102
C	-2.5096	-0.2298	3.3235	C	-0.3315	-2.9573	2.0054
C	-4.4203	0.8312	2.3049	C	0.0093	-4.8239	0.5148
O	-1.4971	-0.9197	3.2729	O	-0.1892	-1.7809	2.3203
C	-4.9341	-2.1031	-1.9178	C	4.2675	-3.6478	-1.9426
C	-0.9704	-4.0623	0.6406	C	3.8609	-0.2273	1.8319
O	-1.5296	-5.0792	1.0281	O	4.7141	-0.7096	2.5643
C	-2.6426	4.6376	1.5141	C	-4.7808	-3.241	1.5641
C	-1.5818	3.6033	1.2136	C	-3.8243	-2.1072	1.2688
C	-1.0488	3.4084	-0.0182	C	-3.4091	-1.7813	0.0194
C	-1.4421	4.3042	-1.2122	C	-3.955	-2.5181	-1.2232
C	-2.2246	5.5693	-0.7637	C	-5.1907	-3.3994	-0.89
C	-0.0429	2.3191	-0.3724	C	-2.3999	-0.6858	-0.3088
C	1.2139	2.88	-1.0595	C	-2.9526	0.3218	-1.3322
C	0.8201	3.6925	-2.3031	C	-3.3847	-0.4105	-2.6117
C	-0.1657	4.8029	-1.9415	C	-4.4148	-1.4944	-2.296
C	2.2134	1.7803	-1.337	C	-1.984	1.4577	-1.5695
C	2.5856	1.2885	-2.5176	C	-1.3411	1.7733	-2.6926
O	2.8442	1.2527	-0.2073	O	-1.7943	2.3078	-0.478
C	-2.3274	3.5056	-2.1979	C	-2.8521	-3.4272	-1.8111
C	-1.1882	2.8088	2.4209	C	-3.3839	-1.389	2.5099
O	-1.7727	2.9092	3.4957	O	-3.7702	-1.7209	3.6267
O	-3.6547	-4.1087	-0.4923	O	5.0812	-2.4852	0.4447
C	-3.2857	5.2491	0.2762	C	-5.0017	-4.1897	0.3935
H	6.5056	1.9337	1.1052	H	-3.4158	5.8401	0.1301
H	4.7939	2.0033	1.4867	H	-3.2325	4.2022	0.7329
H	5.1538	2.2251	-0.928	H	-3.0256	4.2523	-1.7084
H	6.075	0.7285	-0.991	H	-1.7536	5.4641	-1.6405
H	5.8712	0.2005	2.757	H	-1.9657	5.7558	2.1408
H	6.5691	-0.4623	1.2917	H	-1.173	6.4416	0.7356
H	2.3796	-1.7921	-1.1956	H	1.4475	2.4559	-0.8909
H	2.9605	-2.8707	0.0181	H	2.1108	3.365	0.4144
H	1.1762	-0.4315	0.4499	H	0.0693	1.1034	0.6227
H	1.1946	-0.7785	2.8126	H	-0.1005	1.4309	2.9916
H	2.1848	-2.2151	2.7025	H	1.1026	2.7029	3.0037
H	3.554	-0.3737	3.4363	H	-1.0715	3.6992	3.2245
H	3.0104	0.6532	2.138	H	-1.7063	2.8248	1.8599
H	5.7882	-2.6447	1.5583	H	1.0269	6.1889	1.4725
H	5.1196	-2.2161	3.1309	H	0.4273	5.6104	3.025
H	4.1189	-3.0493	1.9414	H	1.6641	4.6992	2.1598
H	4.873	-1.7447	-1.6313	H	0.9703	4.7837	-1.6668
H	0.7342	-3.9466	2.1091	H	2.7053	1.0113	3.3151
H	-0.7637	-2.1793	-3.0706	H	3.7557	0.6371	-2.2446

H	-1.1042	-3.6461	-3.9725	H	5.4998	0.7768	-2.3846
H	-1.5131	-4.918	-1.9063	H	5.8266	0.0576	-0.0566
H	0.0723	-4.1558	-1.8754	H	4.7364	1.4358	-0.1416
H	-3.3951	-3.6977	-3.2508	H	5.8292	-1.5868	-2.0943
H	-3.0571	-2.1241	-3.9455	H	4.6761	-1.3308	-3.3897
H	-4.4084	-2.1783	0.914	H	3.009	-3.8674	0.6363
H	-2.9242	-2.6249	1.6687	H	2.68	-2.5771	1.733
H	-1.8203	-0.5415	0.8107	H	0.9593	-1.6383	0.1872
H	-4.4777	0.1978	-0.4637	H	1.5161	-3.9364	-1.7151
H	-2.9977	1.1284	-0.4498	H	0.3405	-2.6514	-1.8864
H	-3.3156	-0.0564	-2.5877	H	2.3671	-2.2413	-3.2323
H	-1.8346	-0.528	-1.7952	H	2.06	-0.9629	-2.0863
H	-2.8379	0.2464	4.2631	H	-0.9776	-3.6345	2.5898
H	-4.6515	1.2735	3.2709	H	-0.6993	-5.398	1.1056
H	-5.0963	1.0879	1.4967	H	0.4535	-5.3448	-0.3274
H	-5.4426	-1.7152	-1.0313	H	3.6774	-4.4207	-1.4431
H	-5.2559	-1.4954	-2.7719	H	4.1907	-3.8243	-3.0221
H	-5.3145	-3.1168	-2.0866	H	5.3146	-3.815	-1.6661
H	-3.4436	4.2009	2.123	H	-4.418	-3.8375	2.4102
H	-2.184	5.4359	2.1118	H	-5.7445	-2.8094	1.8642
H	-1.5361	6.309	-0.3325	H	-6.0854	-2.7719	-0.7759
H	-2.6924	6.0567	-1.6284	H	-5.4056	-4.0873	-1.7174
H	-0.5314	1.5918	-1.033	H	-1.4886	-1.1526	-0.7025
H	0.2641	1.7418	0.5003	H	-2.0777	-0.1403	0.5791
H	1.702	3.5758	-0.3609	H	-3.8569	0.7779	-0.9016
H	1.7127	4.1463	-2.7521	H	-3.8299	0.2999	-3.3198
H	0.3791	3.0445	-3.0699	H	-2.5191	-0.8558	-3.1166
H	0.3638	5.5258	-1.3054	H	-5.3316	-0.9925	-1.9564
H	-0.4422	5.3451	-2.855	H	-4.6792	-2.0162	-3.2248
H	2.2667	1.5123	-3.5172	H	-1.3173	1.3047	-3.6574
H	-1.8206	2.6232	-2.6006	H	-1.9868	-2.8594	-2.1628
H	-3.2486	3.1539	-1.7224	H	-2.4858	-4.1474	-1.0729
H	-2.6172	4.1264	-3.0538	H	-3.2284	-3.9968	-2.6688
H	-0.3418	2.1184	2.3163	H	-2.6998	-0.5401	2.3887
H	-3.319	-4.6713	0.2381	H	5.1776	-2.2592	1.3945
H	-4.0343	4.5628	-0.1355	H	-4.1536	-4.8777	0.3015
H	-3.8229	6.1627	0.5562	H	-5.8855	-4.809	0.5857
3d-3	X axis(Å)	Y axis(Å)	Z axis(Å)	3d-4	X axis(Å)	Y axis(Å)	Z axis(Å)
C	2.4159	4.0714	-1.5176	C	-1.2246	5.5713	-0.1763
C	2.1778	3.8571	-0.0274	C	-0.9514	4.8531	1.1386
C	1.2814	2.6352	0.2098	C	-1.1926	3.3436	1.0032
C	-0.0979	2.7787	-0.5245	C	-2.6505	3.0224	0.5238
C	0.0678	3.1047	-2.0564	C	-3.0277	3.8114	-0.7863
C	1.1013	4.2482	-2.2689	C	-2.647	5.3143	-0.6583
C	-1.0232	1.5537	-0.3355	C	-2.918	1.5079	0.3336
C	-0.6406	0.3138	-1.1585	C	-2.2915	0.8786	-0.9255
C	-0.4481	0.6525	-2.6405	C	-2.6152	1.697	-2.1856

C	0.4963	1.8404	-2.8452	C	-2.326	3.1893	-2.0198
C	-1.2629	3.6261	-2.6753	C	-4.5634	3.7926	-1.0411
C	1.1057	2.4139	1.6985	C	-0.8537	2.6706	2.313
O	0.3953	3.0685	2.4497	O	-1.5388	2.67	3.3262
O	-0.7915	3.9124	0.0551	O	-3.5671	3.4787	1.5485
C	-1.6309	-0.8128	-0.9916	C	-2.6859	-0.5806	-1.0246
O	-2.9851	-0.4942	-1.0778	O	-2.3104	-1.372	0.0646
C	-1.3139	-2.0803	-0.7356	C	-3.2967	-1.1959	-2.0359
C	-5.4121	-1.028	-2.6796	C	-3.465	-3.0649	2.2227
C	-4.328	-2.041	-2.3322	C	-3.9672	-2.9632	0.7884
C	-3.7208	-1.7352	-0.9581	C	-2.8087	-2.7062	-0.182
C	-4.811	-1.7359	0.1748	C	-1.7017	-3.8152	-0.0901
C	-6.0201	-0.7854	-0.1664	C	-1.2132	-4.0458	1.3909
C	-6.5123	-1.0137	-1.6251	C	-2.4222	-4.1671	2.3625
C	-4.2462	-1.4077	1.5825	C	-0.4902	-3.5509	-1.0236
C	-3.905	0.074	1.8174	C	0.4855	-2.4608	-0.5424
C	-5.0878	0.9846	1.4461	C	0.9161	-2.6936	0.9139
C	-5.6233	0.6989	0.0398	C	-0.2791	-2.8964	1.8472
C	-3.3551	0.2838	3.2188	C	1.6367	-2.3226	-1.5242
C	-1.9223	-0.0763	3.449	C	1.4294	-1.4089	-2.6864
C	-4.0109	0.7962	4.273	C	2.8327	-2.9281	-1.4496
O	-1.2042	-0.5591	2.58	O	0.3994	-0.7656	-2.8504
C	-7.2536	-1.0848	0.7364	C	-0.4331	-5.3863	1.5303
C	-2.6141	-2.7228	-0.661	C	-3.3541	-2.5753	-1.5855
O	-2.7589	-3.9047	-0.3796	O	-3.7759	-3.4882	-2.2825
C	7.8825	-2.257	0.2683	C	6.1597	-1.0902	-0.0974
C	6.9352	-1.0945	0.4592	C	4.92	-0.6315	0.6341
C	5.6396	-1.1047	0.0585	C	4.3258	0.5718	0.4396
C	5.0218	-2.3478	-0.6188	C	4.9028	1.5885	-0.5647
C	5.9198	-3.6074	-0.4715	C	5.944	0.9459	-1.5229
C	4.6675	0.0599	0.208	C	3.0742	1.0528	1.1663
C	3.3497	-0.3544	0.8891	C	1.981	1.6064	0.2245
C	2.6942	-1.5186	0.1406	C	2.5732	2.6947	-0.6848
C	3.6554	-2.6997	0.0294	C	3.7787	2.1687	-1.4582
C	2.4095	0.8175	1.0109	C	0.7502	2.1244	0.9426
C	1.9049	1.2867	2.1497	C	0.4302	1.9905	2.2287
O	2.0384	1.4597	-0.1703	O	-0.1686	2.803	0.1384
C	4.8269	-2.0559	-2.126	C	5.5914	2.7303	0.22
C	7.5876	0.0817	1.1169	C	4.4302	-1.6363	1.6272
O	8.7243	0.0364	1.5757	O	4.7879	-2.8091	1.6082
O	-5.3653	-3.0731	0.2605	O	-2.2864	-5.0702	-0.5173
C	7.3872	-3.3031	-0.7215	C	6.9158	0.0328	-0.7942
H	3.0358	4.9644	-1.6596	H	-1.0793	6.649	-0.0369
H	2.9826	3.2322	-1.9366	H	-0.5014	5.2584	-0.9377
H	3.1517	3.7227	0.4607	H	0.0877	5.0545	1.4298
H	1.7296	4.757	0.4121	H	-1.5844	5.2741	1.9299
H	1.3167	4.3642	-3.3389	H	-2.7921	5.8209	-1.6212

H	0.6613	5.2014	-1.9451	H	-3.3313	5.8053	0.0471
H	-1.0654	1.292	0.7266	H	-2.5856	0.9655	1.2284
H	-2.0526	1.8547	-0.5733	H	-4.0039	1.337	0.3191
H	0.3161	-0.0572	-0.7849	H	-1.2026	0.8752	-0.8152
H	-0.0364	-0.2176	-3.1682	H	-2.0256	1.3194	-3.0311
H	-1.4152	0.8591	-3.115	H	-3.6667	1.5665	-2.4681
H	0.5416	2.0673	-3.9184	H	-2.6481	3.7084	-2.9322
H	1.5104	1.533	-2.5706	H	-1.2424	3.3335	-1.9741
H	-1.5715	4.5788	-2.2304	H	-5.1121	4.3133	-0.2483
H	-1.1482	3.7991	-3.7521	H	-4.8067	4.2982	-1.9832
H	-2.0931	2.9269	-2.5451	H	-4.9707	2.78	-1.1016
H	-0.8489	3.7788	1.0246	H	-3.3107	3.0693	2.4016
H	-0.362	-2.5547	-0.5997	H	-3.6463	-0.8319	-2.9825
H	-4.978	-0.0277	-2.7887	H	-3.0513	-2.1045	2.5501
H	-5.8475	-1.2838	-3.6527	H	-4.3099	-3.2803	2.8873
H	-4.7442	-3.0559	-2.3552	H	-4.5013	-3.8823	0.5163
H	-3.5564	-2.0013	-3.112	H	-4.7005	-2.148	0.7374
H	-7.0391	-1.9761	-1.685	H	-2.9294	-5.1273	2.1958
H	-7.252	-0.2487	-1.8944	H	-2.0673	-4.19	3.4009
H	-4.9701	-1.7341	2.3425	H	0.0613	-4.492	-1.1604
H	-3.3687	-2.036	1.7804	H	-0.8474	-3.3141	-2.0341
H	-3.101	0.3581	1.1388	H	-0.0287	-1.496	-0.536
H	-5.9064	0.8769	2.1658	H	1.585	-3.5562	0.9985
H	-4.7731	2.0349	1.497	H	1.4888	-1.8283	1.2652
H	-6.4926	1.3454	-0.1386	H	0.0999	-3.1016	2.857
H	-4.8738	1.0123	-0.6935	H	-0.8255	-1.9516	1.9292
H	-1.5352	0.1167	4.464	H	2.2685	-1.3365	-3.399
H	-3.5422	0.9316	5.2439	H	3.6142	-2.7772	-2.1888
H	-5.0513	1.0978	4.2104	H	3.0804	-3.6145	-0.6446
H	-7.0253	-1.017	1.8031	H	0.416	-5.4554	0.8452
H	-8.0656	-0.3771	0.5308	H	-0.0421	-5.504	2.548
H	-7.6532	-2.0894	0.5572	H	-1.0756	-6.2519	1.3336
H	8.8591	-1.9022	-0.0835	H	6.8533	-1.5814	0.5963
H	8.046	-2.732	1.2443	H	5.865	-1.8418	-0.8408
H	5.8262	-4.0232	0.5413	H	5.4329	0.3528	-2.2939
H	5.5866	-4.3973	-1.1564	H	6.5027	1.7242	-2.0578
H	4.4683	0.4711	-0.7901	H	3.3736	1.8258	1.8861
H	5.0889	0.887	0.7831	H	2.622	0.253	1.7559
H	3.5952	-0.7048	1.9026	H	1.6425	0.781	-0.4172
H	1.7909	-1.8427	0.6723	H	1.8253	3.0328	-1.4133
H	2.3727	-1.2085	-0.8603	H	2.8507	3.5781	-0.097
H	3.8189	-3.0933	1.0423	H	3.4193	1.3933	-2.1493
H	3.1672	-3.504	-0.536	H	4.1776	2.9759	-2.0862
H	2.023	0.9547	3.1629	H	0.9297	1.505	3.0444
H	4.1295	-1.2322	-2.3076	H	4.8935	3.2796	0.8596
H	5.7707	-1.7838	-2.611	H	6.3859	2.3522	0.8726
H	4.4278	-2.9338	-2.647	H	6.043	3.4589	-0.4633

H	7.0062	1.0097	1.1773	H	3.7262	-1.2801	2.3909
H	-4.6277	-3.7106	0.3663	H	-2.7084	-4.9387	-1.3927
H	7.5376	-2.9507	-1.7483	H	7.5033	0.6006	-0.0638
H	7.9823	-4.2177	-0.6161	H	7.6326	-0.3943	-1.5051
3d-5	X axis(Å)	Y axis(Å)	Z axis(Å)	3d-6	X axis(Å)	Y axis(Å)	Z axis(Å)
C	5.4819	0.2917	1.8185	C	5.6172	1.0227	0.9867
C	5.4999	0.6249	0.3314	C	5.2715	0.9019	-0.4917
C	4.2029	0.1651	-0.3463	C	3.9261	0.187	-0.6849
C	3.9667	-1.3762	-0.1619	C	3.9248	-1.2379	-0.032
C	4.0241	-1.8051	1.3531	C	4.3724	-1.1978	1.4776
C	5.2774	-1.201	2.0501	C	5.6623	-0.3462	1.6535
C	2.6586	-1.8931	-0.8129	C	2.5753	-1.9852	-0.1754
C	1.3706	-1.5339	-0.0535	C	1.4527	-1.5253	0.7715
C	1.4532	-1.8815	1.4363	C	1.9281	-1.4112	2.2279
C	2.7354	-1.3684	2.0959	C	3.2365	-0.6323	2.3667
C	4.1672	-3.3479	1.5059	C	4.7393	-2.6176	2.0012
C	4.2257	0.5611	-1.8048	C	3.5982	0.1399	-2.1601
O	4.8694	0.0174	-2.6913	O	4.0731	-0.6292	-2.984
O	5.0522	-2.0739	-0.821	O	4.9133	-2.0422	-0.7224
C	0.1393	-2.1331	-0.691	C	0.2575	-2.4371	0.5945
O	-0.9213	-1.2505	-0.9091	O	-0.6437	-2.0683	-0.4093
C	-0.0311	-3.3977	-1.0738	C	-0.0261	-3.5371	1.2908
C	-2.3462	0.0166	-3.1663	C	-1.5959	-3.0267	-3.0442
C	-1.8554	-1.4245	-3.1172	C	-1.2814	-3.8968	-1.8336
C	-1.9129	-1.9677	-1.6832	C	-1.6	-3.1499	-0.5326
C	-3.3674	-1.8998	-1.0951	C	-3.1045	-2.702	-0.4703
C	-3.9928	-0.458	-1.2161	C	-3.5425	-1.8955	-1.7519
C	-3.7709	0.131	-2.6392	C	-3.0597	-2.6038	-3.0505
C	-3.4665	-2.4126	0.3653	C	-3.4567	-1.9121	0.8179
C	-2.9165	-1.4503	1.4356	C	-2.9635	-0.4545	0.8432
C	-3.5396	-0.0534	1.2767	C	-3.4085	0.2926	-0.4229
C	-3.3922	0.4888	-0.1465	C	-2.997	-0.4461	-1.6987
C	-3.0636	-2.0543	2.8235	C	-3.363	0.2174	2.146
C	-2.12	-3.1557	3.1812	C	-2.5126	-0.0789	3.3389
C	-3.9237	-1.6802	3.7847	C	-4.3702	1.0848	2.3359
O	-1.2654	-3.5737	2.4086	O	-1.5385	-0.8214	3.2799
C	-5.5379	-0.4887	-1.0201	C	-5.094	-1.8225	-1.8757
C	-1.3609	-3.376	-1.6586	C	-1.2368	-4.0181	0.6508
O	-1.9274	-4.3777	-2.0737	O	-1.8566	-4.9978	1.0422
C	-2.2654	4.3202	2.0717	C	-2.1166	4.9708	1.5081
C	-1.1968	3.3272	1.675	C	-1.3353	3.7213	1.1838
C	-0.5734	3.3369	0.4706	C	-0.9053	3.4253	-0.0669
C	-0.8639	4.4323	-0.5752	C	-1.2497	4.3195	-1.2782
C	-1.6754	5.6147	0.0223	C	-2.1618	5.5256	-0.916
C	0.4477	2.3077	0.0069	C	0.0133	2.2656	-0.422
C	1.7672	2.9454	-0.4683	C	1.3394	2.7898	-1.0055
C	1.4831	3.9784	-1.5706	C	1.0869	3.73	-2.2002

C	0.4708	5.0247	-1.1026	C	0.0916	4.8453	-1.8542
C	2.7684	1.8796	-0.8632	C	2.2776	1.6454	-1.31
C	3.3487	1.6959	-2.0479	C	2.6162	1.1567	-2.5018
O	3.1279	0.9942	0.1564	O	2.8826	1.0621	-0.1937
C	-1.6709	3.8277	-1.748	C	-2.0146	3.5287	-2.3686
C	-0.9098	2.3239	2.7505	C	-1.0395	2.8803	2.3853
O	-1.5069	2.3148	3.8224	O	-1.5876	3.0643	3.4681
O	-4.2107	-2.7677	-1.8932	O	-3.9263	-3.8965	-0.4562
C	-2.8137	5.1383	0.9094	C	-1.9	6.0711	0.4767
H	6.4323	0.6004	2.2696	H	6.5946	1.5081	1.0913
H	4.6985	0.8651	2.3267	H	4.8944	1.6705	1.4949
H	5.6291	1.7095	0.2235	H	5.2394	1.9121	-0.9197
H	6.3713	0.1579	-0.1445	H	6.0713	0.3659	-1.0181
H	5.2321	-1.3892	3.1306	H	5.8815	-0.2141	2.7209
H	6.178	-1.7183	1.6916	H	6.5194	-0.8914	1.235
H	2.5869	-1.5336	-1.8478	H	2.2257	-1.9271	-1.2148
H	2.7352	-2.9831	-0.9236	H	2.7555	-3.0598	-0.0268
H	1.245	-0.4524	-0.1276	H	1.1273	-0.5256	0.4683
H	0.5937	-1.4484	1.9636	H	1.1565	-0.9103	2.8253
H	1.3791	-2.9662	1.5794	H	2.0584	-2.4007	2.6795
H	2.7611	-1.7311	3.132	H	3.5428	-0.6541	3.4209
H	2.6764	-0.2786	2.1746	H	3.0448	0.4215	2.1437
H	5.1085	-3.7122	1.0794	H	5.613	-3.0276	1.4821
H	4.1639	-3.6345	2.5644	H	4.9879	-2.5852	3.0687
H	3.3584	-3.899	1.019	H	3.9266	-3.3382	1.8781
H	5.1087	-1.7628	-1.7491	H	4.7151	-2.0257	-1.6826
H	0.6136	-4.252	-0.9986	H	0.4837	-4.0155	2.1043
H	-1.6756	0.6645	-2.5922	H	-0.9451	-2.1452	-3.0603
H	-2.3132	0.376	-4.2014	H	-1.3783	-3.5889	-3.9599
H	-2.4555	-2.0474	-3.7922	H	-1.8475	-4.8349	-1.8907
H	-0.8268	-1.4504	-3.4995	H	-0.2189	-4.1695	-1.8724
H	-4.4285	-0.384	-3.353	H	-3.6627	-3.5067	-3.2189
H	-4.073	1.1862	-2.6589	H	-3.2387	-1.9564	-3.9186
H	-4.5181	-2.6375	0.5934	H	-4.5474	-1.924	0.9548
H	-2.9765	-3.391	0.4395	H	-3.0838	-2.4548	1.6956
H	-1.8416	-1.316	1.2828	H	-1.8693	-0.4419	0.8203
H	-4.6019	-0.0672	1.5446	H	-4.493	0.4454	-0.4301
H	-3.0627	0.6445	1.9733	H	-2.9644	1.2929	-0.4319
H	-3.8833	1.4692	-0.1968	H	-3.3612	0.1234	-2.5637
H	-2.3337	0.6812	-0.3435	H	-1.9056	-0.4343	-1.7795
H	-2.2326	-3.5796	4.1935	H	-2.8051	0.4166	4.2804
H	-3.9507	-2.154	4.7621	H	-4.5655	1.5437	3.3021
H	-4.6386	-0.8774	3.6366	H	-5.039	1.3767	1.5337
H	-5.8368	-0.9465	-0.0737	H	-5.5716	-1.407	-0.9846
H	-5.9515	0.5267	-1.0372	H	-5.3865	-1.1958	-2.7266
H	-6.0369	-1.0497	-1.8185	H	-5.5348	-2.812	-2.0424
H	-3.111	3.8048	2.5435	H	-3.182	4.7174	1.5737

H	-1.8428	4.9998	2.8229	H	-1.8184	5.3728	2.4839
H	-1.0204	6.2597	0.6241	H	-2.0453	6.3294	-1.6538
H	-2.0742	6.2497	-0.7788	H	-3.2184	5.2264	-0.9626
H	0.0064	1.7191	-0.8076	H	-0.4851	1.602	-1.1377
H	0.6759	1.5828	0.7882	H	0.2312	1.6294	0.4365
H	2.2079	3.4862	0.3822	H	1.8307	3.3975	-0.2305
H	2.4117	4.4913	-1.8516	H	2.0328	4.1869	-2.5177
H	1.1116	3.486	-2.4773	H	0.7117	3.1687	-3.0638
H	0.9482	5.6178	-0.3102	H	0.5687	5.5207	-1.1316
H	0.2718	5.7209	-1.9276	H	-0.0927	5.442	-2.7569
H	3.2483	2.2184	-2.9797	H	2.3043	1.415	-3.4952
H	-1.1145	3.0546	-2.2856	H	-1.4547	2.6774	-2.7648
H	-2.6034	3.3682	-1.4041	H	-2.9612	3.1372	-1.9789
H	-1.9331	4.5986	-2.4818	H	-2.2529	4.1765	-3.2207
H	-0.1298	1.5794	2.5514	H	-0.3166	2.0637	2.264
H	-3.8046	-3.6605	-1.915	H	-3.619	-4.4784	0.2715
H	-3.5273	4.5396	0.3319	H	-2.5776	6.9073	0.6835
H	-3.3711	5.9985	1.2979	H	-0.8786	6.4638	0.5476
3d-7	X axis(Å)	Y axis(Å)	Z axis(Å)	3d-8	X axis(Å)	Y axis(Å)	Z axis(Å)
C	2.1697	4.827	-1.3474	C	1.7404	5.379	-0.664
C	1.8971	4.5666	0.1297	C	1.7941	4.6854	0.6911
C	1.1965	3.2162	0.3228	C	1.135	3.3039	0.6284
C	-0.152	3.1452	-0.4781	C	-0.3499	3.3754	0.1224
C	0.0332	3.5042	-2.0001	C	-0.4897	4.1814	-1.2249
C	0.8818	4.7982	-2.1626	C	0.3042	5.5172	-1.1554
C	-0.8822	1.7889	-0.3336	C	-1.0137	1.9803	-0.0149
C	-0.2725	0.6299	-1.1376	C	-0.58	1.1656	-1.248
C	-0.0619	1.0057	-2.608	C	-0.7061	1.9824	-2.538
C	0.6933	2.3287	-2.766	C	-0.0025	3.3364	-2.4292
C	-1.3318	3.8134	-2.6834	C	-1.969	4.5885	-1.4928
C	0.9845	2.957	1.7985	C	1.2263	2.6439	1.987
O	0.1445	3.4854	2.5147	O	0.5952	2.954	2.9885
O	-1.043	4.1514	0.0664	O	-1.1215	4.1101	1.1055
C	-1.0776	-0.6416	-1.0206	C	-1.3247	-0.1405	-1.3783
O	-2.463	-0.5357	-1.1299	O	-2.6905	-0.1308	-1.1054
C	-0.5719	-1.8508	-0.7857	C	-0.7731	-1.3059	-1.7113
C	-4.7521	-1.4024	-2.7897	C	-5.3267	-0.5681	-2.3628
C	-3.5289	-2.2425	-2.4424	C	-4.0588	-1.3654	-2.6451
C	-2.9992	-1.8782	-1.0509	C	-3.1884	-1.4603	-1.3869
C	-4.0937	-2.0745	0.0607	C	-3.9608	-2.1276	-0.1922
C	-5.4306	-1.3158	-0.2842	C	-5.3361	-1.4149	0.093
C	-5.8578	-1.584	-1.7566	C	-6.1299	-1.1911	-1.227
C	-3.6087	-1.6947	1.4852	C	-3.1238	-2.229	1.1103
C	-3.5066	-0.1838	1.7558	C	-2.945	-0.9066	1.8757
C	-4.8113	0.5398	1.3819	C	-4.2957	-0.2079	2.1088
C	-5.2737	0.207	-0.04	C	-5.1107	-0.0642	0.8198
C	-3.0159	0.0771	3.1703	C	-2.1196	-1.1289	3.1326

C	-1.5464	-0.0473	3.4163	C	-0.6354	-1.2042	2.9733
C	-3.7611	0.4464	4.225	C	-2.5817	-1.2371	4.3892
O	-0.7457	-0.3805	2.5491	O	-0.0658	-1.0972	1.8923
C	-6.6166	-1.8243	0.5882	C	-6.2605	-2.2949	0.9858
C	-1.7576	-2.6886	-0.7513	C	-1.9121	-2.2071	-1.7039
O	-1.7216	-3.8841	-0.4931	O	-1.8148	-3.4077	-1.9168
C	5.8905	-3.1523	-1.3793	C	5.0594	-4.1624	-0.7307
C	4.816	-2.0992	-1.2279	C	4.1464	-3.1539	-0.07
C	4.3819	-1.6342	-0.0297	C	4.4811	-1.8544	0.1262
C	4.9963	-2.1361	1.2928	C	5.8297	-1.2884	-0.3666
C	6.3131	-2.93	1.069	C	6.5445	-2.2537	-1.3518
C	3.2729	-0.6072	0.161	C	3.6183	-0.8288	0.8471
C	3.6862	0.578	1.0547	C	3.3948	0.4455	0.0098
C	4.2128	0.0637	2.4037	C	4.7409	1.063	-0.388
C	5.3524	-0.9343	2.2073	C	5.6096	0.0465	-1.1291
C	2.5567	1.5801	1.1794	C	2.519	1.4784	0.6806
C	1.9232	1.961	2.2875	C	2.1528	1.5265	1.9598
O	2.1489	2.1785	-0.0171	O	1.9767	2.4422	-0.1731
C	3.9802	-3.0596	2.0059	C	6.757	-1.0491	0.8486
C	4.2692	-1.6392	-2.5446	C	2.8398	-3.7493	0.3608
O	4.7231	-2.0196	-3.6188	O	2.5825	-4.9408	0.2234
O	-4.4344	-3.483	0.1094	O	-4.286	-3.4878	-0.5737
C	6.2087	-3.9032	-0.093	C	6.5025	-3.6962	-0.8757
H	2.6458	5.8082	-1.4593	H	2.1899	6.3752	-0.5779
H	2.882	4.0917	-1.738	H	2.3431	4.8303	-1.3962
H	2.8552	4.5851	0.665	H	2.846	4.5959	0.9914
H	1.2907	5.3805	0.5463	H	1.3042	5.312	1.447
H	1.1279	4.9541	-3.2209	H	0.3114	6.0003	-2.141
H	0.2811	5.6675	-1.8618	H	-0.2123	6.2144	-0.4815
H	-0.9318	1.5162	0.7253	H	-0.8298	1.3978	0.8946
H	-1.9339	1.9268	-0.6193	H	-2.104	2.1147	-0.0248
H	0.71	0.4116	-0.7156	H	0.475	0.9038	-1.1357
H	0.5077	0.2151	-3.1138	H	-0.2644	1.4252	-3.3745
H	-1.0246	1.0609	-3.1306	H	-1.7614	2.1266	-2.7997
H	0.7552	2.5677	-3.8357	H	-0.165	3.8889	-3.3639
H	1.7282	2.1821	-2.4411	H	1.0775	3.1655	-2.3755
H	-1.8081	4.7023	-2.2547	H	-2.3418	5.286	-0.7344
H	-1.1942	4.0097	-3.7534	H	-2.0638	5.0917	-2.4625
H	-2.0465	2.9911	-2.5932	H	-2.648	3.7317	-1.5025
H	-1.123	4.0058	1.0324	H	-0.9812	3.7039	1.9861
H	0.4385	-2.1776	-0.6389	H	0.2416	-1.565	-1.9426
H	-4.4775	-0.3446	-2.8696	H	-5.0773	0.4721	-2.1246
H	-5.1268	-1.6999	-3.7761	H	-5.9441	-0.5383	-3.2682
H	-3.7815	-3.3089	-2.4944	H	-4.3204	-2.3655	-3.0124
H	-2.7606	-2.0649	-3.2059	H	-3.5115	-0.8671	-3.4556
H	-6.227	-2.6149	-1.8464	H	-6.5166	-2.1546	-1.5867
H	-6.7033	-0.9373	-2.0245	H	-7.0116	-0.567	-1.0321

H	-4.2845	-2.147	2.2248	H	-3.59	-2.9692	1.776
H	-2.6469	-2.1827	1.6873	H	-2.145	-2.671	0.8847
H	-2.7477	0.2372	1.0971	H	-2.3679	-0.2193	1.2566
H	-5.614	0.2891	2.0837	H	-4.8964	-0.7505	2.8464
H	-4.6653	1.6248	1.4604	H	-4.1242	0.7906	2.5312
H	-6.2302	0.7143	-0.2217	H	-6.0784	0.3901	1.0701
H	-4.5707	0.6501	-0.7523	H	-4.6129	0.6582	0.1659
H	-1.2105	0.1793	4.4425	H	-0.0615	-1.3633	3.9022
H	-3.3343	0.6323	5.2067	H	-1.927	-1.3828	5.244
H	-4.8363	0.5731	4.1513	H	-3.6418	-1.1925	4.6166
H	-6.4184	-1.7468	1.6604	H	-5.7928	-2.5768	1.9327
H	-7.5255	-1.2467	0.3818	H	-7.1887	-1.7627	1.226
H	-6.852	-2.8742	0.3806	H	-6.5472	-3.2241	0.4806
H	5.5976	-3.8935	-2.133	H	5.0696	-5.1013	-0.1637
H	6.8022	-2.6636	-1.7466	H	4.6543	-4.3922	-1.7248
H	7.142	-2.2393	0.8614	H	6.0685	-2.2071	-2.3411
H	6.5918	-3.4741	1.9802	H	7.5871	-1.9461	-1.5009
H	2.4015	-1.1126	0.5964	H	4.1104	-0.5781	1.7957
H	2.9298	-0.2041	-0.7921	H	2.642	-1.227	1.126
H	4.5156	1.1031	0.5585	H	2.8748	0.1393	-0.9099
H	4.5826	0.9033	3.006	H	4.582	1.9306	-1.0411
H	3.4081	-0.4054	2.9824	H	5.269	1.4372	0.4975
H	6.2049	-0.3871	1.7813	H	5.1273	-0.1585	-2.0951
H	5.6817	-1.2957	3.1901	H	6.5771	0.5089	-1.3635
H	2.0304	1.6537	3.3096	H	2.3886	0.8916	2.7915
H	3.0561	-2.5392	2.2762	H	6.3629	-0.2932	1.535
H	3.6919	-3.9076	1.375	H	6.9023	-1.9637	1.4338
H	4.4022	-3.4646	2.933	H	7.7452	-0.7019	0.5254
H	3.4299	-0.9338	-2.523	H	2.1004	-3.0741	0.8089
H	-3.6082	-4.0013	0.2112	H	-3.463	-3.9378	-0.8608
H	5.4372	-4.6563	0.1037	H	7.029	-3.8011	0.0798
H	7.1526	-4.448	-0.2109	H	7.0255	-4.3417	-1.591
3d-9	X axis(Å)	Y axis(Å)	Z axis(Å)	3d-10	X axis(Å)	Y axis(Å)	Z axis(Å)
C	1.4665	5.5072	-0.3819	C	2.7939	4.4943	-0.6672
C	1.3594	4.782	0.9541	C	2.4235	4.1113	0.7606
C	0.509	3.5107	0.8166	C	1.2231	3.155	0.7721
C	-0.9309	3.8349	0.2935	C	-0.0274	3.7876	0.0706
C	-0.8978	4.6638	-1.0434	C	0.3058	4.2949	-1.3819
C	0.0895	5.8614	-0.9301	C	1.6155	5.1356	-1.3901
C	-1.8307	2.587	0.1299	C	-1.2645	2.8569	0.0461
C	-1.5415	1.6996	-1.0965	C	-1.2188	1.7103	-0.9799
C	-1.4144	2.5336	-2.383	C	-0.8153	2.209	-2.3767
C	-0.5031	3.7536	-2.2339	C	0.4298	3.0986	-2.3598
C	-2.2842	5.2997	-1.3561	C	-0.8006	5.2492	-1.9206
C	0.491	2.7692	2.1337	C	0.9257	2.732	2.1945
O	-0.183	3.053	3.1141	O	0.3648	3.4058	3.0472
O	-1.5803	4.6773	1.2783	O	-0.4143	4.9599	0.8299

C	-2.6074	0.6208	-1.1741	C	-2.5426	0.9741	-0.9451
O	-2.6773	-0.2265	-0.064	O	-2.7681	0.2104	0.2048
C	-3.4847	0.3946	-2.1511	C	-3.4971	0.9601	-1.8744
C	-4.515	-0.5641	2.2295	C	-4.5301	0.1909	2.5783
C	-4.9281	-0.3443	0.7789	C	-4.9508	0.5386	1.1554
C	-3.9084	-0.9776	-0.1781	C	-4.133	-0.2658	0.1377
C	-3.753	-2.515	0.083	C	-4.289	-1.8125	0.3577
C	-3.4085	-2.8243	1.5883	C	-3.9749	-2.2369	1.8425
C	-4.361	-2.0478	2.5434	C	-4.6961	-1.2988	2.8535
C	-2.7331	-3.2124	-0.8511	C	-3.4559	-2.6619	-0.6362
C	-1.2548	-2.9224	-0.5342	C	-1.9456	-2.7042	-0.3476
C	-0.9349	-3.1446	0.9519	C	-1.6705	-3.1045	1.1115
C	-1.9323	-2.4659	1.8941	C	-2.4462	-2.2318	2.1029
C	-0.2763	-3.7017	-1.399	C	-1.2418	-3.5607	-1.3864
C	1.0175	-3.0368	-1.726	C	-0.9204	-2.9037	-2.6893
C	-0.4538	-4.9297	-1.9134	C	-0.8535	-4.839	-1.2505
O	1.3012	-1.9129	-1.3266	O	-1.1692	-1.7258	-2.9177
C	-3.6177	-4.3292	1.9281	C	-4.5114	-3.6663	2.1518
C	-4.2981	-0.682	-1.6075	C	-4.527	0.1367	-1.2648
O	-5.1734	-1.2464	-2.2491	O	-5.5618	-0.1748	-1.8387
C	5.4351	-3.4553	-0.4143	C	6.5315	-3.0852	0.2058
C	4.3479	-2.6387	0.2414	C	5.8462	-1.8003	0.6112
C	4.3995	-1.2926	0.3948	C	4.6552	-1.3904	0.1086
C	5.608	-0.48	-0.1111	C	3.8879	-2.2429	-0.9248
C	6.5262	-1.3068	-1.0546	C	4.4535	-3.6859	-1.0369
C	3.3102	-0.4473	1.0491	C	3.9517	-0.0885	0.4739
C	2.8628	0.7515	0.1861	C	2.4887	-0.3075	0.9025
C	4.0778	1.599	-0.2199	C	1.7141	-1.0592	-0.1831
C	5.1312	0.7499	-0.9253	C	2.397	-2.3828	-0.5163
C	1.8292	1.6443	0.838	C	1.829	1.0049	1.237
C	1.4129	1.6432	2.1034	C	1.4029	1.3799	2.441
O	1.2402	2.5819	-0.0144	O	1.6579	1.905	0.1878
C	6.4441	-0.0147	1.1045	C	3.9886	-1.5655	-2.3125
C	3.2045	-3.4721	0.7229	C	6.6364	-1.0136	1.6103
O	3.0343	-4.632	0.3589	O	7.6453	-1.4554	2.1499
O	-5.0339	-3.1421	-0.1776	O	-5.6772	-2.1604	0.1277
C	6.7614	-2.7185	-0.5438	C	5.9724	-3.7101	-1.0657
H	2.0504	6.4256	-0.2495	H	3.6328	5.1998	-0.6465
H	2.0161	4.8936	-1.1046	H	3.1438	3.6144	-1.2187
H	2.3742	4.5367	1.2929	H	3.2984	3.6409	1.2276
H	0.9325	5.4524	1.7104	H	2.2052	5.0135	1.3454
H	0.2101	6.3414	-1.9098	H	1.9113	5.3578	-2.4235
H	-0.3416	6.6272	-0.2706	H	1.4266	6.1082	-0.9152
H	-1.7842	1.9816	1.0448	H	-1.439	2.449	1.0505
H	-2.8803	2.914	0.0965	H	-2.1598	3.4684	-0.1381
H	-0.5879	1.1817	-0.9434	H	-0.4602	0.9858	-0.6677
H	-1.0257	1.9004	-3.1912	H	-0.6257	1.3484	-3.0312

H	-2.4004	2.876	-2.7188	H	-1.6364	2.7653	-2.8431
H	-0.5401	4.3288	-3.1686	H	0.6047	3.4685	-3.3788
H	0.5328	3.4131	-2.1489	H	1.3021	2.4817	-2.1247
H	-2.5751	6.032	-0.5946	H	-0.8665	6.1687	-1.3281
H	-2.2603	5.8288	-2.3163	H	-0.5852	5.5489	-2.9531
H	-3.0875	4.5605	-1.4129	H	-1.7941	4.7932	-1.9151
H	-1.5522	4.2178	2.1442	H	-0.5582	4.6935	1.7625
H	-3.6419	0.8775	-3.096	H	-3.563	1.4308	-2.8358
H	-3.5808	-0.0324	2.4431	H	-3.4925	0.4964	2.7544
H	-5.2745	-0.1315	2.8914	H	-5.1444	0.7598	3.2861
H	-5.929	-0.76	0.608	H	-6.0238	0.3501	1.0261
H	-5.0059	0.7366	0.6045	H	-4.802	1.6158	1.006
H	-5.3618	-2.4996	2.5048	H	-5.7729	-1.5169	2.848
H	-4.0212	-2.1572	3.5814	H	-4.3512	-1.5121	3.8735
H	-2.9246	-4.2918	-0.8077	H	-3.8499	-3.6882	-0.6443
H	-2.9409	-2.9529	-1.8973	H	-3.6357	-2.3119	-1.6607
H	-1.0924	-1.8633	-0.7551	H	-1.5355	-1.6967	-0.4558
H	-0.8962	-4.2185	1.1732	H	-1.9258	-4.1551	1.286
H	0.067	-2.7584	1.1768	H	-0.5979	-3.015	1.3246
H	-1.6853	-2.7529	2.9247	H	-2.2397	-2.5927	3.119
H	-1.7724	-1.3842	1.8528	H	-2.0436	-1.2146	2.0682
H	1.7184	-3.6177	-2.3494	H	-0.4323	-3.5427	-3.4446
H	0.3011	-5.4219	-2.5208	H	-0.344	-5.382	-2.0418
H	-1.3529	-5.5074	-1.7268	H	-1.0424	-5.4014	-0.3418
H	-3.0187	-4.9934	1.2998	H	-4.127	-4.4221	1.4619
H	-3.3418	-4.5331	2.9697	H	-4.2297	-3.9756	3.1654
H	-4.6647	-4.6298	1.8103	H	-5.605	-3.7098	2.0975
H	5.617	-4.3762	0.1534	H	7.6039	-2.9152	0.0492
H	5.0883	-3.7559	-1.4114	H	6.4372	-3.8017	1.032
H	6.0758	-1.3783	-2.0543	H	4.1195	-4.2912	-0.1829
H	7.4899	-0.8003	-1.1912	H	4.061	-4.1824	-1.9333
H	3.6954	-0.0957	2.0149	H	3.9984	0.5837	-0.3929
H	2.4164	-1.031	1.2802	H	4.4547	0.4463	1.2822
H	2.4076	0.3523	-0.73	H	2.4933	-0.9332	1.8071
H	3.7693	2.4035	-0.9	H	0.6955	-1.2579	0.1655
H	4.514	2.0915	0.6578	H	1.6163	-0.4524	-1.0911
H	4.7038	0.4159	-1.8811	H	2.3146	-3.0328	0.3659
H	5.9885	1.3864	-1.18	H	1.8385	-2.8821	-1.3172
H	1.6804	1.032	2.9432	H	1.4115	0.8707	3.3852
H	5.881	0.6429	1.7742	H	3.5252	-0.5741	-2.3307
H	6.7869	-0.8623	1.7081	H	5.0306	-1.4334	-2.6239
H	7.3315	0.5413	0.7805	H	3.4872	-2.167	-3.0797
H	2.5071	-3.0024	1.4278	H	6.2791	-0.0049	1.8512
H	-5.3196	-2.8974	-1.0833	H	-5.9435	-1.8149	-0.7511
H	7.2765	-2.6969	0.4234	H	6.3491	-3.1752	-1.945
H	7.4167	-3.262	-1.2343	H	6.3286	-4.7431	-1.1534
3d-11	X axis(Å)	Y axis(Å)	Z axis(Å)	3d-12	X axis(Å)	Y axis(Å)	Z axis(Å)

C	5.4303	0.6606	1.7256	C	2.3736	4.1787	-1.4141
C	5.4154	0.8649	0.216	C	2.1707	3.8906	0.069
C	4.1529	0.2537	-0.4044	C	1.2901	2.6501	0.2658
C	4.0282	-1.2786	-0.0847	C	-0.1069	2.8177	-0.429
C	4.1442	-1.5768	1.4584	C	0.0213	3.2177	-1.9468
C	5.3516	-0.819	2.0816	C	1.0411	4.3789	-2.1273
C	2.7474	-1.932	-0.6672	C	-1.0196	1.5781	-0.278
C	1.4525	-1.6154	0.0986	C	-0.646	0.3818	-1.1665
C	1.5994	-1.8704	1.6018	C	-0.4893	0.7913	-2.6348
C	2.835	-1.1885	2.1903	C	0.4409	1.996	-2.8045
C	4.4182	-3.0859	1.7291	C	-1.3269	3.7567	-2.5101
C	4.1509	0.5072	-1.8939	C	1.1501	2.3532	1.7451
O	4.8276	-0.0775	-2.7285	O	0.452	2.9633	2.5437
O	5.1486	-1.9581	-0.7058	O	-0.7945	3.9167	0.2202
C	0.2629	-2.3572	-0.4642	C	-1.6227	-0.7606	-1.0305
O	-0.8306	-1.5686	-0.8261	O	-2.9811	-0.4517	-1.0739
C	0.1495	-3.6731	-0.6356	C	-1.2889	-2.0351	-0.8384
C	-2.349	-0.7776	-3.2536	C	-5.4372	-0.9363	-2.6463
C	-1.7814	-2.1597	-2.9573	C	-4.337	-1.9535	-2.3683
C	-1.7982	-2.4452	-1.4502	C	-3.703	-1.704	-0.9949
C	-3.2454	-2.3363	-0.8502	C	-4.7685	-1.7668	0.1596
C	-3.941	-0.9694	-1.2138	C	-5.9929	-0.8135	-0.1123
C	-3.772	-0.6427	-2.7257	C	-6.5145	-0.9802	-1.5691
C	-3.3086	-2.5771	0.6825	C	-4.1764	-1.4973	1.5686
C	-2.7914	-1.4116	1.5498	C	-3.8428	-0.0245	1.8632
C	-3.4464	-0.0829	1.1481	C	-5.0413	0.8904	1.5591
C	-3.366	0.183	-0.3548	C	-5.6048	0.6637	0.1529
C	-2.9357	-1.6217	3.0492	C	-3.2641	0.1269	3.2606
C	-1.9499	-0.918	3.924	C	-1.8239	-0.2309	3.4433
C	-3.8438	-2.3876	3.6757	C	-3.9005	0.586	4.3506
O	-1.0115	-0.2724	3.4727	O	-1.1216	-0.6684	2.5382
C	-5.4784	-1.0265	-0.9721	C	-7.204	-1.1655	0.8018
C	-1.1855	-3.8043	-1.1932	C	-2.5814	-2.6931	-0.7663
O	-1.7179	-4.8863	-1.3986	O	-2.7097	-3.888	-0.5362
C	-2.4841	4.524	1.5686	C	7.6819	-2.4577	0.3839
C	-1.3694	3.5271	1.3404	C	6.8792	-1.1807	0.4497
C	-0.7718	3.3313	0.1382	C	5.6599	-1.0436	-0.1256
C	-1.14	4.1995	-1.0835	C	5.0487	-2.1548	-1.0069
C	-2.0237	5.421	-0.7062	C	5.9923	-3.3757	-1.1956
C	0.302	2.2854	-0.1524	C	4.7176	0.1323	0.0908
C	1.5742	2.8851	-0.7881	C	3.4049	-0.3444	0.7485
C	1.2109	3.7171	-2.031	C	2.7504	-1.4822	-0.0494
C	0.1536	4.7712	-1.7173	C	3.7336	-2.6238	-0.3308
C	2.6169	1.82	-1.0736	C	2.4528	0.8066	0.9496
C	3.206	1.5545	-2.2391	C	1.9686	1.2124	2.1212
O	3.021	1.0514	0.0227	O	2.0487	1.5025	-0.1895
C	-1.9072	3.3485	-2.1219	C	4.7508	-1.6273	-2.4325

C	-1.0071	2.7853	2.5927	C	7.5396	-0.0995	1.2453
O	-1.528	3.0438	3.6742	O	8.5916	-0.269	1.8519
O	-4.0588	-3.3703	-1.4598	O	-5.3091	-3.1117	0.196
C	-3.1118	5.0547	0.2874	C	6.8273	-3.6709	0.038
H	6.3539	1.0829	2.1386	H	2.9827	5.0833	-1.5263
H	4.604	1.2086	2.1922	H	2.9377	3.3661	-1.8855
H	5.4629	1.9427	0.0141	H	3.1563	3.742	0.5285
H	6.3167	0.4239	-0.2282	H	1.7249	4.7639	0.5614
H	5.3339	-0.9207	3.1744	H	1.2317	4.5473	-3.195
H	6.2876	-1.2895	1.7503	H	0.601	5.3119	-1.749
H	2.6278	-1.6527	-1.7221	H	-1.0368	1.2665	0.7712
H	2.9004	-3.0193	-0.7045	H	-2.056	1.8816	-0.4792
H	1.2375	-0.5515	-0.0314	H	0.3215	0.0028	-0.8314
H	0.712	-1.5004	2.1239	H	-0.0827	-0.0495	-3.2118
H	1.637	-2.9463	1.8106	H	-1.4684	1.0113	-3.0777
H	2.907	-1.4554	3.2528	H	0.4593	2.2738	-3.8665
H	2.6805	-0.105	2.1723	H	1.4636	1.6849	-2.5685
H	5.3895	-3.3998	1.3304	H	-1.633	4.6838	-2.0126
H	4.4343	-3.2901	2.8063	H	-1.2378	3.9827	-3.5794
H	3.6632	-3.7401	1.2852	H	-2.1486	3.0446	-2.396
H	5.1814	-1.7109	-1.6542	H	-0.8292	3.7357	1.183
H	0.8299	-4.4744	-0.4197	H	-0.33	-2.5054	-0.7433
H	-1.7066	-0.003	-2.821	H	-5.0142	0.072	-2.719
H	-2.3481	-0.6105	-4.3371	H	-5.8913	-1.152	-3.6206
H	-2.3535	-2.9217	-3.5014	H	-4.7448	-2.9702	-2.4284
H	-0.7561	-2.201	-3.3469	H	-3.5829	-1.8711	-3.1616
H	-4.4101	-1.3137	-3.3169	H	-7.0341	-1.9439	-1.6616
H	-4.1312	0.374	-2.9316	H	-7.2663	-0.2109	-1.7877
H	-4.3504	-2.803	0.9433	H	-4.8809	-1.8646	2.3281
H	-2.7666	-3.496	0.9408	H	-3.2895	-2.1255	1.7191
H	-1.7195	-1.3275	1.3535	H	-3.0564	0.2977	1.1812
H	-4.4943	-0.0643	1.4721	H	-5.8432	0.7423	2.2904
H	-2.9609	0.7486	1.6723	H	-4.7348	1.9404	1.6511
H	-3.9085	1.1127	-0.5685	H	-6.4833	1.3092	0.0227
H	-2.324	0.384	-0.6189	H	-4.8741	1.0173	-0.5811
H	-2.1052	-1.0222	5.0112	H	-1.416	-0.08	4.4573
H	-3.8739	-2.4895	4.7571	H	-3.4116	0.6818	5.3162
H	-4.605	-2.9377	3.1323	H	-4.9442	0.8814	4.3239
H	-5.7363	-1.2943	0.0559	H	-6.9534	-1.1438	1.8655
H	-5.9402	-0.0539	-1.1803	H	-8.0264	-0.4571	0.6458
H	-5.9654	-1.7573	-1.6274	H	-7.5985	-2.1647	0.5856
H	-3.2848	4.0716	2.1667	H	8.4787	-2.3361	-0.3604
H	-2.0833	5.3648	2.1496	H	8.1665	-2.6627	1.3459
H	-1.4075	6.214	-0.2603	H	5.4148	-4.2672	-1.471
H	-2.4771	5.8588	-1.6044	H	6.6822	-3.1938	-2.0316
H	-0.1223	1.5283	-0.8241	H	4.524	0.6269	-0.8683
H	0.5903	1.7369	0.746	H	5.1476	0.908	0.7283

H	2.0221	3.5704	-0.0537	H	3.6639	-0.7505	1.7379
H	2.1044	4.2269	-2.4136	H	1.8938	-1.8802	0.509
H	0.8518	3.0683	-2.8393	H	2.3499	-1.1079	-0.9984
H	0.6054	5.5061	-1.0365	H	3.9605	-3.1233	0.6203
H	-0.0888	5.3164	-2.6387	H	3.2316	-3.3713	-0.9584
H	3.085	1.9844	-3.2148	H	2.1136	0.8323	3.1139
H	-1.3247	2.4963	-2.4837	H	4.0167	-0.8171	-2.4521
H	-2.8362	2.9463	-1.7066	H	5.6625	-1.2451	-2.9072
H	-2.1731	3.9485	-3	H	4.356	-2.4289	-3.0683
H	-0.237	2.0086	2.5127	H	7.0509	0.883	1.2537
H	-3.6057	-4.2331	-1.3495	H	-4.5639	-3.7461	0.2574
H	-3.789	4.3059	-0.1392	H	7.4749	-4.5356	-0.1472
H	-3.7232	5.9354	0.5157	H	6.1809	-3.9337	0.8838

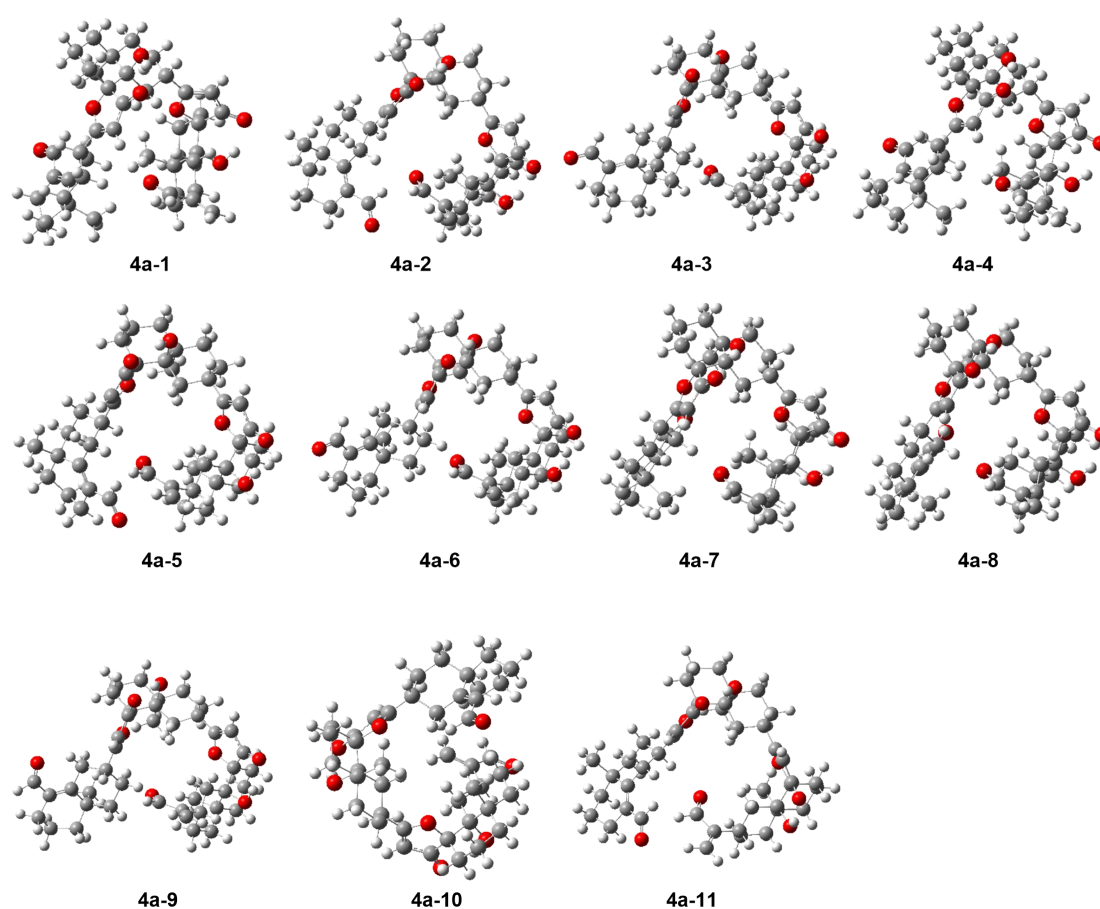


Figure S21. Optimized geometries of predominant conformers for **4a** at the B3LYP/6-31G (d,p) level

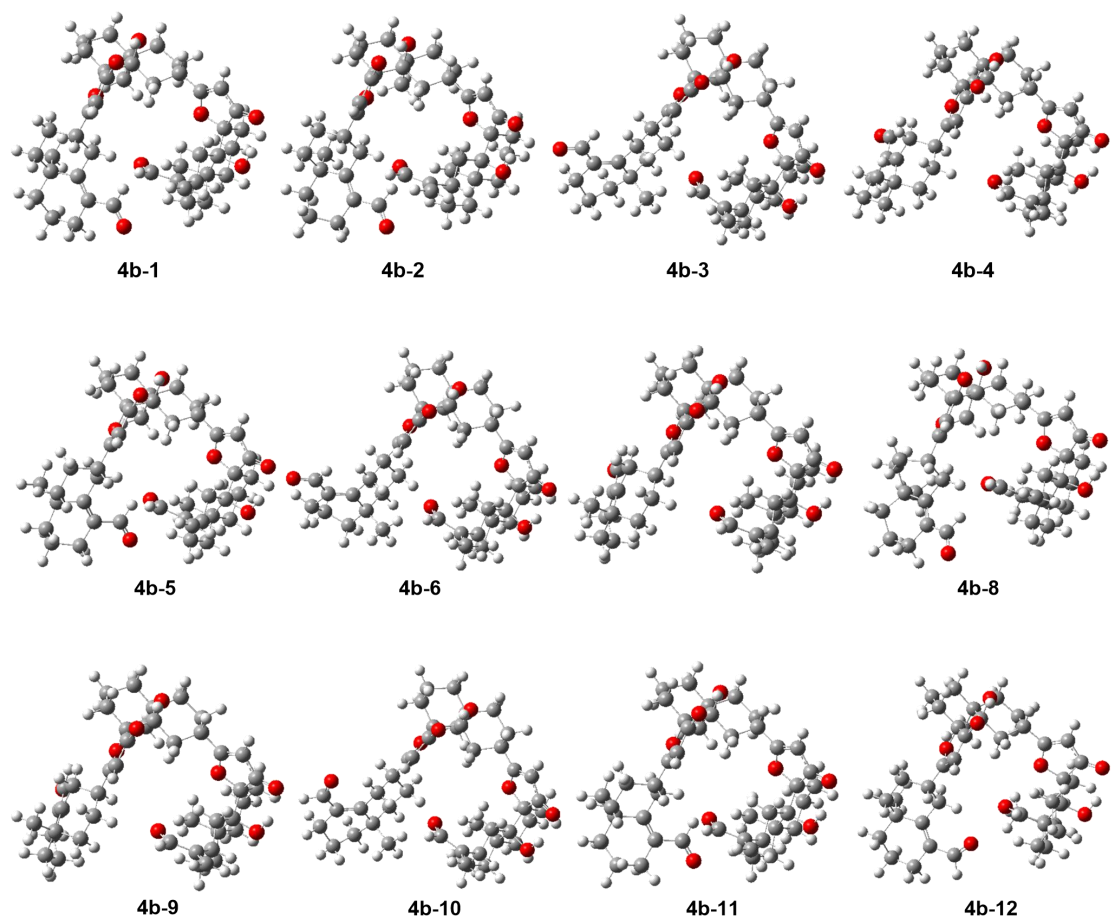
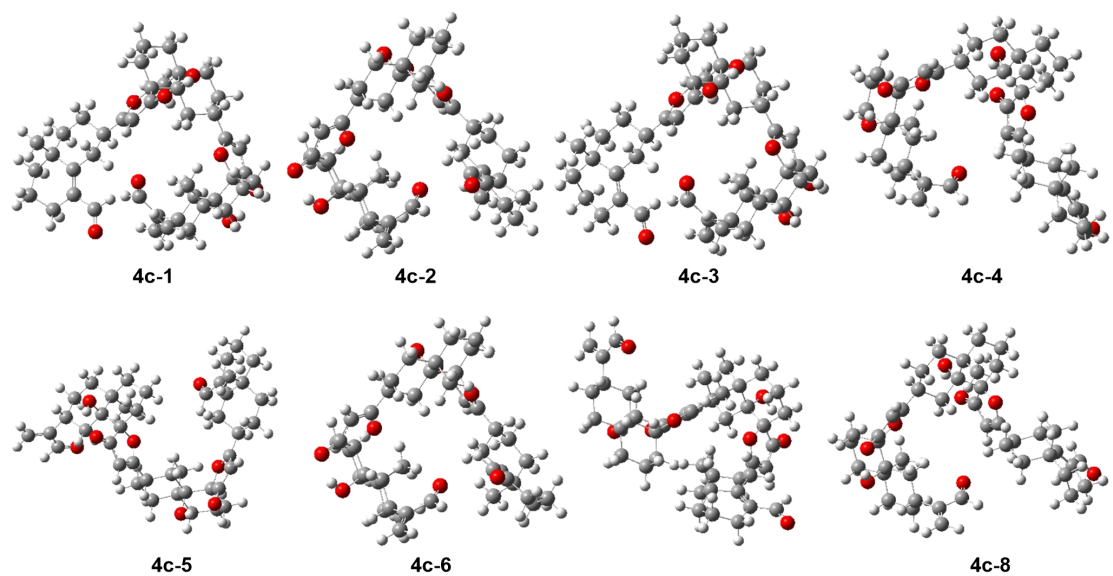


Figure S22. Optimized geometries of predominant conformers for **4b** at the B3LYP/6-31G (d,p) level



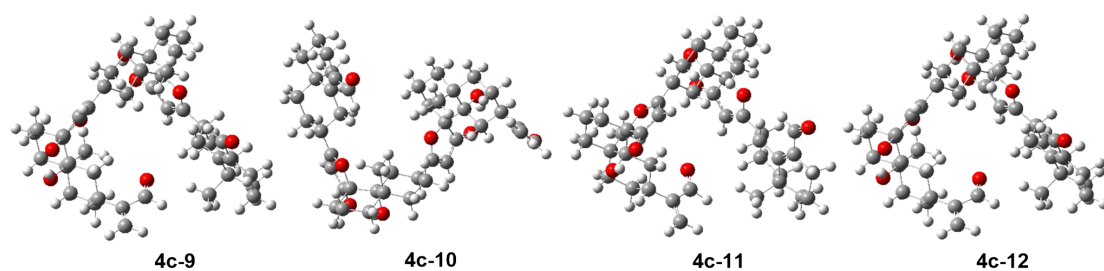


Figure S23. Optimized geometries of predominant conformers for **4c** at the B3LYP/6-31G (d,p) level

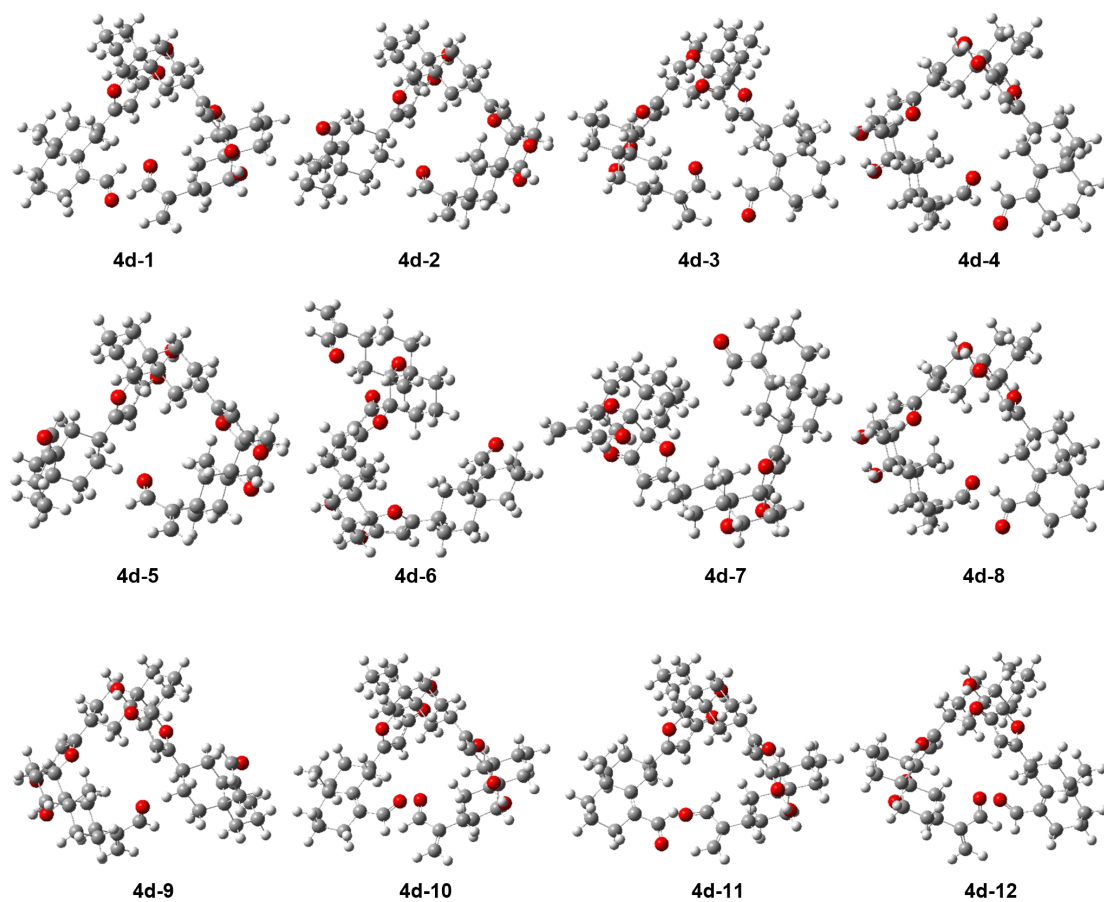


Figure S24. Optimized geometries of predominant conformers for **4d** at the B3LYP/6-31G (d,p) level

Table S8. Conformational analysis of the optimized **4a-4d** at the B3LYP/6-31G(d,p) level in the gas phase

	<i>Conformers</i>	G (Hartree)	ΔG (Kcal/mol)	Population
4a	4a-1	-2273.33080	0.23406123	20.88%
	4a-2	-2273.33117	0	30.99%
	4a-3	-2273.33108	0.05584839	28.21%

	4a-4	-2273.32889	1.43448786	2.75%
	4a-5	-2273.32875	1.5185742	2.39%
	4a-6	-2273.32965	0.95193267	6.21%
	4a-7	-2273.32688	2.69139039	0.33%
	4a-8	-2273.32688	2.69076288	0.33%
	4a-9	-2273.32935	1.1420682	4.51%
	4a-10	-2273.32852	1.66352901	1.87%
	4a-11	-2273.32834	1.77459828	1.55%
	<i>Conformers</i>	G (Hartree)	ΔG (Kcal/mol)	Population
4b	4b-1	-2273.32986	0.76305216	9.82%
	4b-2	-2273.32834	1.71686736	1.96%
	4b-3	-2273.33063	0.27986946	22.21%
	4b-4	-2273.33107	0	35.62%
	4b-5	-2273.32890	1.36546176	3.55%
	4b-6	-2273.32863	1.5311244	2.68%
	4b-7	-2273.32996	0.69841863	10.95%
	4b-8	-2273.32506	3.77321763	0.06%
	4b-9	-2273.32996	0.69841863	10.95%
	4b-10	-2273.32804	1.90386534	1.43%
	4b-11	-2273.32735	2.33747475	0.69%
	4b-12	-2273.32516	3.70732908	0.07%
	<i>Conformers</i>	G (Hartree)	ΔG (Kcal/mol)	Population
4c	4c-1	-2273.33008	1.04605917	6.35%
	4c-2	-2273.32752	2.65122975	0.42%
	4c-3	-2273.32840	2.10090348	1.07%
	4c-4	-2273.33052	0.77120979	10.10%
	4c-5	-2273.33068	0.66955317	12.00%
	4c-6	-2273.32723	2.83446267	0.31%
	4c-7	-2273.33174	0	37.16%
	4c-8	-2273.32894	1.757028	1.91%
	4c-9	-2273.32935	1.50414147	2.93%
	4c-10	-2273.33127	0.2949297	22.58%
	4c-11	-2273.32908	1.6691766	2.22%

	4c-12	-2273.32935	1.50288645	2.94%
	<i>Conformers</i>	G (Hartree)	ΔG (Kcal/mol)	Population
4d	4d-1	-2273.32957	1.13955816	6.09%
	4d-2	-2273.33066	0.45996483	19.18%
	4d-3	-2273.32753	2.4221886	0.70%
	4d-4	-2273.32831	1.93084827	1.60%
	4d-5	-2273.32943	1.2299196	5.23%
	4d-6	-2273.33139	0	41.69%
	4d-7	-2273.32926	1.33785132	4.35%
	4d-8	-2273.32683	2.85893556	0.33%
	4d-9	-2273.33067	0.45306222	19.40%
	4d-10	-2273.32729	2.57216349	0.54%
	4d-11	-2273.32693	2.79994962	0.37%
	4d-12	-2273.32726	2.59098879	0.53%

Functional mPW1PW91		Solvent? PCM		Basis Set 6-311+G(d,p)			Type of Data Unscaled Shifts	
		DP4+	0.00%	0.00%	100.00%	0.00%	-	
Nuclei	sp2?	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	
C		18.3	21.71124	22.37611	21.83125	21.86178		
C		31.1	36.33472	36.31442	36.0008	36.08954		
C		91.9	98.32359	98.26312	98.53558	98.63436		
C		75.3	81.6234	81.69776	81.58459	81.67673		
C		37.5	42.64329	42.47866	42.63939	42.63689		
C		34	36.77877	36.75209	36.57267	36.60723		
C		31.1	34.1448	34.11459	34.98266	34.69681		
C		35.9	41.61404	41.3538	41.1075	40.53564		
C		25.6	28.86024	28.86506	27.36355	26.78691		
C		36.1	38.28298	38.41729	37.97265	37.81802		
C		20.8	21.08743	21.07235	21.10576	20.96887		
C	x	209.7	219.8436	219.74532	219.77354	219.8935		
C	x	197.7	209.27044	209.17991	209.42687	209.98241		
C	x	102	108.72491	108.63837	108.31259	108.07143		
C		18.3	21.90272	21.89574	22.11371	22.21984		
C		31.4	35.78217	35.84291	35.70376	35.43914		
C		92.1	99.19423	99.29608	98.80442	98.67876		
C		75.7	82.00326	82.2298	81.92231	82.10562		
C		37.5	42.54189	42.50907	42.54017	41.27425		
C		34.1	36.6924	36.66143	36.67963	35.99773		
C		32.5	34.42124	34.44377	34.97503	36.11811		
C		33.4	43.20152	43.53183	41.72165	43.35825		
C		26.8	28.13242	28.12192	27.87111	28.14699		
C		36.7	38.53513	38.58971	38.80583	38.85056		
C	x	154.8	162.73587	162.81674	163.05764	162.69117		
C	x	195	206.87033	206.6345	206.54441	206.6166		
C	x	134.2	150.69418	150.64576	149.38595	150.55471		
C		20.5	21.24859	22.88507	21.24496	21.28467		
C	x	209.9	220.01006	219.97521	220.10916	219.84339		
C		24.7	27.79854	27.43069	27.44988	27.47406		
C	x	134.4	141.91186	141.76958	142.04037	141.72484		
C	x	160.1	178.90296	179.45933	178.3352	178.97238		
C		36.9	43.36686	43.62503	43.28358	43.13361		
C		39.6	41.65417	41.5186	41.41964	41.57867		
C		26.9	30.61675	30.80064	31.00308	30.44242		
C		41.8	47.55591	47.15483	47.16475	46.80541		
C		26.3	28.45004	27.58925	27.69221	28.24022		
C		40.9	43.92124	43.69123	43.738	43.64987		
C	x	196.7	208.34031	208.49654	207.91073	208.26769		
C	x	102	108.06812	108.04379	108.41881	108.45609		
C		25.1	26.61205	26.83595	26.38836	26.59271		
C	x	190.8	200.27997	199.23253	198.84677	198.91827		
C		18.3	21.34572	21.32706	21.11142	21.12845		
H		1.95	2.03032	2.06824	2.0057	1.60952		
H		1.55	1.59242	1.61616	1.59104	2.04751		
H		2.48	2.2971	2.29921	2.30236	1.50858		
H		1.5	1.459	1.43686	1.47396	2.29777		
H		2.11	2.12713	2.06209	2.10006	1.18629		
H		1.08	1.18927	1.17159	1.1682	2.12127		
H		1.61	1.03238	1.00422	1.19792	1.81778		
H		2.14	2.08439	2.12611	1.93674	1.38494		
H		3.44	3.48431	3.47177	3.36732	3.36119		
H		1.83	1.6933	1.52526	1.52351	1.91251		
H		1.83	1.91681	2.07406	1.99739	1.64561		
H		1.14	1.20163	1.20062	1.20806	2.09753		
H		2.2	2.08819	2.0912	2.09186	1.19261		
H		1.34	2.04646	1.49023	2.00252	1.44069		
H		1.34	0.48697	2.0054	0.51355	0.47389		
H		1.34	1.60418	0.6261	1.56561	1.97956		

H		5.24	4.88096	4.90019	4.92285	5.04282	
H	x	5.56	5.47046	5.46782	5.47291	5.49489	
H		1.55	1.9878	1.95257	1.89432	1.85661	
H		1.55	1.53724	1.51758	1.46599	1.60262	
H		2.44	2.20933	2.19543	2.22176	2.2072	
H		1.42	1.37651	1.34566	1.26199	1.31136	
H		1.07	2.0409	2.03772	1.06352	1.99153	
H		2.1	1.10479	1.09044	2.05309	1.04603	
H		1.94	0.64394	0.64188	2.05388	0.66246	
H		1.25	2.21502	2.24049	0.81254	2.31038	
H		3.32	2.93977	2.94265	3.03474	2.95208	
H		1.69	1.22692	1.19305	2.21628	1.15057	
H		1.59	2.2167	2.27916	1.21217	2.26023	
H		2.2	1.98945	2.03365	2.02956	1.99122	
H		1.05	1.01316	1.04669	1.07042	1.01753	
H	x	9.5	9.72478	9.71967	9.74732	9.70429	
H	x	5.83	6.37701	6.4061	6.3897	6.41831	
H	x	6.06	6.87201	6.90209	6.87171	6.88525	
H		1.3	1.88661	1.93212	1.88956	1.83713	
H		1.3	0.3175	0.39908	1.72795	0.35205	
H		1.3	1.70042	1.77056	0.3977	1.71461	
H		2.17	2.30485	2.43539	2.02969	2.06732	
H		2.49	2.35133	2.24172	2.59837	2.60432	
H		1.27	1.44791	1.44498	1.40739	1.40845	
H		1.46	1.66976	1.62898	1.68047	1.63398	
H		2.41	2.73732	4.1406	2.51718	2.56053	
H		3.83	4.16208	2.62682	3.89824	3.91234	
H		2.74	2.94943	2.9415	2.94854	3.34559	
H		1.93	2.2313	2.65239	2.17017	2.18687	
H		2.01	2.43049	2.25418	1.82365	1.92243	
H		1.65	1.92814	1.72776	1.94102	1.87098	
H		1.49	1.66574	1.84169	1.61221	1.64391	
H	x	5.95	5.65976	5.6777	5.69197	5.70356	
H		1.12	1.96425	0.8175	1.03717	1.86202	
H		1.12	0.78592	1.99046	1.38198	0.86483	
H		1.12	1.2651	1.17771	1.63462	1.37125	
H	x	10.43	10.53428	10.66374	10.58585	10.54874	
H		5.02	4.75845	4.72221	4.70394	4.68062	
H		1.46	1.65069	1.64785	1.62225	1.65046	
H		1.55	1.68827	1.64713	1.69904	1.69621	





































Functional	Solvent?		Basis Set		Type of Data	
mPW1PW91	PCM		6-311+G(d,p)		Unscaled Shifts	
	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	 0.00%	 0.00%	 100.00%	 0.00%	–	–
sDP4+ (C data)	 12.21%	 3.20%	 66.27%	 18.33%	–	–
sDP4+ (all data)	 0.00%	 0.00%	 100.00%	 0.00%	–	–
uDP4+ (H data)	 0.00%	 0.00%	 100.00%	 0.00%	–	–
uDP4+ (C data)	 2.35%	 3.47%	 90.10%	 4.08%	–	–
uDP4+ (all data)	 0.00%	 0.00%	 100.00%	 0.00%	–	–
DP4+ (H data)	 0.00%	 0.00%	 100.00%	 0.00%	–	–
DP4+ (C data)	 0.47%	 0.18%	 98.12%	 1.23%	–	–
DP4+ (all data)	 0.00%	 0.00%	 100.00%	 0.00%	–	–

Figure S25. DP4+ analysis of experimental NMR data of **4** and unscaled shifts of **4a-4d** (Isomer 1-4)

Table S9. The Cartesian coordinates of the lowest energy conformers for **4a–4d** in the gas phase at the B3LYP/6-31G(d,p) level

4a-1	X axis(Å)	Y axis(Å)	Z axis(Å)	4a-2	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-0.2422	5.7818	-0.6601	C	0.6044	5.8243	-0.3409
C	-0.3579	5.1996	0.7489	C	0.1494	5.0856	0.9179
C	-0.0329	3.6973	0.797	C	0.377	3.5679	0.8349
C	1.3545	3.3986	0.1563	C	1.848	3.2312	0.4532
C	1.4194	3.9266	-1.3255	C	2.2532	3.926	-0.8998
C	1.091	5.4451	-1.3351	C	2.03	5.457	-0.7651
C	1.7771	1.9139	0.2178	C	2.1426	1.7182	0.3906
C	3.1894	1.6945	-0.3735	C	3.6181	1.4203	0.0405
C	3.3236	2.2675	-1.7916	C	4.0904	2.1646	-1.2168
C	2.8601	3.7244	-1.8732	C	3.7594	3.6586	-1.1711
C	0.4457	3.2095	-2.2987	C	1.4607	3.4251	-2.1374
C	-0.1067	3.2086	2.225	C	-0.0213	2.9256	2.1428
O	0.6908	3.4694	3.1158	O	0.5681	3.0424	3.2088
O	2.3605	4.1356	0.9024	O	2.7217	3.7744	1.4776
C	3.5672	0.2365	-0.3483	C	3.8382	-0.0625	-0.1147
O	2.7174	-0.6406	-1.0134	O	2.956	-0.7337	-0.9543
C	4.6272	-0.2802	0.269	C	4.7776	-0.7821	0.4941
C	2.4933	-2.9224	-3.0803	C	2.6433	-2.626	-3.3439
C	3.6805	-2.544	-2.1933	C	3.7948	-2.5438	-2.3406
C	3.2517	-1.9709	-0.8342	C	3.3253	-2.1282	-0.9389
C	2.2495	-2.9155	-0.1071	C	2.1722	-3.0435	-0.4304
C	0.9876	-3.1921	-1.0058	C	0.9597	-3.0399	-1.4343
C	1.457	-3.7921	-2.3593	C	1.4688	-3.4706	-2.8378
C	1.8239	-2.4169	1.2943	C	1.6889	-2.7131	1.001
C	0.8547	-3.3992	1.9898	C	0.5851	-3.6856	1.4759
C	-0.3549	-3.7554	1.1112	C	-0.5808	-3.7893	0.4799
C	0.068	-4.2191	-0.2873	C	-0.1012	-4.0676	-0.9483
C	0.447	-2.9311	3.3732	C	0.1202	-3.3811	2.8864
C	-0.296	-1.6547	3.5585	C	-0.5518	-2.0921	3.2053
C	0.7315	-3.6235	4.4892	C	0.2861	-4.2373	3.9087
O	-0.6125	-0.9137	2.6361	O	-0.7816	-1.2222	2.3734
C	0.1341	-1.9326	-1.3028	C	0.2489	-1.6662	-1.572
C	4.4717	-1.7032	0.0185	C	4.4935	-2.1279	0.0223
O	5.2185	-2.55	0.4899	O	5.1075	-3.1135	0.4077
C	-5.1617	-1.5559	-2.5098	C	-5.9189	-2.057	-0.9087
C	-3.9867	-0.7501	-2.0048	C	-4.8204	-1.4115	-0.0956
C	-3.7818	-0.4593	-0.6962	C	-4.5472	-0.083	-0.1183
C	-4.7776	-0.9116	0.392	C	-5.3565	0.8844	-1.0052
C	-6.123	-1.401	-0.2117	C	-6.2092	0.1355	-2.0664
C	-2.5859	0.3066	-0.1465	C	-3.4631	0.5993	0.7075
C	-2.9948	1.4962	0.7399	C	-2.5288	1.4949	-0.1325
C	-3.8961	1.0119	1.8851	C	-3.357	2.5225	-0.9182
C	-5.1173	0.2709	1.3399	C	-4.4079	1.8316	-1.7845

C	-1.7699	2.2599	1.1892	C	-1.446	2.1897	0.667
C	-1.263	2.3498	2.4175	C	-1.207	2.1022	1.9746
O	-1.1083	2.9576	0.1785	O	-0.5749	2.9827	-0.0804
C	-4.1522	-2.0714	1.2031	C	-6.304	1.716	-0.108
C	-3.0619	-0.3227	-3.1027	C	-4.0832	-2.3917	0.7638
O	-3.2909	-0.5519	-4.2861	O	-4.2858	-3.6008	0.7126
O	2.9004	-4.1973	0.0991	O	2.6709	-4.4074	-0.3874
C	-5.9184	-2.3019	-1.4182	C	-6.9269	-1.0707	-1.4842
H	-1.076	5.4233	-1.2737	H	-0.0967	5.6202	-1.1577
H	-0.353	6.8715	-0.6086	H	0.5506	6.9049	-0.1621
H	0.3134	5.7527	1.4184	H	0.6848	5.499	1.7824
H	-1.3771	5.3815	1.1135	H	-0.9143	5.303	1.0793
H	1.8867	6.0033	-0.8247	H	2.7289	5.8744	-0.0285
H	1.0737	5.821	-2.366	H	2.2593	5.9571	-1.7147
H	1.8045	1.5774	1.2625	H	1.9408	1.2581	1.3671
H	1.0386	1.2826	-0.2895	H	1.4671	1.2328	-0.3228
H	3.9038	2.2353	0.2634	H	4.2359	1.7708	0.8794
H	4.3715	2.2124	-2.1139	H	5.1765	2.0481	-1.3266
H	2.7576	1.6597	-2.508	H	3.6511	1.717	-2.1168
H	2.9208	4.0603	-2.9164	H	4.0625	4.1202	-2.1196
H	3.5699	4.3505	-1.3172	H	4.377	4.1335	-0.398
H	-0.6039	3.438	-2.1042	H	0.4106	3.7234	-2.1272
H	0.6371	3.5243	-3.3319	H	1.8852	3.844	-3.058
H	0.5468	2.1213	-2.2726	H	1.4824	2.3371	-2.2416
H	2.2497	3.9307	1.855	H	2.3959	3.4758	2.3529
H	5.4023	0.1864	0.8457	H	5.5475	-0.4954	1.1839
H	2.0198	-2.0116	-3.463	H	2.3006	-1.6149	-3.5903
H	2.8615	-3.4609	-3.9619	H	3.015	-3.0548	-4.2823
H	4.3077	-3.4326	-2.0458	H	4.2993	-3.5175	-2.2973
H	4.2975	-1.8157	-2.7351	H	4.5343	-1.8279	-2.7219
H	1.8923	-4.7867	-2.1975	H	1.7847	-4.5217	-2.8149
H	0.5962	-3.9446	-3.023	H	0.6511	-3.4181	-3.568
H	2.7083	-2.3234	1.938	H	2.5264	-2.8043	1.7049
H	1.3878	-1.4162	1.2228	H	1.3507	-1.6738	1.057
H	1.4121	-4.3383	2.1245	H	1.044	-4.6853	1.5017
H	-0.9344	-4.5564	1.5879	H	-1.2594	-4.5948	0.7885
H	-1.0374	-2.9039	1.0208	H	-1.1792	-2.8735	0.4833
H	0.5764	-5.1878	-0.1987	H	0.3067	-5.0857	-0.9906
H	-0.8317	-4.4085	-0.8868	H	-0.968	-4.0659	-1.6217
H	-0.5543	-1.3991	4.6004	H	-0.8443	-1.9541	4.2603
H	0.4434	-3.2897	5.4816	H	-0.0469	-4.0227	4.9197
H	1.2733	-4.5647	4.4392	H	0.7662	-5.2007	3.7571
H	0.6109	-1.2372	-1.9964	H	0.8571	-0.9154	-2.0801
H	-0.8198	-2.2138	-1.7647	H	-0.6667	-1.7671	-2.1677
H	-0.0965	-1.3686	-0.3977	H	-0.0434	-1.2424	-0.6077
H	-5.8511	-0.8738	-3.024	H	-6.4735	-2.7811	-0.2992
H	-4.8303	-2.2951	-3.2494	H	-5.4542	-2.6181	-1.7297

H	-6.732	-0.5423	-0.5266	H	-5.5694	-0.2131	-2.8889
H	-6.7131	-1.9307	0.5467	H	-6.942	0.816	-2.5181
H	-1.9742	-0.39	0.4367	H	-3.9528	1.1946	1.4891
H	-1.928	0.6745	-0.9354	H	-2.8396	-0.1226	1.2332
H	-3.5904	2.1904	0.1289	H	-2.014	0.8477	-0.8578
H	-3.3431	0.3575	2.5692	H	-3.8349	3.2345	-0.2344
H	-4.2386	1.8681	2.4799	H	-2.7073	3.1157	-1.5742
H	-5.7225	-0.0864	2.1831	H	-4.9921	2.5964	-2.3125
H	-5.7391	1.0029	0.806	H	-3.8769	1.2632	-2.5609
H	-1.5676	1.9022	3.3434	H	-1.6929	1.542	2.75
H	-3.2572	-1.7644	1.7519	H	-5.7618	2.3424	0.6072
H	-4.8614	-2.4599	1.943	H	-6.9283	2.3852	-0.7113
H	-3.857	-2.9054	0.5568	H	-6.9739	1.0762	0.4769
H	-2.1517	0.2165	-2.814	H	-3.3446	-1.988	1.466
H	3.7735	-4.0404	0.5165	H	3.5117	-4.4171	0.1163
H	-5.3713	-3.2078	-1.1334	H	-7.6338	-0.7591	-0.7068
H	-6.8884	-2.6336	-1.8065	H	-7.5195	-1.5651	-2.2627
4a-3	X axis(Å)	Y axis(Å)	Z axis(Å)	4a-4	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-2.2971	4.8121	-0.4649	C	-1.3456	5.5815	-0.5061
C	-2.1335	4.1633	0.9099	C	-1.3313	4.9439	0.8833
C	-1.1703	2.9642	0.8866	C	-0.7108	3.5364	0.883
C	0.201	3.3545	0.2618	C	0.703	3.5426	0.2309
C	0.0172	3.937	-1.1892	C	0.6487	4.1194	-1.2331
C	-0.9572	5.1457	-1.1283	C	0.0228	5.5407	-1.193
C	1.2444	2.216	0.2575	C	1.4143	2.1716	0.2431
C	2.6033	2.6859	-0.3119	C	2.8367	2.257	-0.359
C	2.462	3.3349	-1.6963	C	2.842	2.8911	-1.7572
C	1.394	4.4318	-1.7148	C	2.0961	4.2277	-1.7895
C	-0.5354	2.9153	-2.2188	C	-0.1696	3.2527	-2.2275
C	-1.0117	2.4144	2.2868	C	-0.6757	3.0002	2.2954
O	-0.4069	2.9516	3.205	O	0.065	3.3831	3.1911
O	0.7716	4.4219	1.0664	O	1.5472	4.442	0.999
C	3.5944	1.5524	-0.3508	C	3.4959	0.9027	-0.3854
O	3.223	0.4244	-1.0738	O	2.8235	-0.105	-1.0678
C	4.7759	1.5316	0.2617	C	4.6479	0.5877	0.2022
C	4.0219	-1.6136	-3.2439	C	2.9988	-2.3393	-3.1874
C	4.9246	-0.7943	-2.3203	C	4.1101	-1.7605	-2.3101
C	4.2928	-0.5373	-0.9441	C	3.6075	-1.3105	-0.9304
C	3.8177	-1.8624	-0.2782	C	2.8202	-2.4457	-0.2116
C	2.8043	-2.626	-1.2093	C	1.6157	-2.9391	-1.0963
C	3.4825	-2.887	-2.5822	C	2.1627	-3.4072	-2.4726
C	3.2232	-1.675	1.1379	C	2.3367	-2.0693	1.2089
C	2.7981	-3.0192	1.7707	C	1.5875	-3.2335	1.8951
C	1.8689	-3.8345	0.8571	C	0.4514	-3.7973	1.0271
C	2.4436	-3.9895	-0.5556	C	0.926	-4.1397	-0.3896
C	2.2347	-2.8499	3.1682	C	1.1247	-2.8795	3.2949
C	0.9942	-2.06	3.3993	C	0.1541	-1.7734	3.52

C	2.8119	-3.3872	4.2563	C	1.5587	-3.5253	4.3905
O	0.3687	-1.5028	2.506	O	-0.3191	-1.0924	2.6186
C	1.4773	-1.8637	-1.4591	C	0.5302	-1.8604	-1.3459
C	5.2704	0.2031	-0.0593	C	4.7696	-0.8309	-0.0899
O	6.3198	-0.2441	0.3832	O	5.6777	-1.5268	0.3439
C	-7.0461	-2.5682	-0.7022	C	-5.166	-2.1213	-2.455
C	-6.2853	-1.3879	-0.1427	C	-3.9531	-1.3603	-1.9777
C	-4.9905	-1.1169	-0.4413	C	-3.6488	-1.2081	-0.666
C	-4.1758	-2.0358	-1.3779	C	-4.4582	-1.9102	0.4451
C	-4.886	-3.3935	-1.637	C	-5.5977	-2.814	-0.1044
C	-4.2044	0.0828	0.0747	C	-2.5712	-0.2824	-0.1219
C	-2.8604	-0.3159	0.7122	C	-3.1954	0.8119	0.767
C	-2.0213	-1.1505	-0.2585	C	-4.0347	0.1861	1.896
C	-2.7986	-2.3701	-0.746	C	-5.0689	-0.8095	1.3528
C	-2.0967	0.8996	1.1714	C	-2.1329	1.7787	1.2358
C	-1.6731	1.1269	2.4127	C	-1.6465	1.9323	2.466
O	-1.8061	1.8595	0.2061	O	-1.6204	2.6146	0.2433
C	-3.9702	-1.3212	-2.7348	C	-3.5509	-2.8428	1.285
C	-7.1216	-0.5337	0.7584	C	-3.1521	-0.7537	-3.0868
O	-8.2564	-0.8482	1.1021	O	-3.4741	-0.8507	-4.2665
O	4.9719	-2.7305	-0.1224	O	3.7086	-3.583	-0.0492
C	-6.3731	-3.2263	-1.8995	C	-6.2283	-2.2643	-1.3717
H	-2.8845	4.1524	-1.1132	H	-2.0953	5.0825	-1.13
H	-2.8844	5.7322	-0.3602	H	-1.6724	6.6246	-0.4192
H	-1.7774	4.9201	1.6206	H	-0.7794	5.5992	1.5694
H	-3.1247	3.8501	1.2623	H	-2.3634	4.9062	1.2549
H	-0.4941	5.9721	-0.5735	H	0.6944	6.2307	-0.6655
H	-1.1455	5.5301	-2.1389	H	-0.0772	5.938	-2.2112
H	1.4226	1.8698	1.2841	H	1.5178	1.8148	1.2763
H	0.8658	1.3501	-0.2977	H	0.8118	1.4218	-0.2823
H	3.0009	3.4537	0.367	H	3.4354	2.9074	0.2944
H	2.2266	2.578	-2.4544	H	3.8771	3.0572	-2.0828
H	3.4223	3.7727	-1.998	H	2.4032	2.2059	-2.4928
H	1.2945	4.8157	-2.7382	H	2.0798	4.6023	-2.821
H	1.7493	5.2781	-1.1127	H	2.6709	4.9648	-1.2141
H	-1.5756	2.6388	-2.0362	H	-1.242	3.2595	-2.0237
H	-0.5085	3.3393	-3.2301	H	-0.0539	3.6321	-3.2502
H	0.0427	1.9879	-2.2459	H	0.1478	2.2066	-2.2372
H	0.7727	4.1335	2.0039	H	1.4877	4.1881	1.9445
H	5.263	2.264	0.876	H	5.3263	1.1811	0.7841
H	3.1914	-0.9885	-3.5899	H	2.3521	-1.5276	-3.5384
H	4.5846	-1.8886	-4.1441	H	3.4446	-2.7774	-4.0884
H	5.8808	-1.3205	-2.2033	H	4.8984	-2.5156	-2.1955
H	5.1535	0.1574	-2.817	H	4.5654	-0.9157	-2.8427
H	4.3147	-3.5926	-2.4608	H	2.7833	-4.3036	-2.3439
H	2.7744	-3.3716	-3.2665	H	1.3332	-3.7066	-3.126
H	3.9775	-1.2291	1.7994	H	3.2003	-1.8226	1.8403

H	2.3861	-0.9712	1.107	H	1.7164	-1.169	1.1703
H	3.7168	-3.6167	1.87	H	2.3171	-4.0506	1.999
H	1.7149	-4.8332	1.2857	H	0.0471	-4.7054	1.4925
H	0.8752	-3.3772	0.7977	H	-0.3839	-3.0919	0.9695
H	3.3309	-4.6337	-0.5059	H	1.6127	-4.9942	-0.3345
H	1.7184	-4.5293	-1.1779	H	0.0671	-4.4854	-0.9791
H	0.6564	-1.997	4.4478	H	-0.1259	-1.5899	4.5714
H	2.4115	-3.2657	5.2584	H	1.2312	-3.2721	5.3945
H	3.7214	-3.9767	4.1723	H	2.2701	-4.3434	4.311
H	1.5918	-0.9941	-2.1092	H	0.85	-1.0719	-2.03
H	0.7442	-2.5142	-1.9511	H	-0.3629	-2.3085	-1.798
H	1.0251	-1.5086	-0.5316	H	0.2163	-1.3706	-0.4227
H	-7.1678	-3.3104	0.0973	H	-5.6341	-1.6133	-3.3065
H	-8.053	-2.2632	-1.0129	H	-4.8483	-3.1119	-2.8034
H	-4.766	-4.056	-0.7687	H	-6.3725	-2.9602	0.6587
H	-4.4198	-3.9142	-2.483	H	-5.2077	-3.8159	-0.3327
H	-4.0398	0.7694	-0.7659	H	-1.8434	-0.8673	0.4481
H	-4.7598	0.662	0.8152	H	-1.9923	0.1997	-0.9116
H	-3.0796	-0.941	1.5902	H	-3.8917	1.395	0.1454
H	-1.6914	-0.5481	-1.1134	H	-3.39	-0.3213	2.6231
H	-1.1132	-1.4955	0.2467	H	-4.5608	0.9751	2.4483
H	-2.179	-2.9235	-1.4635	H	-5.5923	-1.2681	2.2015
H	-2.9413	-3.0393	0.114	H	-5.8266	-0.2449	0.7934
H	-1.7521	0.5311	3.3011	H	-1.8561	1.4126	3.3804
H	-3.3909	-0.3974	-2.6395	H	-2.7639	-2.3108	1.825
H	-3.4311	-1.9651	-3.4393	H	-4.1389	-3.3839	2.036
H	-4.9251	-1.0499	-3.1981	H	-3.0579	-3.5876	0.6488
H	-6.6804	0.4061	1.1116	H	-2.2332	-0.2223	-2.8094
H	5.6845	-2.2246	0.3218	H	4.5441	-3.2709	0.3576
H	-6.5395	-2.6266	-2.8016	H	-7.0186	-2.9396	-1.7191
H	-6.8324	-4.204	-2.0861	H	-6.7021	-1.2953	-1.1738
4a-5	X axis(Å)	Y axis(Å)	Z axis(Å)	4a-6	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-0.0756	5.812	-0.407	C	-2.2195	4.895	-0.4401
C	-0.4238	5.0525	0.8732	C	-2.0974	4.2136	0.9232
C	-0.0271	3.5686	0.8139	C	-1.1593	2.9949	0.8929
C	1.4663	3.3925	0.4122	C	0.2322	3.3693	0.3043
C	1.7693	4.1018	-0.9599	C	0.0901	3.986	-1.1372
C	1.3757	5.6001	-0.8493	C	-0.8597	5.2137	-1.0695
C	1.9296	1.9217	0.3715	C	1.2515	2.2091	0.2964
C	3.4244	1.787	0.0025	C	2.6312	2.6615	-0.2362
C	3.7904	2.5547	-1.2761	C	2.5313	3.3421	-1.6089
C	3.2919	4.0018	-1.2523	C	1.4874	4.4621	-1.6247
C	1.0202	3.4896	-2.1742	C	-0.4628	2.9983	-2.1994
C	-0.3307	2.9128	2.1403	C	-1.0413	2.4113	2.2834
O	0.2626	3.1111	3.1921	O	-0.4454	2.9159	3.2256
O	2.2883	4.0514	1.4113	O	0.8084	4.4069	1.143
C	3.8104	0.3363	-0.1282	C	3.5986	1.5079	-0.2803

O	3.0091	-0.4445	-0.9542	O	3.2144	0.4007	-1.0282
C	4.8257	-0.2617	0.4901	C	4.7698	1.4511	0.3494
C	2.9175	-2.4004	-3.3133	C	3.9994	-1.6205	-3.2179
C	4.0505	-2.1695	-2.3122	C	4.9068	-0.8365	-2.2685
C	3.535	-1.7875	-0.9172	C	4.2603	-0.5866	-0.8978
C	2.4933	-2.8198	-0.3925	C	3.7459	-1.9109	-0.2598
C	1.2902	-2.9726	-1.396	C	2.7298	-2.6371	-1.2175
C	1.8476	-3.366	-2.7921	C	3.4222	-2.8916	-2.5845
C	1.9726	-2.5212	1.0327	C	3.1344	-1.732	1.15
C	0.9863	-3.6046	1.5253	C	2.6699	-3.0758	1.7555
C	-0.1571	-3.8609	0.5311	C	1.7377	-3.857	0.8156
C	0.3538	-4.107	-0.892	C	2.3299	-4.0024	-0.5909
C	0.4854	-3.3276	2.9292	C	2.0878	-2.9145	3.1462
C	-0.3342	-2.1201	3.221	C	0.8617	-2.1	3.3691
C	0.7483	-4.137	3.9691	C	2.6348	-3.4809	4.2352
O	-0.6628	-1.3	2.3718	O	0.2641	-1.5154	2.4741
C	0.4267	-1.6921	-1.5572	C	1.4235	-1.8419	-1.474
C	4.6951	-1.6389	0.0424	C	5.2406	0.1179	0.0131
O	5.416	-2.5421	0.4441	O	6.2737	-0.3592	0.4628
C	-5.5051	-2.5733	-1.1329	C	-6.8158	-2.7308	-0.6286
C	-4.6271	-1.866	-0.1293	C	-6.2076	-1.4189	-0.1949
C	-4.5891	-0.5171	-0.0033	C	-4.987	-0.9981	-0.6063
C	-5.5457	0.3992	-0.7935	C	-4.1686	-1.7817	-1.6552
C	-6.5493	-0.3839	-1.6861	C	-4.9183	-3.0242	-2.2122
C	-3.5774	0.2543	0.8317	C	-4.2377	0.2011	-0.0434
C	-2.7172	1.1836	-0.0561	C	-2.911	-0.2439	0.6083
C	-3.6108	2.1031	-0.9114	C	-2.0573	-1.0903	-0.347
C	-4.6794	1.3228	-1.6855	C	-2.8526	-2.2389	-0.9758
C	-1.6947	2.0007	0.7064	C	-2.1327	0.9441	1.1121
C	-1.4276	1.9682	2.0111	C	-1.7309	1.1351	2.3666
O	-0.9212	2.8613	-0.073	O	-1.8036	1.9194	0.1751
C	-6.4114	1.2529	0.1659	C	-3.8476	-0.8957	-2.8845
C	-3.7793	-2.7952	0.681	C	-7.0623	-0.6512	0.7631
O	-3.7966	-4.0124	0.5284	O	-8.1209	-1.0859	1.2043
O	3.1447	-4.1167	-0.3254	O	4.878	-2.8069	-0.1009
C	-5.9556	-1.6568	-2.2638	C	-5.7796	-3.7102	-1.1664
H	-0.7615	5.513	-1.2073	H	-2.8074	4.2621	-1.1141
H	-0.2491	6.883	-0.2475	H	-2.7893	5.825	-0.327
H	0.0752	5.541	1.7201	H	-1.7402	4.9472	1.6572
H	-1.5025	5.1517	1.0498	H	-3.102	3.9141	1.2489
H	2.0339	6.1088	-0.1328	H	-0.3906	6.0182	-0.488
H	1.5323	6.1037	-1.8118	H	-1.0194	5.6233	-2.0751
H	1.7956	1.4609	1.3592	H	1.4018	1.8379	1.3187
H	1.3038	1.3485	-0.3219	H	0.8659	1.3634	-0.2844
H	4.01	2.2229	0.8243	H	3.0313	3.4061	0.4667
H	4.881	2.5601	-1.4019	H	3.5065	3.7654	-1.8824
H	3.3919	2.0421	-2.1602	H	2.2951	2.6065	-2.3874

H	3.5261	4.4755	-2.2143	H	1.4167	4.8697	-2.6413
H	3.863	4.5595	-0.4989	H	1.8482	5.2875	-0.9975
H	-0.0568	3.6661	-2.1505	H	-1.5124	2.7411	-2.0441
H	1.3795	3.9363	-3.1094	H	-0.4056	3.4425	-3.2007
H	1.1648	2.4094	-2.2597	H	0.0955	2.0591	-2.2343
H	2.013	3.7337	2.2972	H	0.7844	4.0987	2.0739
H	5.5586	0.1221	1.173	H	5.2628	2.1622	0.9837
H	2.461	-1.4397	-3.5764	H	3.1881	-0.9713	-3.5653
H	3.3372	-2.7991	-4.2446	H	4.5688	-1.8938	-4.1144
H	4.6635	-3.078	-2.2532	H	5.8489	-1.3861	-2.146
H	4.7033	-1.3799	-2.706	H	5.1644	0.1173	-2.7466
H	2.2825	-4.3731	-2.7511	H	4.2367	-3.6175	-2.4625
H	1.0304	-3.4207	-3.5226	H	2.7138	-3.3494	-3.2866
H	2.8138	-2.5032	1.7379	H	3.8883	-1.3133	1.8295
H	1.5177	-1.5264	1.0701	H	2.3139	-1.0091	1.1175
H	1.5569	-4.5443	1.571	H	3.5737	-3.6947	1.8602
H	-0.7385	-4.7339	0.8543	H	1.5564	-4.8587	1.2261
H	-0.8575	-3.0207	0.5181	H	0.7549	-3.378	0.7488
H	0.8762	-5.0719	-0.9167	H	3.2022	-4.6667	-0.5386
H	-0.5063	-4.2167	-1.5651	H	1.6025	-4.5164	-1.2323
H	-0.6436	-1.9959	4.273	H	0.5079	-2.0448	4.4128
H	0.3902	-3.9421	4.9755	H	2.2206	-3.365	5.2324
H	1.3389	-5.0401	3.8375	H	3.532	-4.0896	4.1569
H	0.9462	-0.8847	-2.0767	H	1.5668	-0.964	-2.1069
H	-0.4695	-1.9073	-2.1522	H	0.6848	-2.468	-1.989
H	0.0846	-1.2891	-0.6004	H	0.9637	-1.4933	-0.5476
H	-4.9726	-3.4171	-1.5878	H	-7.3239	-3.2203	0.2108
H	-6.3788	-2.9842	-0.6119	H	-7.5754	-2.5315	-1.3948
H	-6.9164	0.2535	-2.5003	H	-4.2054	-3.7451	-2.6321
H	-7.4361	-0.6642	-1.1004	H	-5.5727	-2.728	-3.044
H	-4.1048	0.8289	1.6023	H	-4.0628	0.928	-0.8453
H	-2.9055	-0.4068	1.378	H	-4.8121	0.745	0.7098
H	-2.1489	0.5422	-0.7462	H	-3.1658	-0.8809	1.4685
H	-4.0866	2.8629	-0.2792	H	-1.6225	-0.4663	-1.1372
H	-2.9988	2.6542	-1.6371	H	-1.2118	-1.5162	0.2043
H	-5.3173	2.0393	-2.2187	H	-2.2098	-2.7532	-1.7017
H	-4.1748	0.7275	-2.4582	H	-3.0741	-2.9721	-0.189
H	-1.8419	1.3798	2.8068	H	-1.8401	0.5214	3.2395
H	-6.9909	0.6145	0.8437	H	-3.2283	-0.027	-2.6445
H	-5.826	1.9336	0.7899	H	-3.3064	-1.47	-3.646
H	-7.1214	1.8702	-0.3974	H	-4.7677	-0.5168	-3.3453
H	-3.144	-2.3472	1.4544	H	-6.7141	0.3483	1.0524
H	3.9805	-4.0211	0.1775	H	5.5949	-2.3242	0.3618
H	-6.7023	-2.1719	-2.8789	H	-6.2869	-4.5752	-1.6088
H	-5.1103	-1.4206	-2.9211	H	-5.1574	-4.0916	-0.3481
4a-7	X axis(Å)	Y axis(Å)	Z axis(Å)	4a-8	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-1.5638	5.5763	-0.5137	C	-2.0834	5.4253	-0.502

C	-1.5613	4.9312	0.8727	C	-1.9861	4.7973	0.8893
C	-0.909	3.5388	0.8753	C	-1.2268	3.4604	0.8788
C	0.517	3.5822	0.2518	C	0.1731	3.6145	0.2142
C	0.4784	4.1651	-1.2102	C	0.0456	4.1758	-1.2511
C	-0.1821	5.571	-1.1752	C	-0.7274	5.5233	-1.2088
C	1.2635	2.2295	0.2732	C	1.0344	2.3316	0.229
C	2.696	2.3577	-0.2954	C	2.4357	2.5813	-0.3757
C	2.7122	2.9928	-1.693	C	2.3574	3.1876	-1.7836
C	1.9336	4.3104	-1.7374	C	1.4684	4.4342	-1.8227
C	-0.299	3.2843	-2.2248	C	-0.6844	3.2229	-2.235
C	-0.8879	2.9902	2.2831	C	-1.1183	2.9202	2.2857
O	-0.1855	3.3935	3.201	O	-0.4346	3.3906	3.1854
O	1.3235	4.4987	1.0425	O	0.9178	4.607	0.974
C	3.4009	1.0263	-0.3037	C	3.2672	1.3256	-0.3735
O	2.7824	-0.0045	-1.0023	O	2.7382	0.2207	-1.0306
C	4.5479	0.7522	0.3135	C	4.4499	1.1827	0.2201
C	3.1046	-2.2134	-3.1321	C	3.2451	-2.0009	-3.1214
C	4.167	-1.5963	-2.2212	C	4.253	-1.2502	-2.2502
C	3.6095	-1.1785	-0.8521	C	3.6833	-0.8609	-0.8777
C	2.8515	-2.3515	-0.1631	C	3.0676	-2.0895	-0.1442
C	1.6933	-2.8882	-1.0834	C	1.9605	-2.775	-1.0261
C	2.2957	-3.3214	-2.4479	C	2.5801	-3.1741	-2.3929
C	2.3154	-2.0089	1.2473	C	2.5188	-1.7655	1.2657
C	1.602	-3.2123	1.9039	C	1.9487	-3.0179	1.9686
C	0.5119	-3.8138	1.0028	C	0.9245	-3.7697	1.1037
C	1.036	-4.1226	-0.4043	C	1.4582	-4.0566	-0.3041
C	1.0949	-2.8966	3.2976	C	1.4202	-2.7116	3.3565
C	0.0674	-1.8415	3.5143	C	0.2776	-1.7763	3.5487
C	1.5382	-3.5325	4.3953	C	1.9442	-3.2508	4.4704
O	-0.4227	-1.1768	2.6103	O	-0.295	-1.2033	2.6304
C	0.5709	-1.8542	-1.3543	C	0.7259	-1.8782	-1.2949
C	4.7292	-0.6599	0.0221	C	4.764	-0.2112	-0.0425
O	5.6505	-1.3237	0.4779	O	5.7572	-0.7671	0.4074
C	-4.5742	-2.6535	-2.7083	C	-4.6184	-2.8697	-2.7035
C	-3.6684	-1.5992	-2.1313	C	-3.7283	-1.7861	-2.1557
C	-3.5604	-1.3276	-0.8105	C	-3.545	-1.5477	-0.8359
C	-4.4362	-2.0404	0.2318	C	-4.253	-2.3908	0.2379
C	-5.6027	-2.8246	-0.4333	C	-5.3949	-3.2602	-0.3609
C	-2.5796	-0.3253	-0.2207	C	-2.6409	-0.4538	-0.2842
C	-3.2761	0.7164	0.6698	C	-3.3517	0.4456	0.7441
C	-4.0748	0.0071	1.7771	C	-3.9547	-0.4072	1.8708
C	-5.0718	-0.9941	1.1871	C	-4.8981	-1.4704	1.3076
C	-2.2722	1.726	1.1779	C	-2.4209	1.5382	1.2207
C	-1.8141	1.8785	2.4191	C	-1.9315	1.7262	2.4449
O	-1.7832	2.6035	0.2117	O	-2.0487	2.4598	0.2429
C	-3.5719	-3.037	1.0389	C	-3.2195	-3.3282	0.9049
C	-2.877	-0.8763	-3.1695	C	-3.0396	-1.0134	-3.2335

O	-2.7721	0.3422	-3.2182	O	-1.8554	-0.7069	-3.2125
O	3.783	-3.4525	0.0133	O	4.1161	-3.0783	0.0455
C	-5.1503	-3.6018	-1.6624	C	-4.9945	-3.9249	-1.6704
H	-2.2898	5.0636	-1.1544	H	-2.7856	4.8492	-1.1148
H	-1.9163	6.6111	-0.4276	H	-2.515	6.4295	-0.4132
H	-1.038	5.5949	1.5729	H	-1.4952	5.5068	1.5676
H	-2.5992	4.8671	1.2241	H	-3.0039	4.6548	1.2746
H	0.4629	6.274	-0.6321	H	-0.1254	6.2838	-0.6944
H	-0.2726	5.9708	-2.1933	H	-0.8827	5.9014	-2.2274
H	1.3531	1.8698	1.3067	H	1.1804	1.9923	1.2629
H	0.6941	1.4668	-0.2701	H	0.522	1.5162	-0.2942
H	3.2589	3.0272	0.3707	H	2.947	3.3152	0.2635
H	3.7487	3.1855	-1.9988	H	3.364	3.4619	-2.1246
H	2.3046	2.2973	-2.4368	H	1.988	2.4459	-2.5021
H	1.9286	4.6875	-2.7682	H	1.403	4.7937	-2.8577
H	2.4782	5.0601	-1.1489	H	1.9638	5.2359	-1.2599
H	-1.3754	3.266	-2.0437	H	-1.7512	3.1226	-2.026
H	-0.1707	3.6706	-3.2434	H	-0.6128	3.6043	-3.261
H	0.0424	2.2458	-2.2317	H	-0.2616	2.2148	-2.2386
H	1.2442	4.2407	1.9852	H	0.8981	4.3462	1.919
H	5.1894	1.3696	0.912	H	5.0404	1.8758	0.7873
H	2.4338	-1.4265	-3.4943	H	2.4836	-1.3013	-3.4833
H	3.592	-2.6247	-4.0243	H	3.7548	-2.3776	-4.0162
H	4.9827	-2.3191	-2.0907	H	5.1445	-1.8778	-2.1229
H	4.6009	-0.7292	-2.7355	H	4.5795	-0.3545	-2.7941
H	2.9498	-4.192	-2.3093	H	3.3305	-3.9621	-2.2484
H	1.4971	-3.6498	-3.1254	H	1.81	-3.6072	-3.044
H	3.1508	-1.7297	1.9027	H	3.3293	-1.3794	1.8978
H	1.6561	-1.1371	1.2002	H	1.7695	-0.9704	1.2071
H	2.3636	-3.9987	2.0152	H	2.7944	-3.7101	2.0966
H	0.1341	-4.7422	1.45	H	0.6651	-4.7222	1.5834
H	-0.3503	-3.1427	0.9299	H	-0.0115	-3.2073	1.028
H	1.7559	-4.9486	-0.3386	H	2.2677	-4.7943	-0.2308
H	0.2073	-4.498	-1.0184	H	0.6676	-4.5394	-0.8928
H	-0.24	-1.6817	4.5619	H	-0.038	-1.6178	4.594
H	1.1788	-3.306	5.3947	H	1.5696	-3.0313	5.4656
H	2.2903	-4.3139	4.3223	H	2.7818	-3.9415	4.4148
H	0.8754	-1.0461	-2.0223	H	0.9295	-1.0521	-1.9789
H	-0.2891	-2.3357	-1.8346	H	-0.0813	-2.462	-1.7533
H	0.2119	-1.3875	-0.4358	H	0.3286	-1.4395	-0.3784
H	-5.3981	-2.1506	-3.2307	H	-5.5315	-2.4031	-3.0949
H	-4.0392	-3.2497	-3.4573	H	-4.13	-3.3718	-3.5477
H	-6.3976	-2.1317	-0.742	H	-6.2815	-2.6401	-0.5523
H	-6.0619	-3.5122	0.288	H	-5.7097	-4.0265	0.3586
H	-1.8461	-0.8789	0.3759	H	-1.7708	-0.9263	0.1838
H	-1.9899	0.1818	-0.9888	H	-2.2478	0.1854	-1.0788
H	-3.9983	1.2709	0.0526	H	-4.1879	0.948	0.2355

H	-3.4034	-0.5125	2.4709	H	-3.167	-0.8886	2.4617
H	-4.6264	0.7465	2.3713	H	-4.518	0.2316	2.5628
H	-5.5935	-1.5034	2.0074	H	-5.289	-2.0749	2.1362
H	-5.8376	-0.4204	0.6468	H	-5.7636	-0.9511	0.8731
H	-2.0143	1.331	3.319	H	-2.0492	1.16	3.348
H	-2.7938	-2.5392	1.6248	H	-2.4352	-2.7771	1.4317
H	-4.1867	-3.6059	1.7459	H	-3.7004	-3.9821	1.6415
H	-3.0661	-3.7563	0.3854	H	-2.7187	-3.9683	0.1702
H	-2.4221	-1.5258	-3.9362	H	-3.6796	-0.771	-4.0989
H	4.5915	-3.1084	0.4483	H	4.8919	-2.6348	0.4484
H	-4.4023	-4.3537	-1.3855	H	-4.1549	-4.6111	-1.5108
H	-5.9977	-4.1488	-2.0916	H	-5.825	-4.5306	-2.0512
4a-9	X axis(Å)	Y axis(Å)	Z axis(Å)	4a-10	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-2.3674	4.7683	-0.5394	C	4.1515	-4.1217	0.7297
C	-2.2339	4.1147	0.8362	C	3.5944	-3.9281	-0.6805
C	-1.2533	2.9295	0.8356	C	2.7463	-2.653	-0.8153
C	0.1294	3.3414	0.2509	C	3.5182	-1.3986	-0.3104
C	-0.0217	3.9295	-1.2017	C	4.0056	-1.5884	1.1736
C	-1.0139	5.1244	-1.162	C	4.8686	-2.8768	1.2606
C	1.1872	2.2161	0.2689	C	2.73	-0.0785	-0.4486
C	2.5551	2.7063	-0.2602	C	3.5615	1.1427	0.0057
C	2.4442	3.3634	-1.6436	C	4.1518	0.9648	1.4127
C	1.3623	4.446	-1.6857	C	4.884	-0.3701	1.5755
C	-0.5311	2.9062	-2.2518	C	2.8557	-1.7001	2.2105
C	-1.1262	2.3778	2.2383	C	2.2991	-2.4954	-2.2503
O	-0.5446	2.9173	3.1706	O	3.0033	-2.1619	-3.1931
O	0.6649	4.4117	1.0762	O	4.7122	-1.2474	-1.1217
C	3.5605	1.5848	-0.2801	C	2.731	2.3966	-0.0811
O	3.2277	0.4627	-1.0305	O	1.6368	2.4788	0.7737
C	4.7209	1.5695	0.3717	C	2.9364	3.4092	-0.9197
C	4.1222	-1.5344	-3.1995	C	0.2013	4.2374	2.8892
C	4.9843	-0.7182	-2.2353	C	1.0933	4.6644	1.7232
C	4.3039	-0.488	-0.8776	C	0.9769	3.7365	0.5041
C	3.8234	-1.828	-0.246	C	-0.5057	3.5296	0.0775
C	2.8514	-2.5909	-1.2207	C	-1.365	2.9838	1.2769
C	3.5778	-2.8237	-2.5739	C	-1.2482	3.9727	2.4683
C	3.1795	-1.6668	1.1511	C	-0.6751	2.6168	-1.1589
C	2.7476	-3.0237	1.752	C	-2.155	2.4716	-1.5955
C	1.8638	-3.8408	0.7957	C	-3.0422	2.0288	-0.4173
C	2.4884	-3.9682	-0.5982	C	-2.8494	2.899	0.8293
C	2.1275	-2.8768	3.128	C	-2.3566	1.5583	-2.7973
C	0.8704	-2.1015	3.3152	C	-3.6238	1.7258	-3.572
C	2.6653	-3.4209	4.2328	C	-1.4985	0.639	-3.2721
O	0.2815	-1.538	2.4014	O	-4.4929	2.5326	-3.2683
C	1.5228	-1.8426	-1.5035	C	-0.9498	1.5746	1.7772
C	5.2424	0.2517	0.0493	C	1.8141	4.2865	-0.6301
O	6.2827	-0.1885	0.5193	O	1.5816	5.3021	-1.2706

C	-7.0626	-2.6684	-0.7077	C	-4.4946	-2.4304	2.7036
C	-6.2808	-1.516	-0.1363	C	-3.1133	-2.1924	2.1362
C	-5.0213	-1.1928	-0.5096	C	-2.8027	-2.3409	0.8242
C	-4.2288	-2.0585	-1.5044	C	-3.8534	-2.8296	-0.196
C	-4.9326	-3.4174	-1.7819	C	-5.1198	-3.4068	0.4945
C	-4.2628	0.0266	-0.0057	C	-1.438	-2.0568	0.2108
C	-2.9101	-0.3622	0.6121	C	-0.8919	-3.2476	-0.5983
C	-2.0693	-1.161	-0.3929	C	-1.9003	-3.6495	-1.6847
C	-2.8295	-2.3814	-0.9142	C	-3.2633	-3.9693	-1.0706
C	-2.1652	0.8568	1.0903	C	0.4923	-2.9341	-1.1198
C	-1.7821	1.0865	2.3444	C	0.8754	-2.7594	-2.383
O	-1.8511	1.8182	0.1332	O	1.4811	-2.8366	-0.1404
C	-4.0755	-1.3024	-2.8444	C	-4.2825	-1.6481	-1.0968
C	-7.038	-0.7486	0.8958	C	-2.127	-1.7665	3.1802
O	-6.5575	-0.3885	1.9628	O	-2.4206	-1.6672	4.367
O	4.9828	-2.684	-0.063	O	-1.0601	4.8195	-0.2783
C	-6.4364	-3.2636	-1.9641	C	-5.5896	-2.5396	1.6505
H	-2.9265	4.1039	-1.2076	H	3.34	-4.4078	1.4079
H	-2.9706	5.6794	-0.4471	H	4.8523	-4.9651	0.7262
H	-1.9092	4.8728	1.5603	H	4.4309	-3.8997	-1.3907
H	-3.2303	3.7858	1.1584	H	2.9983	-4.8126	-0.9393
H	-0.5783	5.9537	-0.5895	H	5.7982	-2.7443	0.6919
H	-1.1784	5.5123	-2.1754	H	5.1743	-3.0571	2.2992
H	1.3415	1.8662	1.2981	H	2.4596	0.0836	-1.5005
H	0.8353	1.3486	-0.3011	H	1.7854	-0.1337	0.105
H	2.9248	3.4739	0.4345	H	4.4068	1.2478	-0.6892
H	3.4067	3.8161	-1.9149	H	4.8545	1.7818	1.622
H	2.2406	2.609	-2.4134	H	3.367	1.0444	2.1748
H	1.2862	4.8348	-2.7093	H	5.2172	-0.4693	2.6166
H	1.6892	5.2933	-1.0691	H	5.7999	-0.3447	0.9711
H	-1.5716	2.6132	-2.0988	H	2.2729	-2.6176	2.1099
H	-0.4833	3.3367	-3.2595	H	3.2603	-1.7071	3.23
H	0.0612	1.9875	-2.2686	H	2.1509	-0.8664	2.1529
H	0.6356	4.1197	2.0123	H	4.4561	-1.2729	-2.0679
H	5.1776	2.2991	1.012	H	3.6885	3.5618	-1.6696
H	3.2955	-0.9142	-3.5632	H	0.6249	3.3462	3.3651
H	4.7171	-1.7893	-4.0848	H	0.2142	5.021	3.6564
H	5.9421	-1.2352	-2.0937	H	0.8299	5.6912	1.438
H	5.2183	0.2429	-2.7109	H	2.1315	4.6977	2.0776
H	4.4146	-3.5205	-2.4349	H	-1.7152	4.9315	2.2083
H	2.899	-3.3071	-3.288	H	-1.8063	3.5907	3.3327
H	3.9057	-1.222	1.844	H	-0.1249	3.0413	-2.0086
H	2.3369	-0.971	1.1003	H	-0.2346	1.6351	-0.9555
H	3.6695	-3.6106	1.8802	H	-2.4859	3.474	-1.9026
H	1.7108	-4.8473	1.2059	H	-4.1007	2.0699	-0.7013
H	0.8655	-3.3985	0.7076	H	-2.8409	0.9804	-0.1699
H	3.3826	-4.6009	-0.5269	H	-3.2436	3.9023	0.6226

H	1.7926	-4.5094	-1.2523	H	-3.4683	2.4975	1.6421
H	0.4857	-2.0555	4.3484	H	-3.7407	1.0697	-4.4511
H	2.2224	-3.3141	5.2185	H	-1.7151	0.0427	-4.1544
H	3.5834	-4.0003	4.1795	H	-0.5405	0.4475	-2.802
H	1.6474	-0.9606	-2.1348	H	0.0216	1.559	2.275
H	0.8167	-2.4948	-2.0316	H	-1.673	1.204	2.5134
H	1.0329	-1.5099	-0.5868	H	-0.9051	0.8385	0.9722
H	-7.1402	-3.4477	0.0612	H	-4.4696	-3.3559	3.2933
H	-8.0857	-2.3548	-0.9481	H	-4.7717	-1.6201	3.3892
H	-4.7608	-4.1113	-0.9475	H	-4.9143	-4.4132	0.8844
H	-4.5016	-3.8978	-2.6693	H	-5.9335	-3.5226	-0.2324
H	-4.1113	0.71	-0.8516	H	-1.5246	-1.1775	-0.4402
H	-4.8348	0.6113	0.7195	H	-0.6951	-1.7802	0.9605
H	-3.1078	-1.0121	1.477	H	-0.7849	-4.1054	0.082
H	-1.7595	-0.5294	-1.2344	H	-2.0093	-2.8535	-2.4309
H	-1.1493	-1.5042	0.0918	H	-1.5389	-4.5353	-2.2222
H	-2.2127	-2.8924	-1.6646	H	-3.9646	-4.2264	-1.875
H	-2.9377	-3.0853	-0.0771	H	-3.1492	-4.8778	-0.4628
H	-1.8924	0.491	3.2295	H	0.3258	-2.781	-3.3041
H	-3.4965	-0.3792	-2.743	H	-3.4529	-1.2523	-1.6888
H	-3.5584	-1.9217	-3.5865	H	-5.0608	-1.9562	-1.8044
H	-5.0483	-1.0244	-3.2647	H	-4.6814	-0.8142	-0.5095
H	-8.097	-0.5642	0.6487	H	-1.1057	-1.5455	2.8482
H	5.672	-2.1759	0.4142	H	-0.4716	5.2499	-0.9333
H	-6.6538	-2.6274	-2.8298	H	-5.8698	-1.5417	1.2945
H	-6.8897	-4.2397	-2.1719	H	-6.4897	-2.9728	2.1018
4a-11	X axis(Å)	Y axis(Å)	Z axis(Å)				
C	-0.9518	5.5836	-1.3163				
C	-1.4516	5.0971	0.0422				
C	-0.8774	3.7264	0.4377				
C	0.6754	3.6942	0.3289				
C	1.1622	4.1338	-1.1001				
C	0.5732	5.5314	-1.4326				
C	1.3001	2.3323	0.7059				
C	2.8422	2.3691	0.66				
C	3.3885	2.9318	-0.6657				
C	2.7129	4.2384	-1.0878				
C	0.7593	3.1543	-2.2342				
C	-1.3424	3.3882	1.8344				
O	-0.9531	3.9081	2.8714				
O	1.2132	4.6704	1.2607				
C	3.4073	1.0009	0.9533				
O	3.5028	0.1167	-0.1182				
C	3.825	0.5684	2.1412				
C	5.7742	-1.2565	-1.6924				
C	5.6889	-0.9632	-0.196				
C	4.2485	-1.0298	0.3453				

C	3.5646	-2.3777	-0.0224				
C	3.5936	-2.6205	-1.5787				
C	5.0628	-2.5552	-2.0783				
C	2.1231	-2.526	0.5192				
C	1.5154	-3.9044	0.1648				
C	1.6196	-4.2409	-1.3329				
C	3.0337	-4.0377	-1.8801				
C	0.0987	-4.0792	0.6716				
C	-1.0073	-3.2465	0.1274				
C	-0.2461	-4.9921	1.5952				
O	-0.832	-2.2585	-0.5749				
C	2.7555	-1.6002	-2.395				
C	4.2752	-0.7809	1.8368				
O	4.6222	-1.5804	2.6953				
C	-5.691	-3.414	0.008				
C	-4.9132	-2.3105	0.6815				
C	-4.8483	-1.0376	0.2211				
C	-5.6184	-0.6049	-1.0412				
C	-6.1195	-1.8216	-1.8687				
C	-4.0344	0.0723	0.8725				
C	-3.1345	0.8458	-0.1168				
C	-3.9738	1.3747	-1.2876				
C	-4.7145	0.2335	-1.9813				
C	-2.3413	1.9659	0.5248				
C	-2.318	2.3133	1.8107				
O	-1.5103	2.6847	-0.338				
C	-6.8421	0.2375	-0.6087				
C	-4.2336	-2.7504	1.9374				
O	-3.9816	-3.9275	2.1727				
O	4.3408	-3.4489	0.5782				
C	-6.721	-2.912	-0.9958				
H	-1.4143	4.9902	-2.1125				
H	-1.2886	6.6151	-1.4746				
H	-1.19	5.8459	0.8012				
H	-2.548	5.0569	0.0112				
H	0.9987	6.2879	-0.7603				
H	0.8641	5.8323	-2.4472				
H	1.0087	2.0659	1.7306				
H	0.9148	1.5336	0.0612				
H	3.182	3.0464	1.4566				
H	4.4686	3.1043	-0.5716				
H	3.2748	2.2009	-1.4752				
H	3.0811	4.5248	-2.0814				
H	3.0377	5.0376	-0.4092				
H	-0.3191	3.1076	-2.3978				
H	1.2022	3.4704	-3.1866				
H	1.0971	2.1309	-2.0513				

H	0.8098	4.5208	2.1418				
H	3.841	1.048	3.1005				
H	5.358	-0.4143	-2.256				
H	6.8286	-1.3238	-1.9861				
H	6.3251	-1.6777	0.3424				
H	6.1207	0.03	-0.0171				
H	5.6354	-3.398	-1.6695				
H	5.0963	-2.6695	-3.1693				
H	2.1286	-2.4428	1.6139				
H	1.4958	-1.7078	0.1531				
H	2.133	-4.654	0.682				
H	1.3273	-5.2866	-1.4955				
H	0.9161	-3.6411	-1.9207				
H	3.6904	-4.8062	-1.4523				
H	3.0269	-4.2216	-2.9622				
H	-2.0226	-3.5701	0.4027				
H	-1.268	-5.1159	1.9468				
H	0.4964	-5.6511	2.0366				
H	3.1725	-0.5914	-2.3816				
H	2.7132	-1.8976	-3.45				
H	1.7235	-1.5235	-2.0435				
H	-4.9797	-4.0758	-0.5028				
H	-6.2157	-4.0229	0.7546				
H	-5.287	-2.2611	-2.4354				
H	-6.8581	-1.4989	-2.6133				
H	-4.7329	0.7612	1.3651				
H	-3.3837	-0.3188	1.6588				
H	-2.3992	0.1357	-0.5217				
H	-4.6821	2.1368	-0.941				
H	-3.3298	1.8668	-2.0275				
H	-5.3109	0.6458	-2.8055				
H	-3.9617	-0.4185	-2.446				
H	-2.8272	1.9182	2.6681				
H	-6.5541	1.1529	-0.0818				
H	-7.4374	0.5398	-1.478				
H	-7.5011	-0.3203	0.0655				
H	-3.9582	-1.9641	2.6542				
H	4.437	-3.2586	1.5355				
H	-7.6067	-2.5377	-0.4701				
H	-7.0598	-3.7463	-1.6209				
4b-1	X axis(Å)	Y axis(Å)	Z axis(Å)	4b-2	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-2.4491	5.2487	-0.2917	C	-2.3402	5.2771	-0.2427
C	-2.278	4.566	1.0653	C	-2.2106	4.5649	1.1036
C	-1.3876	3.3126	0.9909	C	-1.3369	3.3005	1.0241
C	-0.0186	3.6333	0.3265	C	0.0517	3.6134	0.3974
C	-0.2174	4.2521	-1.1082	C	-0.1048	4.2639	-1.0283
C	-1.1147	5.5151	-0.9943	C	-0.986	5.5377	-0.9089

C	0.9538	2.4352	0.2673	C	1.0067	2.4014	0.3352
C	2.3164	2.8367	-0.3427	C	2.3891	2.7927	-0.2357
C	2.1661	3.5151	-1.7117	C	2.281	3.5034	-1.5924
C	1.1669	4.674	-1.6749	C	1.2983	4.6764	-1.554
C	-0.8652	3.2837	-2.1341	C	-0.7427	3.3264	-2.0885
C	-1.2258	2.7286	2.3768	C	-1.2137	2.6871	2.4013
O	-0.5342	3.1894	3.2748	O	-0.5402	3.1236	3.3248
O	0.6402	4.6499	1.1289	O	0.7077	4.6031	1.2349
C	3.2447	1.6551	-0.4366	C	3.2981	1.5967	-0.336
O	2.7708	0.5373	-1.1154	O	2.8249	0.5092	-1.0626
C	4.4672	1.5897	0.0856	C	4.5026	1.4918	0.2206
C	3.3434	-1.4768	-3.3734	C	3.433	-1.4311	-3.3739
C	4.3371	-0.6967	-2.5126	C	4.4131	-0.701	-2.4554
C	3.8216	-0.4537	-1.0862	C	3.8581	-0.5001	-1.0372
C	3.3712	-1.7799	-0.4058	C	3.3652	-1.842	-0.42
C	2.2849	-2.5217	-1.2687	C	2.2918	-2.5307	-1.3414
C	2.8496	-2.7592	-2.6962	C	2.895	-2.7272	-2.7593
C	2.875	-1.5993	1.0473	C	2.8304	-1.7067	1.0245
C	2.4849	-2.9444	1.7	C	2.3976	-3.0683	1.6135
C	1.5183	-3.7719	0.8386	C	1.4381	-3.8411	0.6949
C	1.9808	-3.8989	-0.6154	C	1.9419	-3.9243	-0.7487
C	1.9783	-2.766	3.1186	C	1.8589	-2.9383	3.0253
C	0.7309	-1.9982	3.3927	C	0.6242	-2.1516	3.302
C	2.611	-3.2794	4.1872	C	2.4508	-3.5134	4.0859
O	0.0555	-1.4613	2.5222	O	-0.0123	-1.5573	2.4396
C	0.9414	-1.7547	-1.3967	C	0.9674	-1.7332	-1.4805
C	4.8863	0.2453	-0.2701	C	4.9082	0.1513	-0.1649
O	5.9485	-0.2404	0.0943	O	5.949	-0.3665	0.2165
C	-4.3049	-4.3422	-0.759	C	-4.6087	-4.143	-0.6635
C	-3.4224	-3.2534	-0.1955	C	-3.5451	-3.1521	-0.258
C	-3.6067	-1.9332	-0.44	C	-3.5826	-1.8423	-0.6038
C	-4.8314	-1.4283	-1.23	C	-4.7141	-1.2651	-1.4787
C	-5.8836	-2.5476	-1.4687	C	-5.6929	-2.3499	-2.0081
C	-2.6765	-0.8155	0.0164	C	-2.6225	-0.7724	-0.1053
C	-3.42	0.2371	0.8512	C	-3.3817	0.2404	0.7703
C	-4.6173	0.8023	0.0695	C	-4.6016	0.8286	0.0329
C	-5.5439	-0.3116	-0.4179	C	-5.4913	-0.2546	-0.5925
C	-2.4905	1.3399	1.2881	C	-2.463	1.3319	1.2544
C	-2.0164	1.5166	2.5195	C	-2.0144	1.4775	2.4993
O	-2.1049	2.2571	0.3145	O	-2.0533	2.2692	0.3104
C	-4.3788	-0.8827	-2.6043	C	-4.1571	-0.5524	-2.7355
C	-2.3265	-3.7786	0.6761	C	-2.4916	-3.7393	0.626
O	-2.1105	-4.9778	0.8191	O	-2.4164	-4.9414	0.8596
O	4.521	-2.6652	-0.3401	O	4.497	-2.7501	-0.3549
C	-5.239	-3.8658	-1.8645	C	-5.931	-3.4716	-1.0124
H	-3.096	4.6369	-0.9301	H	-2.9808	4.6879	-0.9082
H	-2.9769	6.1996	-0.1514	H	-2.8574	6.2328	-0.0953

H	-1.8543	5.2874	1.7758	H	-1.7933	5.2656	1.8382
H	-3.2741	4.3062	1.4462	H	-3.2189	4.312	1.4562
H	-0.5848	6.3022	-0.4421	H	-0.4578	6.3054	-0.3285
H	-1.3129	5.9287	-1.9914	H	-1.155	5.9744	-1.9016
H	1.1465	2.0603	1.2811	H	1.1706	2.0031	1.3451
H	0.5055	1.6035	-0.2882	H	0.5584	1.5882	-0.2471
H	2.7791	3.5702	0.3331	H	2.849	3.5029	0.4663
H	3.1397	3.9002	-2.0419	H	3.2677	3.8806	-1.8911
H	1.8594	2.7856	-2.4712	H	1.9815	2.7957	-2.375
H	1.0552	5.0815	-2.6878	H	1.2163	5.1066	-2.5604
H	1.5931	5.4865	-1.0723	H	1.7224	5.4697	-0.9248
H	-0.8467	3.7232	-3.139	H	-0.2354	2.3606	-2.1586
H	-0.3456	2.3239	-2.1957	H	-1.7986	3.1204	-1.9026
H	-1.9135	3.0669	-1.9201	H	-0.6953	3.7862	-3.0833
H	0.6629	4.3394	2.0591	H	0.7026	4.275	2.1593
H	5.0309	2.3071	0.65	H	5.0621	2.1808	0.8233
H	2.494	-0.8328	-3.6266	H	2.6036	-0.7623	-3.6295
H	3.8198	-1.7353	-4.3267	H	3.9342	-1.6643	-4.321
H	5.2868	-1.2461	-2.4819	H	5.3517	-1.2686	-2.4162
H	4.5476	0.2593	-3.0091	H	4.6554	0.2681	-2.9101
H	3.6839	-3.4715	-2.6552	H	3.7143	-3.4569	-2.72
H	2.0859	-3.2264	-3.3311	H	2.1424	-3.1559	-3.4333
H	3.6745	-1.1622	1.6599	H	3.6195	-1.3084	1.6757
H	2.0433	-0.8888	1.0769	H	2.0111	-0.9822	1.0574
H	3.4103	-3.5365	1.7608	H	3.3097	-3.681	1.6733
H	1.4115	-4.7774	1.2655	H	1.2978	-4.8592	1.0802
H	0.5185	-3.333	0.8535	H	0.4472	-3.3812	0.6976
H	2.8698	-4.5418	-0.6474	H	2.8192	-4.5832	-0.778
H	1.2096	-4.4289	-1.1892	H	1.1787	-4.4177	-1.3643
H	0.4358	-1.9323	4.4539	H	0.3012	-2.1269	4.3569
H	2.2501	-3.155	5.2037	H	2.0666	-3.4238	5.0976
H	3.5261	-3.8544	4.0705	H	3.3542	-4.1061	3.9672
H	1.0191	-0.8463	-1.9972	H	1.079	-0.8074	-2.0483
H	0.1875	-2.3814	-1.8888	H	0.2155	-2.3281	-2.0134
H	0.5295	-1.4616	-0.4281	H	0.535	-1.4638	-0.5141
H	-3.6945	-5.1579	-1.1653	H	-4.2433	-4.7223	-1.5206
H	-4.9012	-4.7634	0.0606	H	-4.8077	-4.8553	0.1462
H	-6.473	-2.7173	-0.557	H	-6.6525	-1.8957	-2.2858
H	-6.6013	-2.2418	-2.2403	H	-5.2934	-2.7986	-2.9285
H	-1.8246	-1.1825	0.5899	H	-1.7905	-1.1814	0.4685
H	-2.2284	-0.3488	-0.8706	H	-2.1438	-0.2764	-0.958
H	-3.8131	-0.2603	1.7501	H	-3.7645	-0.3015	1.648
H	-5.188	1.4885	0.7083	H	-5.2034	1.4225	0.7329
H	-4.2794	1.3938	-0.7902	H	-4.2814	1.5241	-0.7524
H	-6.0255	-0.7513	0.4667	H	-6.0009	-0.7869	0.2214
H	-6.3501	0.1316	-1.0165	H	-6.2792	0.2344	-1.1795
H	-2.1523	0.9429	3.4155	H	-2.1706	0.8825	3.3779

H	-5.2406	-0.5668	-3.2036	H	-4.9747	-0.203	-3.3774
H	-3.719	-0.014	-2.5175	H	-3.5441	0.3231	-2.5047
H	-3.8349	-1.6403	-3.1792	H	-3.5362	-1.2342	-3.329
H	-1.7279	-3.0398	1.2209	H	-1.7763	-3.0438	1.0774
H	5.2694	-2.1776	0.0638	H	5.241	-2.2918	0.0895
H	-4.6858	-3.7564	-2.8043	H	-6.6167	-4.2116	-1.4408
H	-6.0118	-4.6225	-2.0426	H	-6.41	-3.0836	-0.1057
4b-3	X axis(Å)	Y axis(Å)	Z axis(Å)	4b-4	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-0.6888	5.6528	-0.745	C	-2.1594	5.0457	0.2875
C	-1.009	4.9244	0.5608	C	-1.8775	4.2155	1.5405
C	-0.45	3.4922	0.5904	C	-0.9838	2.998	1.2603
C	1.0746	3.4756	0.2739	C	0.3227	3.4082	0.5177
C	1.3726	4.1492	-1.1171	C	-0.0059	4.1673	-0.8214
C	0.7975	5.5927	-1.1117	C	-0.8894	5.4018	-0.493
C	1.7245	2.0762	0.3462	C	1.2795	2.2289	0.2476
C	3.2488	2.1396	0.0933	C	2.5765	2.6703	-0.4681
C	3.5906	2.8566	-1.2205	C	2.3005	3.5033	-1.7276
C	2.9115	4.2253	-1.325	C	1.3231	4.6524	-1.4638
C	0.7754	3.3894	-2.3313	C	-0.7462	3.3063	-1.8805
C	-0.7459	2.8576	1.9291	C	-0.683	2.2759	2.5531
O	-0.2226	3.1516	2.9956	O	-0.0124	2.7136	3.4784
O	1.7482	4.2845	1.2766	O	1.0535	4.3401	1.3569
C	3.862	0.7643	0.1305	C	3.4332	1.4754	-0.8026
O	3.3472	-0.1735	-0.7576	O	2.7854	0.3943	-1.3904
C	4.8322	0.3693	0.9517	C	4.7353	1.3527	-0.5567
C	3.9864	-2.267	-2.9309	C	2.7169	-1.6711	-3.6502
C	4.8637	-1.7879	-1.7734	C	3.9295	-0.95	-3.0585
C	4.0513	-1.4131	-0.5248	C	3.7633	-0.6523	-1.5618
C	3.0938	-2.5655	-0.0999	C	3.4023	-1.9407	-0.7626
C	2.1304	-2.9581	-1.2808	C	2.0968	-2.6128	-1.3296
C	2.9847	-3.3511	-2.517	C	2.3007	-2.9055	-2.8421
C	2.2876	-2.2693	1.1874	C	3.2784	-1.7223	0.7631
C	1.3789	-3.4537	1.587	C	2.971	-3.0384	1.5137
C	0.4756	-3.9191	0.434	C	1.7571	-3.7834	0.9343
C	1.2713	-4.18	-0.8499	C	1.8554	-3.9566	-0.5854
C	0.6011	-3.1849	2.8605	C	2.8649	-2.8347	3.0124
C	-0.3894	-2.0759	2.9311	C	1.8035	-1.9617	3.5842
C	0.7605	-3.9141	3.978	C	3.7048	-3.4101	3.8893
O	-0.6336	-1.3225	1.997	O	0.9719	-1.3764	2.9016
C	1.1553	-1.8287	-1.7023	C	0.8139	-1.7543	-1.1663
C	4.9865	-1.0325	0.601	C	5.0132	7.00E-04	-1.0149
O	5.7467	-1.7889	1.19	O	6.1113	-0.5283	-0.908
C	-7.1333	-1.6403	-0.9253	C	-6.2588	-2.1276	-1.9979
C	-6.2288	-0.7203	-0.137	C	-5.5052	-0.99	-1.3466
C	-4.8749	-0.7498	-0.2126	C	-4.7581	-1.1285	-0.223
C	-4.1481	-1.7279	-1.161	C	-4.5851	-2.5027	0.4584
C	-5.1136	-2.3821	-2.1878	C	-5.0714	-3.6728	-0.4409

C	-3.9289	0.1296	0.5985	C	-4.0245	0.0035	0.4874
C	-2.9108	0.8811	-0.2835	C	-2.5323	-0.308	0.711
C	-2.128	-0.1136	-1.1479	C	-2.3793	-1.625	1.4849
C	-3.0674	-0.9781	-1.9845	C	-3.0862	-2.7693	0.7609
C	-1.9556	1.7712	0.4807	C	-1.8339	0.8731	1.346
C	-1.7446	1.8109	1.7952	C	-1.2664	0.9445	2.5487
O	-1.2237	2.6629	-0.3041	O	-1.7363	2.0016	0.5331
C	-3.4875	-2.8498	-0.3252	C	-5.3988	-2.5232	1.7742
C	-6.9883	0.215	0.7521	C	-5.6847	0.3101	-2.0685
O	-8.2139	0.2654	0.7671	O	-6.3296	0.4052	-3.1079
O	3.8977	-3.741	0.1862	O	4.477	-2.9005	-0.949
C	-6.4168	-2.831	-1.5487	C	-6.3949	-3.3651	-1.1205
H	-1.2937	5.2325	-1.5561	H	-2.8594	4.5047	-0.3587
H	-0.9937	6.7023	-0.6548	H	-2.6728	5.9703	0.5777
H	-0.6056	5.5051	1.4003	H	-1.4081	4.8616	2.2934
H	-2.099	4.9115	0.6893	H	-2.8375	3.8928	1.9637
H	1.354	6.2145	-0.3983	H	-0.3141	6.1288	0.0949
H	0.9417	6.06	-2.0942	H	-1.173	5.9199	-1.418
H	1.5771	1.6478	1.3463	H	1.5752	1.7631	1.1971
H	1.2393	1.3899	-0.3573	H	0.7626	1.4533	-0.3284
H	3.6971	2.7256	0.9082	H	3.1394	3.3073	0.2289
H	4.677	2.9957	-1.2931	H	3.2423	3.9226	-2.1049
H	3.3092	2.2381	-2.0814	H	1.9146	2.866	-2.5327
H	3.1415	4.6639	-2.3044	H	1.1207	5.1724	-2.409
H	3.3624	4.8982	-0.5842	H	1.8128	5.391	-0.8163
H	1.0548	2.3326	-2.3474	H	-0.2407	2.3584	-2.0831
H	-0.3146	3.4331	-2.373	H	-1.7738	3.0664	-1.6008
H	1.1318	3.8295	-3.2707	H	-0.8113	3.8455	-2.8336
H	1.4686	3.9722	2.1632	H	1.1338	3.9528	2.2541
H	5.3656	0.8994	1.7169	H	5.4331	2.0312	-0.1054
H	3.4574	-1.4116	-3.3653	H	1.8772	-0.9713	-3.7259
H	4.6283	-2.6585	-3.7293	H	2.9474	-1.9765	-4.6778
H	5.5871	-2.5764	-1.5291	H	4.8244	-1.5629	-3.2255
H	5.4495	-0.9262	-2.1183	H	4.0832	-0.0177	-3.6168
H	3.5407	-4.2747	-2.3098	H	3.0693	-3.6784	-2.9732
H	2.3321	-3.5775	-3.3698	H	1.3806	-3.3202	-3.2732
H	2.9774	-2.093	2.0231	H	4.2267	-1.3373	1.1603
H	1.7071	-1.3496	1.0679	H	2.5232	-0.9596	0.975
H	2.0505	-4.2992	1.7988	H	3.8342	-3.6991	1.3436
H	-0.0432	-4.8427	0.7211	H	1.6798	-4.7756	1.3973
H	-0.3096	-3.1839	0.2305	H	0.8235	-3.2664	1.1796
H	1.9105	-5.0589	-0.6959	H	2.6644	-4.6646	-0.8066
H	0.5738	-4.4557	-1.6513	H	0.9359	-4.4327	-0.9497
H	-0.9087	-1.9605	3.8979	H	1.8029	-1.8648	4.6833
H	0.2067	-3.7231	4.8925	H	3.6302	-3.2618	4.9625
H	1.4656	-4.7409	4.0094	H	4.5077	-4.0594	3.5496
H	1.6444	-1.0063	-2.228	H	0.8021	-0.87	-1.8064

H	0.3905	-2.2135	-2.3877	H	-0.0745	-2.3366	-1.4401
H	0.6357	-1.3935	-0.8472	H	0.6656	-1.4091	-0.14
H	-7.9336	-2.0322	-0.2856	H	-7.2694	-1.8069	-2.2792
H	-7.6144	-1.0534	-1.7183	H	-5.7381	-2.399	-2.9254
H	-5.355	-1.6699	-2.9889	H	-4.3286	-3.8849	-1.2223
H	-4.6303	-3.2373	-2.6767	H	-5.1656	-4.5944	0.1471
H	-4.461	0.8711	1.1971	H	-4.1004	0.9487	-0.0525
H	-3.407	-0.5096	1.3218	H	-4.5155	0.1873	1.4521
H	-3.4851	1.5388	-0.9527	H	-2.0642	-0.4534	-0.2739
H	-1.4454	0.4183	-1.8227	H	-1.3181	-1.8799	1.5839
H	-1.504	-0.7508	-0.5138	H	-2.7751	-1.5289	2.5028
H	-3.554	-0.3233	-2.7207	H	-2.5472	-2.951	-0.1794
H	-2.4703	-1.6962	-2.5615	H	-2.98	-3.6861	1.3551
H	-2.1553	1.23	2.5978	H	-1.1713	0.2166	3.3315
H	-2.9874	-3.5795	-0.9727	H	-5.3337	-3.5037	2.2601
H	-2.7322	-2.4673	0.3671	H	-5.0444	-1.784	2.4991
H	-4.2231	-3.3919	0.2788	H	-6.4589	-2.3108	1.5978
H	-6.4039	0.8724	1.4066	H	-5.2091	1.1976	-1.6344
H	4.613	-3.4859	0.8063	H	5.3286	-2.4583	-0.7485
H	-6.2288	-3.5973	-0.7882	H	-7.1841	-3.2131	-0.3753
H	-7.0637	-3.2936	-2.3032	H	-6.7072	-4.2173	-1.7352
4b-5	X axis(Å)	Y axis(Å)	Z axis(Å)	4b-6	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-3.0069	4.8558	-0.4161	C	-1.1368	5.528	-0.674
C	-2.4899	4.3844	0.945	C	-1.3536	4.7767	0.6401
C	-1.534	3.189	0.8313	C	-0.6868	3.3908	0.6451
C	-0.3746	3.484	-0.1673	C	0.8223	3.4906	0.2748
C	-0.9382	3.8561	-1.5891	C	1.0182	4.1857	-1.1239
C	-1.8891	5.0762	-1.4429	C	0.3357	5.5812	-1.0935
C	0.6626	2.3464	-0.2773	C	1.5795	2.1452	0.3197
C	1.8143	2.696	-1.2461	C	3.0847	2.3255	0.0127
C	1.2985	3.1326	-2.6235	C	3.323	3.0662	-1.3107
C	0.247	4.2427	-2.5177	C	2.5384	4.379	-1.3865
C	-1.7177	2.711	-2.2905	C	0.4375	3.3831	-2.3184
C	-0.9975	2.8094	2.193	C	-0.8876	2.7352	1.9914
O	-0.2893	3.5103	2.9032	O	-0.3464	3.0631	3.0389
O	0.3523	4.6467	0.3105	O	1.4674	4.3482	1.2556
C	2.7883	1.5518	-1.3712	C	3.8036	1.0019	0.0245
O	2.2497	0.2716	-1.4547	O	3.3255	0.0235	-0.8399
C	4.1147	1.6622	-1.3611	C	4.8352	0.6863	0.8042
C	2.2088	-2.4299	-2.9117	C	4.0174	-2.0414	-3.0244
C	3.3478	-1.4136	-2.8211	C	4.9083	-1.4883	-1.911
C	3.356	-0.6575	-1.4853	C	4.127	-1.1598	-0.6301
C	3.3499	-1.6378	-0.2718	C	3.2745	-2.3733	-0.1543
C	2.126	-2.6224	-0.3418	C	2.2905	-2.846	-1.2878
C	2.1547	-3.37	-1.7031	C	3.1156	-3.19	-2.558
C	3.392	-0.9339	1.1039	C	2.5069	-2.1213	1.1654
C	3.4218	-1.9406	2.2774	C	1.7025	-3.3619	1.6144

C	2.3235	-3.0142	2.1879	C	0.7858	-3.9038	0.5062
C	2.2509	-3.6652	0.8037	C	1.5413	-4.1214	-0.8096
C	3.4306	-1.2405	3.6228	C	0.9627	-3.1321	2.9178
C	2.2665	-0.4143	4.0491	C	-0.0972	-2.0918	3.0211
C	4.4604	-1.3187	4.4821	C	1.2188	-3.8355	4.0339
O	1.261	-0.2627	3.3656	O	-0.4337	-1.3702	2.0904
C	0.748	-1.9274	-0.1925	C	1.2191	-1.7938	-1.6735
C	4.545	0.2755	-1.4239	C	5.0806	-0.7017	0.4505
O	5.7206	-0.06	-1.3749	O	5.9217	-1.3943	1.007
C	-3.8472	-4.2314	-1.5457	C	-7.0078	-1.7855	-1.1503
C	-3.201	-2.8811	-1.3432	C	-6.1953	-0.993	-0.1544
C	-3.6268	-1.9664	-0.437	C	-4.8466	-1.0878	-0.0605
C	-4.8606	-2.2361	0.4485	C	-4.0448	-2.1109	-0.8947
C	-5.2565	-3.7384	0.458	C	-4.9426	-3.022	-1.7784
C	-2.9834	-0.6035	-0.2105	C	-3.9574	-0.1704	0.7687
C	-2.7163	-0.2905	1.2788	C	-2.9951	0.6206	-0.1465
C	-4.0034	-0.4381	2.0956	C	-2.1819	-0.3298	-1.0396
C	-4.5885	-1.8378	1.9228	C	-3.0717	-1.3164	-1.8034
C	-2.1093	1.0772	1.4846	C	-2.072	1.5696	0.5845
C	-1.3875	1.452	2.5391	C	-1.819	1.6243	1.891
O	-2.2851	2.0094	0.4684	O	-1.4268	2.5059	-0.2241
C	-6.0515	-1.4128	-0.099	C	-3.2472	-3.0707	0.022
C	-2.0616	-2.6349	-2.2816	C	-7.0181	-0.0634	0.6806
O	-1.5646	-3.5225	-2.9668	O	-8.2316	0.0525	0.5461
O	4.546	-2.4583	-0.3466	O	4.1725	-3.4853	0.1045
C	-5.236	-4.3529	-0.9321	C	-6.1684	-2.3023	-2.3121
H	-3.7317	4.13	-0.8013	H	-1.7366	5.0632	-1.4643
H	-3.5618	5.7924	-0.2842	H	-1.5171	6.5512	-0.5696
H	-1.9885	5.2236	1.4438	H	-0.9654	5.3859	1.4665
H	-3.3528	4.1224	1.5706	H	-2.4341	4.6812	0.8075
H	-1.3162	5.9638	-1.1443	H	0.8684	6.2434	-0.3985
H	-2.3397	5.3217	-2.4131	H	0.4087	6.0586	-2.0791
H	1.1131	2.1549	0.7055	H	1.5012	1.7064	1.3231
H	0.1697	1.416	-0.5804	H	1.1234	1.4241	-0.3682
H	2.3596	3.549	-0.8171	H	3.5153	2.9447	0.8125
H	2.135	3.4988	-3.2327	H	4.3923	3.2877	-1.4222
H	0.8842	2.2747	-3.167	H	3.0585	2.4278	-2.1624
H	-0.1206	4.4831	-3.5235	H	2.6989	4.8343	-2.3722
H	0.7342	5.1559	-2.1524	H	2.963	5.0841	-0.6602
H	-1.1579	1.7723	-2.3154	H	0.7954	2.3506	-2.3475
H	-2.682	2.4971	-1.8257	H	-0.6535	3.3441	-2.3213
H	-1.9397	2.9803	-3.3304	H	0.7258	3.8492	-3.2686
H	0.5805	4.5046	1.2533	H	1.2451	4.0137	2.1504
H	4.7481	2.5247	-1.2847	H	5.358	1.2594	1.5454
H	1.255	-1.9023	-3.0221	H	3.4095	-1.2307	-3.441
H	2.3308	-3.0257	-3.8242	H	4.6499	-2.3944	-3.8479
H	4.3022	-1.9356	-2.966	H	5.6967	-2.2203	-1.6937

H	3.249	-0.7086	-3.6564	H	5.4144	-0.5904	-2.2881
H	3.0261	-4.0364	-1.7452	H	3.7452	-4.0692	-2.3691
H	1.2746	-4.0191	-1.7954	H	2.4439	-3.4715	-3.3791
H	4.3021	-0.3242	1.1788	H	3.2186	-1.888	1.9682
H	2.5511	-0.2404	1.1991	H	1.8584	-1.2459	1.0649
H	4.3748	-2.4838	2.1903	H	2.4408	-4.1553	1.8046
H	2.5147	-3.7956	2.9349	H	0.348	-4.8589	0.8236
H	1.3418	-2.5997	2.4395	H	-0.0586	-3.2292	0.3318
H	3.1439	-4.2868	0.6591	H	2.2482	-4.9506	-0.6771
H	1.4	-4.3583	0.7806	H	0.8311	-4.4552	-1.577
H	2.3571	0.067	5.0378	H	-0.5798	-1.9983	4.0089
H	4.4651	-0.8153	5.4443	H	0.6926	-3.6718	4.9696
H	5.3454	-1.9017	4.2407	H	1.9796	-4.612	4.0421
H	0.4893	-1.3018	-1.0482	H	1.6241	-0.9439	-2.2263
H	-0.0481	-2.676	-0.1041	H	0.4548	-2.2395	-2.3215
H	0.6848	-1.2932	0.6951	H	0.7073	-1.3881	-0.7993
H	-3.9339	-4.4596	-2.6151	H	-7.4851	-2.6248	-0.6293
H	-3.1912	-4.9947	-1.1076	H	-7.8099	-1.1703	-1.5752
H	-4.5629	-4.3074	1.0923	H	-4.3643	-3.434	-2.615
H	-6.2519	-3.8683	0.9012	H	-5.2896	-3.8879	-1.1973
H	-2.0306	-0.5041	-0.7356	H	-4.5292	0.5489	1.3583
H	-3.6484	0.1544	-0.6446	H	-3.4044	-0.7676	1.5026
H	-1.9916	-1.0325	1.6456	H	-3.6211	1.2419	-0.8048
H	-3.7972	-0.2742	3.161	H	-1.5916	0.2437	-1.7658
H	-4.7374	0.3226	1.8037	H	-1.4618	-0.8836	-0.4292
H	-3.8852	-2.5521	2.3732	H	-3.6403	-0.7522	-2.5544
H	-5.5141	-1.9111	2.5084	H	-2.4275	-2.0078	-2.3618
H	-1.0979	0.911	3.4196	H	-2.1633	1.019	2.7066
H	-6.9621	-1.608	0.4792	H	-2.7086	-3.8185	-0.5723
H	-5.8688	-0.3343	-0.057	H	-2.5034	-2.5615	0.6388
H	-6.2661	-1.6548	-1.1456	H	-3.9163	-3.6074	0.7052
H	-1.6831	-1.6066	-2.3476	H	-6.4931	0.5135	1.4518
H	5.3218	-1.8726	-0.4725	H	4.8951	-3.1731	0.6888
H	-5.9755	-3.8661	-1.5781	H	-6.768	-2.9875	-2.9222
H	-5.5207	-5.4101	-0.8775	H	-5.8715	-1.4728	-2.9648
4b-7	X axis(Å)	Y axis(Å)	Z axis(Å)	4b-8	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-2.2292	5.0656	0.2156	C	3.9712	-4.1251	-0.2524
C	-1.9423	4.2634	1.4855	C	3.5418	-3.6391	1.1323
C	-1.0464	3.0422	1.2297	C	2.3066	-2.7253	1.0813
C	0.2572	3.4386	0.4747	C	1.1339	-3.4002	0.3119
C	-0.0769	4.1677	-0.8797	C	1.5728	-3.8098	-1.1435
C	-0.962	5.4072	-0.5758	C	2.8167	-4.7363	-1.053
C	1.2154	2.2554	0.2273	C	-0.161	-2.5592	0.2674
C	2.5093	2.6832	-0.5021	C	-1.3064	-3.3072	-0.4518
C	2.228	3.4887	-1.7783	C	-0.8965	-3.8011	-1.8469
C	1.2493	4.6414	-1.5363	C	0.4132	-4.5937	-1.8196
C	-0.8184	3.2823	-1.9178	C	1.9232	-2.6102	-2.0643

C	-0.7411	2.3489	2.5371	C	1.9021	-2.3366	2.4861
O	-0.0707	2.8087	3.4518	O	1.3975	-3.0774	3.3191
O	0.9885	4.3899	1.2913	O	0.7932	-4.6318	1.0034
C	3.3662	1.4824	-0.8143	C	-2.545	-2.4538	-0.531
O	2.718	0.3889	-1.3783	O	-2.4157	-1.22	-1.1601
C	4.6692	1.3661	-0.5698	C	-3.7394	-2.7739	-0.0386
C	2.6467	-1.7181	-3.5996	C	-3.5336	0.5922	-3.3893
C	3.8596	-0.9842	-3.0245	C	-4.259	-0.4734	-2.5669
C	3.697	-0.6593	-1.5332	C	-3.716	-0.5909	-1.1343
C	3.3403	-1.9333	-0.7093	C	-3.6943	0.7909	-0.4168
C	2.0345	-2.6181	-1.2605	C	-2.8584	1.841	-1.2384
C	2.235	-2.9382	-2.7678	C	-3.4468	1.9436	-2.6722
C	3.2199	-1.6869	0.8123	C	-3.2005	0.7298	1.0481
C	2.9168	-2.9894	1.5879	C	-3.2404	2.1164	1.7302
C	1.7031	-3.7475	1.0255	C	-2.5162	3.1998	0.9153
C	1.7977	-3.9485	-0.491	C	-2.9716	3.229	-0.5474
C	2.8137	-2.7581	3.0829	C	-2.7697	2.0657	3.1708
C	1.7517	-1.8771	3.6411	C	-1.3698	1.6834	3.5045
C	3.657	-3.3153	3.9683	C	-3.572	2.357	4.2088
O	0.9173	-1.306	2.95	O	-0.5297	1.3793	2.6661
C	0.7505	-1.7591	-1.1094	C	-1.3504	1.4982	-1.3542
C	4.9474	0.0056	-1.0019	C	-4.5338	-1.6006	-0.3601
O	6.0464	-0.52	-0.8872	O	-5.6957	-1.4626	-0.0026
C	-5.7136	-2.3865	-2.1777	C	3.1353	5.1263	-0.9931
C	-5.251	-1.139	-1.4636	C	2.3988	4.0006	-0.3066
C	-4.7331	-1.1551	-0.2109	C	2.68	2.6913	-0.5003
C	-4.6744	-2.4501	0.627	C	3.8083	2.2349	-1.4405
C	-5.3209	-3.6717	-0.0841	C	4.8288	3.3811	-1.6561
C	-4.0642	0.0282	0.4747	C	2.0335	1.5267	0.2172
C	-2.577	-0.2826	0.7503	C	3.0315	0.8947	1.2075
C	-2.4277	-1.5853	1.5577	C	4.4877	0.9495	0.6872
C	-3.1804	-2.7545	0.9112	C	4.5563	1.0024	-0.8432
C	-1.8874	0.9158	1.3615	C	2.6099	-0.5129	1.5445
C	-1.3185	1.0151	2.5616	C	2.1679	-0.9288	2.7291
O	-1.7981	2.0284	0.5261	O	2.6808	-1.4494	0.5182
C	-5.4435	-2.2839	1.9609	C	3.2042	1.8199	-2.8018
C	-5.3727	0.1008	-2.2934	C	1.3629	4.4719	0.6639
O	-5.8062	0.0905	-3.4408	O	1.0959	5.6591	0.8193
O	4.4163	-2.8946	-0.8807	O	-5.0558	1.2946	-0.3676
C	-5.1127	-3.6564	-1.5881	C	4.1481	4.6874	-2.047
H	-2.9298	4.5092	-0.4169	H	4.4176	-3.2939	-0.8095
H	-2.7438	5.9952	0.487	H	4.7652	-4.873	-0.1402
H	-1.4724	4.9268	2.223	H	3.3408	-4.5105	1.7685
H	-2.9004	3.9478	1.9181	H	4.3885	-3.1108	1.5892
H	-0.3866	6.1479	-0.0053	H	2.5397	-5.6902	-0.5856
H	-1.2491	5.9046	-1.511	H	3.1744	-4.9872	-2.0597
H	1.515	1.8111	1.1858	H	-0.5018	-2.3455	1.289

H	0.6982	1.4664	-0.3298	H	0.0273	-1.5876	-0.2036
H	3.0737	3.3356	0.1791	H	-1.5506	-4.196	0.1474
H	3.168	3.9015	-2.1672	H	-1.6875	-4.4415	-2.2583
H	1.8411	2.8337	-2.5685	H	-0.8025	-2.9577	-2.5419
H	1.0432	5.1406	-2.4918	H	0.6868	-4.8665	-2.8469
H	1.7395	5.3947	-0.9063	H	0.239	-5.5426	-1.2961
H	-0.3116	2.3311	-2.1011	H	1.1333	-1.8551	-2.0948
H	-1.8447	3.0465	-1.6301	H	2.8431	-2.0995	-1.7742
H	-0.8871	3.8005	-2.8822	H	2.0799	-2.9521	-3.0947
H	1.0719	4.0225	2.1965	H	0.6519	-4.4251	1.9516
H	5.3675	2.0544	-0.1345	H	-4.0727	-3.6469	0.4885
H	1.8055	-1.0212	-3.6858	H	-2.5297	0.2357	-3.6446
H	2.8749	-2.0419	-4.6221	H	-4.0563	0.7261	-4.344
H	4.7551	-1.5986	-3.1827	H	-5.3301	-0.2349	-2.5452
H	4.0101	-0.0621	-3.6003	H	-4.1659	-1.4343	-3.089
H	3.0046	-3.712	-2.8868	H	-4.4534	2.3799	-2.6337
H	1.3144	-3.3624	-3.1888	H	-2.8438	2.6311	-3.2791
H	4.1685	-1.2929	1.1999	H	-3.8504	0.0631	1.6299
H	2.4638	-0.9217	1.0121	H	-2.1967	0.2962	1.0927
H	3.781	-3.6515	1.4282	H	-4.2983	2.4184	1.7518
H	1.6291	-4.7312	1.5068	H	-2.7027	4.1845	1.3628
H	0.7691	-3.2282	1.2637	H	-1.4327	3.0546	0.951
H	2.6076	-4.6589	-0.7014	H	-4.0072	3.5905	-0.5865
H	0.8783	-4.433	-0.8441	H	-2.3757	3.9735	-1.0909
H	1.7534	-1.7603	4.7383	H	-1.1179	1.6852	4.5789
H	3.5847	-3.1474	5.0387	H	-3.2385	2.3229	5.2417
H	4.4605	-3.9691	3.6387	H	-4.6076	2.6467	4.0496
H	0.7352	-0.887	-1.766	H	-1.1492	0.6386	-1.9965
H	-0.1378	-2.348	-1.3691	H	-0.7957	2.3385	-1.7891
H	0.605	-1.3947	-0.0894	H	-0.8996	1.2819	-0.3839
H	-6.8088	-2.4336	-2.1336	H	2.4219	5.8135	-1.4643
H	-5.4336	-2.3549	-3.2375	H	3.669	5.7001	-0.2236
H	-4.9293	-4.6085	0.3321	H	5.4084	3.5469	-0.7378
H	-6.4037	-3.6879	0.104	H	5.553	3.1052	-2.4331
H	-4.1246	0.9426	-0.1181	H	1.1219	1.7998	0.7483
H	-4.5901	0.265	1.4072	H	1.7018	0.7965	-0.5328
H	-2.0876	-0.4559	-0.2202	H	3.0073	1.4858	2.1346
H	-1.3681	-1.8552	1.6325	H	4.9753	1.8468	1.0907
H	-2.7842	-1.4462	2.5851	H	5.0722	0.0978	1.0563
H	-2.6678	-3.015	-0.0244	H	5.607	1.003	-1.1595
H	-3.0911	-3.6321	1.5642	H	4.1325	0.0698	-1.2371
H	-1.2163	0.3036	3.3585	H	2.0066	-0.395	3.6454
H	-5.4391	-3.2208	2.5308	H	3.9931	1.5619	-3.5176
H	-5.0212	-1.5152	2.6137	H	2.5528	0.9434	-2.7057
H	-6.4898	-2.0108	1.7783	H	2.5962	2.616	-3.2443
H	-5.0717	1.0475	-1.8282	H	0.8487	3.7057	1.2575
H	5.2676	-2.4471	-0.6909	H	-5.6337	0.5968	0.0069

H	-5.5903	-4.5331	-2.0404	H	3.649	4.58	-3.0168
H	-4.0444	-3.7179	-1.8275	H	4.9004	5.4738	-2.1803
4b-9	X axis(Å)	Y axis(Å)	Z axis(Å)	4b-10	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-1.6337	5.3728	-0.6905	C	-0.6398	5.6506	-0.8307
C	-1.5931	4.8145	0.7313	C	-1.0021	4.9378	0.4726
C	-0.83	3.4851	0.8334	C	-0.4599	3.4996	0.5301
C	0.5869	3.5809	0.1925	C	1.0723	3.4636	0.2541
C	0.498	4.066	-1.3022	C	1.4146	4.1226	-1.1339
C	-0.2512	5.4252	-1.3476	C	0.855	5.572	-1.1561
C	1.3955	2.2695	0.2811	C	1.7046	2.0577	0.354
C	2.8021	2.3908	-0.3474	C	3.2359	2.1029	0.1416
C	2.7801	2.9934	-1.7607	C	3.6211	2.8074	-1.1672
C	1.9379	4.2677	-1.8487	C	2.9592	4.1817	-1.3006
C	-0.23	3.0768	-2.2527	C	0.8423	3.3587	-2.3575
C	-0.7621	3.0585	2.281	C	-0.7985	2.8834	1.8673
O	-0.1314	3.6206	3.1662	O	-0.2905	3.1777	2.9414
O	1.3504	4.5837	0.911	O	1.7289	4.2734	1.2677
C	3.4801	1.0441	-0.3687	C	3.8333	0.7216	0.2034
O	2.7848	0.018	-0.9998	O	3.3449	-0.2114	-0.7044
C	4.6591	0.7465	0.1716	C	4.7672	0.3176	1.0615
C	2.8939	-2.1656	-3.15	C	4.0389	-2.3153	-2.8477
C	4.0413	-1.594	-2.3154	C	4.8788	-1.8457	-1.659
C	3.5945	-1.1723	-0.9078	C	4.0249	-1.4585	-0.4423
C	2.8601	-2.333	-0.1738	C	3.0385	-2.5986	-0.0513
C	1.6232	-2.8364	-1.0084	C	2.1151	-2.9821	-1.2666
C	2.111	-3.2631	-2.4203	C	3.0101	-3.387	-2.4698
C	2.4352	-1.9945	1.2741	C	2.1892	-2.2882	1.2037
C	1.7558	-3.1959	1.9711	C	1.2455	-3.4556	1.5717
C	0.5913	-3.7747	1.1507	C	0.3862	-3.9198	0.3847
C	0.9993	-4.0701	-0.2969	C	1.2286	-4.1941	-0.8656
C	1.3592	-2.8886	3.4015	C	0.4113	-3.1623	2.8038
C	0.3583	-1.829	3.6995	C	-0.5538	-2.0284	2.815
C	1.8779	-3.5368	4.4581	C	0.4939	-3.8888	3.9312
O	-0.183	-1.1488	2.8368	O	-0.7133	-1.2685	1.8681
C	0.4975	-1.7818	-1.179	C	1.1677	-1.8433	-1.7257
C	4.7819	-0.6749	-0.1132	C	4.9217	-1.0858	0.717
O	5.714	-1.3583	0.2884	O	5.6538	-1.8485	1.3329
C	-4.3234	-2.9506	-2.2564	C	-7.1717	-1.5895	-1.0066
C	-3.8271	-1.5499	-1.9886	C	-6.246	-0.719	-0.1991
C	-4.1228	-0.8665	-0.8557	C	-4.8976	-0.7247	-0.319
C	-5.0784	-1.4355	0.212	C	-4.1855	-1.6667	-1.3051
C	-5.7077	-2.7974	-0.1937	C	-5.1714	-2.2913	-2.3325
C	-3.4857	0.4509	-0.4379	C	-3.9652	0.1637	0.4958
C	-2.654	0.2584	0.8521	C	-2.9457	0.9247	-0.3774
C	-3.5265	-0.3474	1.9703	C	-2.1678	-0.0549	-1.2643
C	-4.2603	-1.6159	1.5161	C	-3.1145	-0.8951	-2.1182
C	-1.9301	1.5233	1.2685	C	-1.9902	1.8042	0.3993

C	-1.5147	1.835	2.4955	C	-1.8162	1.8578	1.719
O	-1.6137	2.4211	0.2497	O	-1.2181	2.6702	-0.3767
C	-6.2691	-0.4783	0.4638	C	-3.5149	-2.8102	-0.5079
C	-2.9344	-1.0194	-3.067	C	-6.9743	0.1309	0.7906
O	-2.6314	-1.6744	-4.0591	O	-6.6021	0.3139	1.9421
O	3.7789	-3.4541	-0.0742	O	3.8169	-3.7828	0.2675
C	-4.7545	-3.6742	-0.9868	C	-6.4689	-2.7576	-1.6874
H	-2.3197	4.7739	-1.2995	H	-1.227	5.2287	-1.654
H	-2.0582	6.3837	-0.6672	H	-0.9362	6.7038	-0.7583
H	-1.1318	5.5626	1.389	H	-0.6145	5.5219	1.3171
H	-2.6255	4.6877	1.0817	H	-2.0952	4.938	0.5723
H	0.3434	6.1985	-0.8439	H	1.3985	6.1941	-0.433
H	-0.363	5.7603	-2.3866	H	1.0309	6.0294	-2.1381
H	1.5335	1.9889	1.3339	H	1.5258	1.6387	1.353
H	0.8343	1.4502	-0.1824	H	1.2311	1.371	-0.357
H	3.3922	3.0667	0.2875	H	3.6686	2.6896	0.9645
H	3.806	3.2263	-2.0747	H	4.7105	2.935	-1.2105
H	2.4085	2.2604	-2.4873	H	3.3576	2.1856	-2.0315
H	1.904	4.6007	-2.8941	H	3.22	4.6101	-2.2768
H	2.4483	5.0681	-1.2979	H	3.3969	4.856	-0.5532
H	0.1783	2.0639	-2.2042	H	1.1123	2.2994	-2.3583
H	-1.3006	2.9972	-2.055	H	-0.2458	3.4118	-2.4279
H	-0.1378	3.41	-3.2937	H	1.2272	3.7882	-3.2905
H	1.283	4.3993	1.8715	H	1.4191	3.9721	2.1484
H	5.3599	1.3538	0.7108	H	5.2755	0.843	1.8468
H	2.2183	-1.355	-3.4451	H	3.5362	-1.4541	-3.3014
H	3.2983	-2.5744	-4.0837	H	4.7048	-2.7152	-3.6218
H	4.8405	-2.3433	-2.2493	H	5.5824	-2.6429	-1.3868
H	4.4646	-0.736	-2.8533	H	5.488	-0.992	-1.9828
H	2.7524	-4.1506	-2.3423	H	3.5474	-4.3166	-2.2409
H	1.2562	-3.5631	-3.0399	H	2.387	-3.6074	-3.3459
H	3.3205	-1.7326	1.8681	H	2.8491	-2.1213	2.0651
H	1.7871	-1.113	1.2818	H	1.6311	-1.3586	1.0595
H	2.5123	-3.9936	2.0176	H	1.8944	-4.3083	1.822
H	0.2416	-4.706	1.6146	H	-0.1519	-4.8373	0.6555
H	-0.2692	-3.0968	1.1549	H	-0.3842	-3.1795	0.1465
H	1.7079	-4.9084	-0.2985	H	1.8524	-5.0787	-0.6835
H	0.1195	-4.4233	-0.85	H	0.5602	-4.4662	-1.6926
H	0.1227	-1.6796	4.767	H	-1.1317	-1.9003	3.7462
H	1.5956	-3.3163	5.4833	H	-0.1025	-3.6778	4.8139
H	2.6159	-4.3234	4.3228	H	1.1753	-4.7325	4.0031
H	0.7716	-0.9589	-1.8419	H	1.6852	-1.0258	-2.2314
H	-0.3943	-2.242	-1.6214	H	0.4274	-2.2212	-2.4412
H	0.1921	-1.3389	-0.2286	H	0.6173	-1.4028	-0.8926
H	-5.162	-2.8991	-2.9619	H	-7.969	-1.991	-0.3689
H	-3.541	-3.5575	-2.7277	H	-7.6569	-0.9648	-1.7675
H	-6.0524	-3.3398	0.6957	H	-5.4239	-1.5558	-3.1088

H	-6.6018	-2.6302	-0.8107	H	-4.6976	-3.133	-2.8533
H	-2.8372	0.8538	-1.2169	H	-4.5182	0.9124	1.0693
H	-4.2582	1.2148	-0.2921	H	-3.4478	-0.467	1.2294
H	-1.8684	-0.4735	0.617	H	-3.52	1.5941	-1.035
H	-2.908	-0.6098	2.8369	H	-1.4856	0.4887	-1.93
H	-4.2517	0.3947	2.326	H	-1.5433	-0.7079	-0.647
H	-3.5126	-2.4087	1.3801	H	-3.6078	-0.2204	-2.8315
H	-4.9165	-1.9509	2.3298	H	-2.5227	-1.5967	-2.7202
H	-1.5902	1.2986	3.4216	H	-2.2684	1.2995	2.5157
H	-6.9731	-0.9152	1.1821	H	-3.0058	-3.5113	-1.1793
H	-5.9683	0.492	0.868	H	-2.767	-2.442	0.2003
H	-6.8192	-0.2844	-0.4648	H	-4.2454	-3.3813	0.0753
H	-2.5597	0.0048	-2.9504	H	-7.9205	0.5581	0.4169
H	4.623	-3.1315	0.3055	H	4.5086	-3.5349	0.9164
H	-5.2465	-4.6174	-1.2508	H	-6.271	-3.5526	-0.9595
H	-3.8776	-3.9327	-0.3814	H	-7.1298	-3.1895	-2.448
4b-11	X axis(Å)	Y axis(Å)	Z axis(Å)	4b-12	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-3.0434	4.8387	-0.3615	C	-0.9587	5.5786	-0.5235
C	-2.5591	4.3152	0.9925	C	-1.0753	4.911	0.8454
C	-1.5876	3.1347	0.8563	C	-0.5081	3.478	0.8605
C	-0.4048	3.4816	-0.097	C	0.9527	3.4457	0.3226
C	-0.9337	3.9073	-1.5172	C	1.0401	4.0692	-1.1209
C	-1.9002	5.112	-1.3467	C	0.4606	5.5099	-1.0912
C	0.6454	2.3584	-0.2255	C	1.6094	2.0484	0.3431
C	1.819	2.7559	-1.1485	C	3.0791	2.0931	-0.1428
C	1.3362	3.2459	-2.5198	C	3.2299	2.7877	-1.5048
C	0.2722	4.3422	-2.3964	C	2.5319	4.1478	-1.5489
C	-1.683	2.7856	-2.2862	C	0.2806	3.2599	-2.2059
C	-1.0853	2.7046	2.216	C	-0.6157	2.927	2.2649
O	-0.4046	3.3826	2.9736	O	0.0963	3.2332	3.2122
O	0.2976	4.6296	0.448	O	1.7654	4.2878	1.1849
C	2.8047	1.6242	-1.2948	C	3.6715	0.7087	-0.1939
O	2.2781	0.3434	-1.4306	O	3.0412	-0.1985	-1.0365
C	4.1297	1.744	-1.2564	C	4.7233	0.2774	0.4983
C	2.2853	-2.3187	-2.9584	C	3.2634	-2.3127	-3.2441
C	3.4147	-1.2972	-2.8192	C	4.3209	-1.8938	-2.2207
C	3.392	-0.5764	-1.4642	C	3.7092	-1.468	-0.8788
C	3.3698	-1.5882	-0.2771	C	2.7545	-2.5623	-0.3167
C	2.1539	-2.5779	-0.3965	C	1.6091	-2.8827	-1.3494
C	2.2144	-3.29	-1.7756	C	2.2565	-3.3276	-2.6898
C	3.3816	-0.9206	1.1172	C	2.1641	-2.2183	1.0694
C	3.3943	-1.9572	2.2645	C	1.2191	-3.3195	1.5999
C	2.3046	-3.0342	2.1254	C	0.1451	-3.7201	0.5773
C	2.2639	-3.6495	0.7238	C	0.7423	-4.045	-0.7944
C	3.3719	-1.2919	3.6274	C	0.5929	-2.9926	2.9424
C	2.1938	-0.4845	4.0512	C	-0.1863	-1.7371	3.1357
C	4.385	-1.3856	4.5048	C	0.6895	-3.804	4.0091

O	1.2008	-0.3229	3.352	O	-0.2008	-0.8219	2.3218
C	0.7684	-1.8955	-0.2556	C	0.6528	-1.6933	-1.6396
C	4.5723	0.3632	-1.3549	C	4.7999	-1.1226	0.1099
O	5.7495	0.0353	-1.2963	O	5.6175	-1.9033	0.578
C	-3.6949	-4.3345	-1.436	C	-5.3191	-3.2685	-0.6171
C	-3.1726	-2.9195	-1.4124	C	-4.2244	-2.4022	-0.0548
C	-3.6903	-1.954	-0.6154	C	-3.9644	-1.141	-0.469
C	-4.977	-2.1844	0.205	C	-4.8646	-0.4296	-1.4922
C	-5.5797	-3.6056	0.0155	C	-6.172	-1.2244	-1.7737
C	-3.0559	-0.5917	-0.3735	C	-2.7938	-0.2997	0.0214
C	-2.7493	-0.3709	1.1286	C	-3.2677	1.0374	0.6086
C	-3.9941	-0.6109	1.9963	C	-4.1226	1.8056	-0.415
C	-4.641	-1.9684	1.7019	C	-5.2858	0.9549	-0.9284
C	-2.1594	0.9922	1.4067	C	-2.1094	1.8739	1.0921
C	-1.4722	1.3311	2.496	C	-1.7178	1.9851	2.3602
O	-2.3151	1.9637	0.4244	O	-1.4032	2.6038	0.1362
C	-6.0836	-1.1929	-0.2335	C	-4.1018	-0.2544	-2.8253
C	-2.0162	-2.6884	-2.3317	C	-3.4407	-3.078	1.0197
O	-1.4656	-3.5937	-2.9487	O	-3.1904	-2.5667	2.1042
O	4.5727	-2.3988	-0.3506	O	3.515	-3.7864	-0.1405
C	-4.5185	-4.6713	-0.1985	C	-5.922	-2.7205	-1.9058
H	-3.7501	4.1232	-0.7966	H	-1.668	5.1169	-1.2191
H	-3.6111	5.764	-0.2061	H	-1.2607	6.6293	-0.438
H	-2.0806	5.1374	1.5397	H	-0.5546	5.5296	1.5878
H	-3.4361	4.019	1.5823	H	-2.1341	4.9077	1.1349
H	-1.3444	5.9911	-0.9956	H	1.1062	6.1609	-0.4873
H	-2.3264	5.394	-2.318	H	0.4618	5.9386	-2.1016
H	1.0715	2.1304	0.7604	H	1.6154	1.6557	1.3684
H	0.1688	1.4373	-0.5791	H	1.0217	1.3407	-0.2524
H	2.3462	3.5938	-0.6701	H	3.6533	2.6801	0.5879
H	2.1853	3.6439	-3.0903	H	4.2951	2.9303	-1.7286
H	0.9445	2.4083	-3.1097	H	2.8395	2.1514	-2.3085
H	-0.0706	4.6216	-3.4009	H	2.6147	4.5582	-2.5635
H	0.7411	5.2431	-1.9802	H	3.0786	4.8447	-0.9005
H	-1.1135	1.8538	-2.3348	H	0.5753	2.2075	-2.2325
H	-2.6571	2.5441	-1.857	H	-0.8036	3.2844	-2.0808
H	-1.8798	3.0962	-3.3197	H	0.4815	3.6736	-3.2017
H	0.5016	4.4502	1.39	H	1.6288	3.9937	2.1112
H	4.7546	2.6083	-1.1395	H	5.3541	0.7805	1.2053
H	1.3299	-1.7952	-3.0743	H	2.7374	-1.4232	-3.6083
H	2.4297	-2.89	-3.8832	H	3.7627	-2.7447	-4.1197
H	4.3756	-1.8085	-2.9594	H	5.0186	-2.7274	-2.0698
H	3.3266	-0.5711	-3.6376	H	4.9084	-1.0712	-2.6483
H	3.0913	-3.9491	-1.8177	H	2.7718	-4.2877	-2.5561
H	1.3412	-3.9426	-1.9015	H	1.4788	-3.5061	-3.4433
H	4.2868	-0.3085	1.2256	H	2.9728	-2.1059	1.8032
H	2.5354	-0.2339	1.2144	H	1.6613	-1.2511	1.0131

H	4.3522	-2.4926	2.1826	H	1.8451	-4.2124	1.747
H	2.4855	-3.8335	2.8558	H	-0.4009	-4.6008	0.9394
H	1.3154	-2.6318	2.3674	H	-0.5996	-2.9241	0.4733
H	3.164	-4.2611	0.5809	H	1.3388	-4.9627	-0.7135
H	1.4187	-4.3475	0.6659	H	-0.0724	-4.2791	-1.4917
H	2.2616	-0.0274	5.0532	H	-0.7428	-1.6597	4.0852
H	4.3672	-0.9072	5.4794	H	0.2353	-3.57	4.9674
H	5.2786	-1.9566	4.2662	H	1.2347	-4.742	3.9506
H	0.516	-1.2572	-1.1041	H	1.113	-0.903	-2.2359
H	-0.0228	-2.6514	-0.1909	H	-0.2186	-2.0322	-2.2133
H	0.6878	-1.2775	0.6419	H	0.2742	-1.2262	-0.7269
H	-4.3007	-4.4746	-2.3398	H	-4.943	-4.2796	-0.8147
H	-2.8674	-5.0523	-1.4856	H	-6.1083	-3.3637	0.1397
H	-6.2043	-3.8756	0.8763	H	-6.8927	-1.0716	-0.9586
H	-6.2484	-3.6199	-0.8565	H	-6.6595	-0.8508	-2.6829
H	-2.1185	-0.4639	-0.9203	H	-2.1949	-0.8304	0.7627
H	-3.7283	0.1848	-0.757	H	-2.1098	-0.122	-0.8182
H	-1.995	-1.1185	1.4166	H	-3.9108	0.8148	1.4729
H	-3.7217	-0.5798	3.0592	H	-4.5231	2.7178	0.0453
H	-4.7243	0.194	1.848	H	-3.5122	2.1331	-1.2654
H	-3.959	-2.7568	2.0472	H	-5.986	0.814	-0.0933
H	-5.55	-2.0608	2.31	H	-5.8321	1.5214	-1.6935
H	-1.2025	0.758	3.3625	H	-2.0827	1.5117	3.2506
H	-7.0106	-1.3744	0.3233	H	-4.7416	0.2105	-3.5844
H	-5.8155	-0.145	-0.0731	H	-3.2166	0.3812	-2.7246
H	-6.3098	-1.3048	-1.3008	H	-3.7601	-1.2161	-3.2235
H	-1.6831	-1.6498	-2.4591	H	-3.1402	-4.1134	0.787
H	5.3467	-1.8052	-0.4467	H	4.3186	-3.5782	0.3805
H	-4.9929	-5.6508	-0.3281	H	-5.2532	-2.9237	-2.7501
H	-3.8691	-4.7458	0.682	H	-6.8633	-3.2398	-2.1196
4c-1	X axis(Å)	Y axis(Å)	Z axis(Å)	4c-2	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-0.7154	5.8082	-0.3467	C	0.0056	5.6327	1.1087
C	-0.8146	4.9733	0.9299	C	-0.0436	5.2572	-0.3723
C	-0.3112	3.5329	0.7375	C	-0.3165	3.7598	-0.5912
C	1.121	3.5077	0.1287	C	-1.5967	3.301	0.1694
C	1.1824	4.3034	-1.2248	C	-1.4988	3.6256	1.7025
C	0.676	5.7523	-0.9846	C	-1.2214	5.1436	1.8838
C	1.7032	2.0893	-0.0559	C	-1.9626	1.816	-0.0405
C	3.1635	2.1188	-0.5722	C	-3.2979	1.4299	0.651
C	3.2936	2.9753	-1.846	C	-3.2941	1.8356	2.1381
C	2.6599	4.3623	-1.7017	C	-2.8585	3.2852	2.3705
C	0.3424	3.6775	-2.3691	C	-0.3937	2.8338	2.4501
C	-0.3688	2.7994	2.0575	C	-0.4181	3.4744	-2.0714
O	0.3611	2.9892	3.0208	O	-1.3367	3.8056	-2.8085
O	2.0077	4.1989	1.0491	O	-2.7173	4.0725	-0.3422
C	3.7125	0.714	-0.7204	C	-3.637	-0.0366	0.4497
O	3.503	-0.1238	0.374	O	-3.0349	-0.6647	-0.6378

C	4.3754	0.1972	-1.7537	C	-4.4361	-0.7874	1.2071
C	4.8328	-1.9092	2.4804	C	-3.2819	-2.4382	-3.1321
C	5.3014	-1.6084	1.0556	C	-4.1859	-2.3979	-1.8979
C	4.1307	-1.3908	0.0855	C	-3.4185	-2.0562	-0.6133
C	3.1294	-2.5825	0.13	C	-2.1969	-3.0023	-0.4142
C	2.5868	-2.8126	1.5892	C	-1.2261	-2.9258	-1.6511
C	3.7931	-3.0336	2.5436	C	-2.0234	-3.2924	-2.9333
C	1.9581	-2.4587	-0.8708	C	-1.427	-2.7608	0.9046
C	1.0248	-3.6903	-0.8219	C	-0.2342	-3.7293	1.0718
C	0.539	-4.0105	0.6013	C	0.6968	-3.7316	-0.1508
C	1.6961	-4.087	1.6029	C	-0.0746	-3.9515	-1.4571
C	-0.1194	-3.5892	-1.8098	C	0.526	-3.5069	2.3649
C	-1.1256	-2.5003	-1.6906	C	1.1508	-2.1882	2.6574
C	-0.2927	-4.4578	-2.82	C	0.6747	-4.4601	3.3
O	-1.0766	-1.6269	-0.8317	O	1.0575	-1.2221	1.9092
C	1.7321	-1.6413	2.1437	C	-0.5744	-1.5341	-1.8638
C	4.6503	-1.1613	-1.314	C	-4.3424	-2.0965	0.5801
O	5.1987	-1.9936	-2.0239	O	-4.9049	-3.0898	1.02
C	-5.7542	-2.9921	-0.4986	C	5.7153	-1.241	1.3424
C	-4.618	-2.2424	0.1558	C	4.4535	-0.4328	1.147
C	-4.6177	-0.9024	0.361	C	3.9285	-0.1385	-0.0681
C	-5.8035	-0.0242	-0.0879	C	4.6329	-0.5661	-1.3694
C	-6.775	-0.7814	-1.0362	C	6.092	-1.0365	-1.1179
C	-3.4887	-0.1222	1.0254	C	2.609	0.5891	-0.2977
C	-2.9996	1.0661	0.1714	C	2.7445	1.7931	-1.2482
C	-4.1787	1.9878	-0.1727	C	3.3779	1.3472	-2.5765
C	-5.2943	1.2141	-0.8716	C	4.7115	0.6365	-2.3466
C	-1.8866	1.8739	0.8015	C	1.416	2.5029	-1.4097
C	-1.4184	1.7944	2.0459	C	0.7341	2.7183	-2.5336
O	-1.2682	2.7915	-0.0498	O	0.8627	3.0061	-0.2309
C	-6.5935	0.4334	1.1609	C	3.847	-1.7283	-2.0219
C	-3.4941	-3.1384	0.5709	C	3.8264	-0.007	2.4387
O	-3.3952	-4.2938	0.1685	O	4.2233	-0.408	3.5294
O	3.8527	-3.7879	-0.238	O	-2.685	-4.3685	-0.3512
C	-7.0531	-2.1999	-0.5672	C	6.1987	-1.9565	0.0871
H	-1.4731	5.473	-1.0635	H	0.9204	5.2312	1.5587
H	-0.9615	6.8511	-0.1137	H	0.0771	6.723	1.2008
H	-0.2418	5.4698	1.7237	H	-0.8172	5.8588	-0.8667
H	-1.8618	4.9709	1.2589	H	0.9114	5.5428	-0.8318
H	1.3764	6.2913	-0.3334	H	-2.0918	5.7256	1.5536
H	0.6573	6.3076	-1.931	H	-1.0887	5.3787	2.9476
H	1.7022	1.5765	0.9143	H	-2.0836	1.6292	-1.1154
H	1.0745	1.4874	-0.7224	H	-1.1515	1.1612	0.2992
H	3.7805	2.5975	0.2016	H	-4.0987	1.9945	0.1532
H	4.3541	3.1063	-2.0968	H	-4.2998	1.7155	2.5603
H	2.8401	2.4567	-2.6995	H	-2.6428	1.1616	2.7085
H	2.7269	4.8863	-2.6639	H	-2.8069	3.472	3.4509

H	3.264	4.952	-1.0001	H	-3.6458	3.9504	1.9926
H	-0.7334	3.7303	-2.1912	H	0.6166	3.1189	2.1502
H	0.522	4.211	-3.3106	H	-0.4549	3.0195	3.5295
H	0.5859	2.6269	-2.5469	H	-0.4772	1.7532	2.3081
H	1.915	3.7885	1.9352	H	-2.7381	3.9785	-1.3183
H	4.6648	0.6202	-2.6961	H	-5.0066	-0.5525	2.0849
H	4.4271	-0.9969	2.9316	H	-3.001	-1.4162	-3.4101
H	5.6995	-2.1876	3.0919	H	-3.8521	-2.833	-3.9816
H	5.9335	-2.4349	0.7067	H	-4.6851	-3.3696	-1.7925
H	5.943	-0.7183	1.0842	H	-4.9788	-1.6598	-2.0745
H	3.4415	-3.1364	3.5782	H	-1.3815	-3.1923	-3.8179
H	4.2938	-3.98	2.3008	H	-2.3245	-4.3475	-2.898
H	1.4054	-1.5321	-0.6897	H	-1.1038	-1.7179	0.9582
H	2.3496	-2.3896	-1.8941	H	-2.0957	-2.9221	1.7602
H	1.635	-4.5525	-1.1299	H	-0.664	-4.7408	1.1251
H	-0.1882	-3.2673	0.945	H	1.2637	-2.7961	-0.2116
H	0.0083	-4.9713	0.6017	H	1.4433	-4.5293	-0.045
H	2.2993	-4.9754	1.3759	H	-0.4718	-4.9747	-1.4641
H	1.2872	-4.254	2.6077	H	0.6278	-3.8986	-2.2988
H	-1.9409	-2.5173	-2.4338	H	1.7103	-2.1205	3.6065
H	-1.1199	-4.3898	-3.52	H	1.2205	-4.2969	4.225
H	0.3953	-5.2858	-2.9686	H	0.2483	-5.4501	3.162
H	2.316	-0.7424	2.3507	H	-1.2701	-0.7823	-2.2413
H	0.924	-1.3503	1.4675	H	-0.1415	-1.135	-0.9444
H	1.2669	-1.9246	3.0958	H	0.2316	-1.5941	-2.605
H	-5.4454	-3.2705	-1.5144	H	6.5041	-0.5645	1.6962
H	-5.9588	-3.9245	0.0419	H	5.5701	-1.9992	2.1215
H	-6.3513	-0.8356	-2.0485	H	6.7459	-0.1704	-0.9456
H	-7.7211	-0.2339	-1.132	H	6.4887	-1.5455	-2.0053
H	-3.8504	0.234	1.9985	H	1.8921	-0.1269	-0.7143
H	-2.6239	-0.7503	1.2472	H	2.1559	0.9321	0.6332
H	-2.6023	0.6566	-0.7682	H	3.4306	2.5162	-0.7833
H	-4.5641	2.473	0.7324	H	2.6985	0.6853	-3.127
H	-3.8481	2.7964	-0.8372	H	3.5531	2.2195	-3.219
H	-6.1283	1.8982	-1.0753	H	5.1105	0.3074	-3.3148
H	-4.9131	0.897	-1.8524	H	5.4224	1.3797	-1.9593
H	-1.6952	1.1712	2.8739	H	0.9323	2.4429	-3.5513
H	-7.4699	1.0265	0.8752	H	4.3549	-2.0863	-2.9249
H	-6.9487	-0.4194	1.7498	H	3.7427	-2.5798	-1.3407
H	-5.9931	1.0546	1.8329	H	2.8353	-1.4375	-2.3202
H	-2.7449	-2.7203	1.2554	H	2.9855	0.6954	2.3824
H	4.3159	-3.6255	-1.0865	H	-3.4054	-4.4109	0.312
H	-7.5419	-2.1919	0.4137	H	5.6138	-2.8694	-0.0732
H	-7.747	-2.6931	-1.2578	H	7.2387	-2.2744	0.2245
4c-3	X axis(Å)	Y axis(Å)	Z axis(Å)	4c-4	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-1.0876	5.6849	-0.4254	C	2.2109	5.0966	-0.5088
C	-1.1158	4.876	0.8714	C	1.866	4.1423	-1.6537

C	-0.5189	3.4682	0.7051	C	1.0831	2.9085	-1.1825
C	0.9051	3.5258	0.08	C	-0.1706	3.3121	-0.3514
C	0.8989	4.2916	-1.2918	C	0.2288	4.2069	0.8788
C	0.2974	5.7081	-1.079	C	1.0001	5.4525	0.3617
C	1.5812	2.1466	-0.0784	C	-1.0283	2.1136	0.1085
C	3.0317	2.264	-0.61	C	-2.2912	2.5553	0.8799
C	3.0906	3.096	-1.9051	C	-1.9482	3.5013	2.0433
C	2.3642	4.4395	-1.7868	C	-1.067	4.6746	1.5994
C	0.0923	3.5831	-2.4115	C	1.1145	3.4888	1.9323
C	-0.5131	2.763	2.0416	C	0.7026	2.0492	-2.3683
O	0.2169	3.019	2.9894	O	-0.0556	2.3707	-3.2726
O	1.7517	4.2974	0.9742	O	-1.0267	4.1278	-1.1928
C	3.6749	0.8971	-0.7307	C	-3.0867	1.3329	1.2775
O	3.5214	0.0687	0.3799	O	-3.6912	0.6618	0.2151
C	4.3715	0.4058	-1.7542	C	-3.2774	0.8312	2.496
C	4.9379	-1.6143	2.5143	C	-6.4415	-0.2366	-0.8395
C	5.3962	-1.3048	1.0879	C	-5.9659	-0.113	0.6076
C	4.2204	-1.1645	0.1101	C	-4.4681	-0.4205	0.7689
C	3.2859	-2.409	0.1653	C	-4.0986	-1.8003	0.1489
C	2.7492	-2.6506	1.6247	C	-4.5221	-1.8732	-1.3659
C	3.9612	-2.7935	2.5869	C	-6.0407	-1.5671	-1.4828
C	2.1148	-2.361	-0.8419	C	-2.61	-2.1911	0.311
C	1.2489	-3.64	-0.7821	C	-2.319	-3.5945	-0.2719
C	0.7746	-3.9702	0.6427	C	-2.8082	-3.7535	-1.7215
C	1.9293	-3.9715	1.6501	C	-4.2638	-3.3114	-1.8955
C	0.1059	-3.6096	-1.7756	C	-0.8693	-4.0078	-0.1131
C	-0.9571	-2.5742	-1.6716	C	0.2103	-3.2768	-0.8295
C	-0.0167	-4.4963	-2.7775	C	-0.484	-5.0421	0.6533
O	-0.9619	-1.6945	-0.8175	O	0.0223	-2.2595	-1.485
C	1.8289	-1.5214	2.1612	C	-3.7531	-0.8892	-2.2875
C	4.7325	-0.9242	-1.2904	C	-4.0953	-0.3416	2.2311
O	5.3366	-1.7309	-1.9843	O	-4.3998	-1.1513	3.0965
C	-5.5662	-3.1322	-0.7287	C	7.0573	-2.6406	0.4246
C	-4.5241	-2.4434	0.1179	C	6.2376	-1.5852	-0.2821
C	-4.6161	-1.1454	0.4953	C	5.1219	-1.021	0.2434
C	-5.8715	-0.3013	0.1967	C	4.5835	-1.4505	1.6257
C	-6.9988	-1.1091	-0.5057	C	5.248	-2.7587	2.1375
C	-3.4933	-0.344	1.1406	C	4.2935	0.07	-0.4263
C	-3.073	0.8423	0.2409	C	2.7983	-0.2873	-0.4973
C	-4.2884	1.7076	-0.1419	C	2.2498	-0.611	0.8985
C	-5.4402	0.875	-0.7147	C	3.0577	-1.7292	1.5521
C	-1.9905	1.7199	0.8304	C	2.005	0.8225	-1.1351
C	-1.5018	1.6982	2.0693	C	1.321	0.7369	-2.2739
O	-1.4336	2.647	-0.0529	O	1.9643	2.0305	-0.4475
C	-6.4948	0.2442	1.5051	C	4.8625	-0.3241	2.6492
C	-3.3564	-3.3126	0.4599	C	6.8039	-1.211	-1.6168
O	-3.1769	-4.411	-0.0572	O	7.7465	-1.8097	-2.1246

O	4.0758	-3.5774	-0.1846	O	-4.866	-2.8213	0.8422
C	-6.4621	-2.1497	-1.4731	C	6.7502	-2.7702	1.9107
H	-1.8283	5.2819	-1.1248	H	3.0008	4.6547	0.1086
H	-1.4015	6.714	-0.2136	H	2.6357	6.0177	-0.9254
H	-0.5686	5.4284	1.6461	H	1.2878	4.6903	-2.4086
H	-2.1567	4.8116	1.2139	H	2.8004	3.8354	-2.141
H	0.9664	6.3089	-0.4492	H	0.3284	6.0925	-0.2252
H	0.2309	6.238	-2.0378	H	1.3368	6.0657	1.2073
H	1.6236	1.6579	0.9032	H	-1.3592	1.5459	-0.7712
H	0.9892	1.4879	-0.7244	H	-0.4368	1.4206	0.7183
H	3.6208	2.8025	0.146	H	-2.9306	3.1262	0.1913
H	4.1372	3.2935	-2.1706	H	-2.8736	3.9005	2.4779
H	2.666	2.5267	-2.741	H	-1.4438	2.9566	2.8497
H	2.3858	4.943	-2.7619	H	-0.8145	5.283	2.4773
H	2.9332	5.0861	-1.1064	H	-1.6548	5.3287	0.9426
H	-0.9828	3.5664	-2.222	H	2.126	3.2819	1.5773
H	0.2251	4.1055	-3.3669	H	1.2306	4.1156	2.825
H	0.4056	2.5478	-2.5685	H	0.691	2.5368	2.2625
H	1.6977	3.9008	1.8698	H	-1.1971	3.6436	-2.0283
H	4.6324	0.829	-2.7048	H	-2.9237	1.1452	3.4586
H	4.4804	-0.7204	2.9527	H	-6.0488	0.6004	-1.4272
H	5.8155	-1.8372	3.1328	H	-7.5334	-0.1387	-0.8684
H	6.0751	-2.099	0.752	H	-6.5591	-0.7908	1.235
H	5.987	-0.3801	1.1083	H	-6.1866	0.9041	0.9563
H	3.6108	-2.903	3.6212	H	-6.3439	-1.5588	-2.5375
H	4.5144	-3.7137	2.3578	H	-6.6219	-2.3689	-1.0089
H	1.5119	-1.4635	-0.6748	H	-1.9654	-1.4317	-0.1423
H	2.5072	-2.2834	-1.8643	H	-2.3493	-2.22	1.3771
H	1.9056	-4.4718	-1.0782	H	-2.9163	-4.3032	0.3213
H	0.0054	-3.2649	0.9749	H	-2.1752	-3.19	-2.4153
H	0.2978	-4.9589	0.6519	H	-2.7214	-4.8048	-2.0252
H	2.5813	-4.8283	1.4363	H	-4.9133	-4.0298	-1.379
H	1.5254	-4.1489	2.6551	H	-4.5321	-3.379	-2.9578
H	-1.7643	-2.6389	-2.4212	H	1.2234	-3.7015	-0.7273
H	-0.8443	-4.4795	-3.4803	H	0.5539	-5.3421	0.763
H	0.7144	-5.2884	-2.915	H	-1.2138	-5.6307	1.2035
H	2.3617	-0.5895	2.3601	H	-4.0019	0.1575	-2.1029
H	1.0097	-1.2831	1.4779	H	-2.6681	-0.9813	-2.1927
H	1.375	-1.8185	3.1146	H	-3.9998	-1.0789	-3.3394
H	-5.0949	-3.7779	-1.4791	H	6.8755	-3.6049	-0.0672
H	-6.1745	-3.7778	-0.0831	H	8.1283	-2.4257	0.3239
H	-7.6819	-0.4327	-1.0348	H	4.8192	-3.6288	1.6213
H	-7.6113	-1.6312	0.2427	H	5.0363	-2.9037	3.2044
H	-3.8251	0.0066	2.1249	H	4.4367	1.0036	0.1333
H	-2.6045	-0.948	1.335	H	4.629	0.2881	-1.4422
H	-2.6659	0.4172	-0.6877	H	2.6989	-1.1894	-1.1179
H	-4.6377	2.277	0.7284	H	2.2618	0.2781	1.5404

H	-3.9959	2.4538	-0.8921	H	1.1997	-0.9207	0.8287
H	-6.2931	1.54	-0.9016	H	2.6603	-1.9145	2.5583
H	-5.1292	0.4921	-1.6957	H	2.8797	-2.6494	0.979
H	-1.7343	1.0847	2.9177	H	1.1803	-0.0857	-2.9495
H	-7.4119	0.8068	1.2931	H	4.5298	-0.6147	3.6524
H	-6.7573	-0.5749	2.1854	H	5.9305	-0.0879	2.7099
H	-5.8308	0.9165	2.055	H	4.3463	0.6082	2.3992
H	-2.6551	-2.9311	1.214	H	6.3409	-0.366	-2.1406
H	4.5349	-3.3999	-1.0323	H	-4.7345	-2.7066	1.8071
H	-7.2934	-2.6911	-1.939	H	7.2295	-1.9563	2.4666
H	-5.9038	-1.6668	-2.284	H	7.1793	-3.7035	2.2933
4c-5	X axis(Å)	Y axis(Å)	Z axis(Å)	4c-6	X axis(Å)	Y axis(Å)	Z axis(Å)
C	3.5944	-4.0381	-2.2938	C	0.9664	5.5527	1.0663
C	4.1777	-3.747	-0.9112	C	0.8687	5.1622	-0.4081
C	3.3153	-2.7783	-0.0899	C	0.3406	3.7312	-0.6059
C	1.8285	-3.2419	-0.0229	C	-1.0071	3.5154	0.145
C	1.2313	-3.439	-1.4649	C	-0.8696	3.8494	1.6735
C	2.119	-4.4477	-2.2432	C	-0.3356	5.2999	1.8315
C	0.9254	-2.3031	0.8047	C	-1.6209	2.1108	-0.0418
C	-0.5359	-2.7941	0.878	C	-3.0086	1.9742	0.6408
C	-1.1253	-3.1338	-0.5006	C	-2.9503	2.4058	2.1195
C	-0.2024	-4.0239	-1.3365	C	-2.2741	3.7632	2.3295
C	1.1312	-2.1329	-2.299	C	0.0742	2.8939	2.4502
C	3.9064	-2.6193	1.2918	C	0.2098	3.4432	-2.0835
O	3.9713	-3.4876	2.1511	O	-0.633	3.9099	-2.8375
O	1.7803	-4.5372	0.6284	O	-1.9725	4.4575	-0.3955
C	-1.3933	-1.7668	1.5728	C	-3.5951	0.5846	0.4642
O	-1.4187	-0.4986	1.0008	O	-3.1108	-0.1576	-0.6104
C	-2.1273	-1.9646	2.6648	C	-4.514	-0.0015	1.2309
C	-1.0323	2.5118	1.4849	C	-3.721	-1.8462	-3.1013
C	-1.4822	1.4356	2.4735	C	-4.5874	-1.6338	-1.858
C	-2.2968	0.3178	1.8042	C	-3.7548	-1.4494	-0.5814
C	-3.4868	0.8935	0.9812	C	-2.7387	-2.6151	-0.3941
C	-2.9828	1.927	-0.0939	C	-1.786	-2.7304	-1.6418
C	-2.1784	3.0472	0.6214	C	-2.6532	-2.9313	-2.9153
C	-4.3699	-0.1883	0.3196	C	-1.9207	-2.5298	0.9154
C	-5.5566	0.4225	-0.4606	C	-0.9435	-3.7175	1.0709
C	-5.1268	1.5208	-1.4475	C	-0.0449	-3.9043	-0.1619
C	-4.2138	2.5642	-0.7962	C	-0.858	-3.9638	-1.4599
C	-6.4155	-0.6355	-1.1261	C	-0.1409	-3.6542	2.356
C	-5.8407	-1.5222	-2.1763	C	0.7525	-2.4968	2.6326
C	-7.7087	-0.8292	-0.8169	C	-0.1878	-4.6126	3.2964
O	-4.6687	-1.4792	-2.528	O	0.8531	-1.5342	1.8813
C	-2.0829	1.3102	-1.1979	C	-0.8752	-1.4942	-1.8623
C	-2.7657	-0.6708	2.8491	C	-4.6588	-1.3131	0.6199
O	-3.595	-0.4544	3.7222	O	-5.3868	-2.1852	1.0742
C	2.0122	4.9427	-1.813	C	5.6466	-1.9055	1.3133

C	2.0225	3.4605	-1.5138	C	4.3677	-1.1233	1.1467
C	2.698	2.9071	-0.4758	C	3.8216	-0.8542	-0.0637
C	3.5573	3.7707	0.4697	C	4.4201	-1.4164	-1.3689
C	3.8012	5.1981	-0.0931	C	5.6609	-2.3248	-1.1383
C	2.6875	1.4277	-0.1149	C	2.6284	0.0594	-0.3007
C	4.1007	0.8286	0.0448	C	3.0241	1.2598	-1.1848
C	4.9128	1.6486	1.058	C	3.6811	0.7859	-2.496
C	4.955	3.1238	0.6629	C	4.8265	-0.2048	-2.2476
C	3.9925	-0.6412	0.3867	C	1.8425	2.185	-1.3814
C	4.3409	-1.2505	1.5185	C	1.2277	2.5013	-2.5197
O	3.4412	-1.438	-0.6162	O	1.3643	2.7887	-0.217
C	2.8403	3.8969	1.835	C	3.3899	-2.2958	-2.1207
C	1.1915	2.6728	-2.4799	C	3.7918	-0.6409	2.4407
O	0.6335	3.1893	-3.4426	O	4.2094	-1.0236	3.5302
O	-4.3488	1.627	1.8914	O	-3.4839	-3.8598	-0.3234
C	2.5391	5.8099	-0.6773	C	6.5002	-1.8921	0.0511
H	3.7206	-3.1599	-2.9364	H	1.7923	5.0076	1.5365
H	4.1733	-4.8411	-2.7657	H	1.2254	6.6157	1.1401
H	4.2932	-4.696	-0.3719	H	0.2175	5.8796	-0.9239
H	5.1882	-3.3388	-1.0415	H	1.8639	5.2681	-0.8586
H	2.0505	-5.4414	-1.7817	H	-1.0881	6.0168	1.4777
H	1.7465	-4.5655	-3.2687	H	-0.1766	5.5302	2.8927
H	1.2988	-2.2427	1.8356	H	-1.7625	1.9259	-1.1146
H	0.969	-1.2848	0.4025	H	-0.9379	1.3332	0.3196
H	-0.548	-3.7169	1.4749	H	-3.6955	2.6575	0.1218
H	-2.0878	-3.6458	-0.3707	H	-3.966	2.4701	2.5299
H	-1.3522	-2.2183	-1.0608	H	-2.4311	1.6424	2.7124
H	-0.6463	-4.1626	-2.3307	H	-2.2018	3.9616	3.4067
H	-0.1693	-5.0229	-0.8833	H	-2.9309	4.5458	1.9281
H	2.1039	-1.7267	-2.5827	H	1.1215	2.9933	2.1584
H	0.5942	-2.3195	-3.2371	H	0.0356	3.1094	3.5251
H	0.594	-1.3366	-1.7771	H	-0.1939	1.8412	2.3273
H	2.2994	-4.4949	1.4586	H	-1.9988	4.3491	-1.37
H	-2.2748	-2.8419	3.2644	H	-5.036	0.3446	2.1021
H	-0.2392	2.1107	0.846	H	-3.2477	-0.8984	-3.3809
H	-0.5816	3.3433	2.0393	H	-4.3656	-2.1192	-3.9454
H	-2.0734	1.9089	3.2679	H	-5.2643	-2.4906	-1.7471
H	-0.5896	1.0184	2.9574	H	-5.224	-0.7558	-2.0267
H	-1.7697	3.7489	-0.1171	H	-2.0134	-2.9581	-3.8066
H	-2.8466	3.6382	1.2612	H	-3.1554	-3.9066	-2.8761
H	-3.7588	-0.8276	-0.3239	H	-1.3951	-1.5723	0.9631
H	-4.793	-0.8441	1.0919	H	-2.5983	-2.5542	1.7789
H	-6.1884	0.9249	0.2872	H	-1.5658	-4.623	1.1293
H	-4.6211	1.0913	-2.319	H	0.6967	-3.1007	-0.2303
H	-6.0169	2.0291	-1.8406	H	0.5283	-4.8351	-0.0633
H	-4.803	3.1481	-0.0774	H	-1.4496	-4.8884	-1.463
H	-3.8865	3.2789	-1.5622	H	-0.1676	-4.049	-2.309

H	-6.5416	-2.2437	-2.6297	H	1.3285	-2.5466	3.5728
H	-8.3216	-1.5871	-1.2955	H	0.389	-4.5642	4.2156
H	-8.1991	-0.2205	-0.0619	H	-0.8157	-5.4904	3.1692
H	-1.1037	0.9966	-0.8313	H	-1.4143	-0.6174	-2.2261
H	-2.5381	0.4396	-1.6769	H	-0.3566	-1.1939	-0.9496
H	-1.8902	2.0459	-1.988	H	-0.1092	-1.709	-2.6171
H	2.6196	5.1169	-2.7106	H	6.2539	-1.4867	2.1249
H	0.9941	5.2799	-2.0435	H	5.3997	-2.9374	1.5919
H	4.5637	5.169	-0.8837	H	6.2869	-2.3548	-2.0391
H	4.1999	5.8554	0.6899	H	5.3413	-3.3613	-0.9605
H	2.1276	1.3038	0.8215	H	1.8211	-0.5106	-0.7705
H	2.1454	0.8301	-0.8494	H	2.1982	0.4387	0.6271
H	4.6157	0.8965	-0.9243	H	3.785	1.8396	-0.641
H	4.4934	1.5515	2.0664	H	2.9375	0.3193	-3.1529
H	5.9403	1.2667	1.1092	H	4.0772	1.6498	-3.0448
H	5.5232	3.6785	1.4207	H	5.2041	-0.5522	-3.2178
H	5.5301	3.2035	-0.2701	H	5.6539	0.3387	-1.7724
H	4.768	-0.874	2.4279	H	1.3922	2.1838	-3.5311
H	2.7045	2.9308	2.3307	H	3.835	-2.7273	-3.0252
H	3.4134	4.5312	2.5212	H	3.0488	-3.1254	-1.4899
H	1.8442	4.34	1.7293	H	2.4988	-1.7482	-2.4381
H	1.095	1.5952	-2.3011	H	2.9591	0.071	2.3884
H	-4.5722	1.0434	2.6465	H	-4.1898	-3.7613	0.3496
H	1.7715	5.9225	0.0968	H	7.3508	-2.5719	0.1752
H	2.751	6.8173	-1.0538	H	6.9145	-0.8908	-0.1179
4c-7	X axis(Å)	Y axis(Å)	Z axis(Å)	4c-8	X axis(Å)	Y axis(Å)	Z axis(Å)
C	2.6908	4.1474	2.2274	C	2.1448	5.192	-0.5388
C	3.0738	4.1628	0.7476	C	1.8327	4.219	-1.6773
C	2.2378	3.19	-0.0968	C	1.0753	2.9714	-1.2012
C	0.7101	3.4039	0.1209	C	-0.1945	3.3521	-0.3833
C	0.3367	3.2805	1.645	C	0.1733	4.2678	0.8412
C	1.1834	4.3002	2.4543	C	0.9183	5.5268	0.3182
C	-0.1738	2.4633	-0.7257	C	-1.0257	2.137	0.0817
C	-1.6826	2.7083	-0.5057	C	-2.3048	2.5532	0.8405
C	-2.0742	2.7211	0.9804	C	-1.9948	3.5202	1.996
C	-1.1679	3.623	1.8211	C	-1.1394	4.7105	1.5469
C	0.5672	1.8678	2.2483	C	1.0677	3.5816	1.9084
C	2.6199	3.3267	-1.5541	C	0.724	2.093	-2.382
O	2.4091	4.3001	-2.2643	O	-0.0293	2.3913	-3.2983
O	0.3741	4.7558	-0.2838	O	-1.064	4.1386	-1.2387
C	-2.5052	1.6813	-1.2421	C	-3.0694	1.3138	1.2464
O	-2.1579	0.3495	-1.0388	O	-3.6459	0.6127	0.1877
C	-3.5379	1.933	-2.0428	C	-3.2557	0.8216	2.4695
C	-1.422	-2.3015	-2.435	C	-6.3663	-0.3676	-0.8731
C	-2.3126	-1.1667	-2.9402	C	-5.9032	-0.2144	0.5751
C	-3.0737	-0.456	-1.8099	C	-4.3991	-0.4824	0.7493
C	-3.8535	-1.4678	-0.9202	C	-3.9914	-1.8602	0.1488

C	-2.8893	-2.567	-0.3356	C	-4.4041	-1.9631	-1.3671
C	-2.1606	-3.274	-1.5111	C	-5.929	-1.6959	-1.4967
C	-4.6652	-0.8031	0.2143	C	-2.4945	-2.2117	0.3239
C	-5.4499	-1.8362	1.0547	C	-2.1655	-3.6151	-0.2388
C	-4.5739	-2.9974	1.5546	C	-2.6431	-3.8057	-1.6886
C	-3.7342	-3.6194	0.4348	C	-4.1079	-3.4013	-1.8764
C	-6.231	-1.186	2.1805	C	-0.7066	-3.9896	-0.0669
C	-5.5195	-0.4601	3.2699	C	0.3576	-3.2433	-0.7904
C	-7.5717	-1.2245	2.2587	C	-0.2992	-5.001	0.7183
O	-4.3028	-0.3275	3.3093	O	0.1459	-2.2442	-1.4665
C	-1.8154	-2.0203	0.6439	C	-3.654	-0.9724	-2.297
C	-3.9858	0.5965	-2.4008	C	-4.0385	-0.3766	2.2129
O	-4.9921	0.3847	-3.0637	O	-4.3265	-1.1844	3.0858
C	6.4415	-3.9094	0.5007	C	6.6721	-2.8908	0.4249
C	6.1239	-2.4369	0.3755	C	6.0797	-1.674	-0.2445
C	4.8635	-1.9417	0.3023	C	5.106	-0.9198	0.321
C	3.6341	-2.8774	0.3201	C	4.6079	-1.1821	1.759
C	4.0218	-4.3665	0.1033	C	5.3777	-2.3277	2.4742
C	4.5087	-0.4619	0.2099	C	4.3266	0.1789	-0.3891
C	3.551	-0.1539	-0.9554	C	2.8302	-0.1879	-0.4569
C	2.291	-1.0241	-0.8758	C	2.2594	-0.5077	0.9363
C	2.6521	-2.5054	-0.8227	C	3.1034	-1.5511	1.6758
C	3.1605	1.3009	-0.9898	C	2.0328	0.903	-1.1204
C	3.2333	2.104	-2.0484	C	1.3615	0.7919	-2.2646
O	2.6359	1.8297	0.1843	O	1.9705	2.1205	-0.4514
C	2.9195	-2.7489	1.6866	C	4.7965	0.0722	2.6478
C	7.3503	-1.5783	0.3687	C	6.6398	-1.4096	-1.6064
O	8.4833	-2.0446	0.31	O	7.4432	-2.1602	-2.1496
O	-4.8131	-2.1616	-1.7606	O	-4.7372	-2.8913	0.8508
C	5.249	-4.7664	0.9048	C	5.7808	-3.4459	1.5291
H	3.0498	3.2205	2.6881	H	2.9397	4.775	0.0894
H	3.2152	4.9612	2.7424	H	2.551	6.1191	-0.9605
H	2.9595	5.1853	0.3651	H	1.2481	4.7462	-2.4421
H	4.1405	3.9178	0.6648	H	2.7782	3.93	-2.1538
H	0.8944	5.3246	2.1854	H	0.2363	6.1445	-0.2805
H	0.9724	4.1994	3.5266	H	1.2329	6.1562	1.1604
H	0.0285	2.6231	-1.7931	H	-1.3361	1.5533	-0.7949
H	0.0822	1.4186	-0.5172	H	-0.4217	1.4646	0.7021
H	-1.9217	3.6995	-0.9162	H	-2.9547	3.0994	0.1417
H	-3.1104	3.0689	1.0838	H	-2.9334	3.9006	2.4189
H	-2.0618	1.7037	1.3908	H	-1.4836	2.9971	2.8123
H	-1.4569	3.5345	2.8762	H	-0.9089	5.3337	2.4205
H	-1.3572	4.6688	1.5471	H	-1.7379	5.3433	0.8791
H	1.6224	1.6017	2.3344	H	2.0862	3.3943	1.5628
H	0.158	1.8154	3.2647	H	1.1627	4.2202	2.7952
H	0.0854	1.0758	1.6688	H	0.6639	2.6236	2.2459
H	0.7421	4.9177	-1.1777	H	-1.2147	3.6438	-2.0717

H	-3.9951	2.8597	-2.3312	H	-2.9187	1.1569	3.431
H	-0.554	-1.8802	-1.9183	H	-5.9902	0.4713	-1.469
H	-1.0219	-2.8544	-3.2932	H	-7.4599	-0.2967	-0.91
H	-3.0216	-1.5738	-3.6725	H	-6.4833	-0.8991	1.2072
H	-1.6825	-0.4506	-3.4833	H	-6.1514	0.8011	0.9098
H	-1.4447	-4.0101	-1.1234	H	-6.226	-1.7086	-2.5532
H	-2.8819	-3.8428	-2.1121	H	-6.4933	-2.5056	-1.0158
H	-4.0044	-0.2007	0.8444	H	-1.8662	-1.4426	-0.1361
H	-5.3991	-0.1081	-0.2145	H	-2.2391	-2.22	1.3916
H	-6.1854	-2.2901	0.3736	H	-2.748	-4.3306	0.3609
H	-3.9111	-2.672	2.3635	H	-2.0204	-3.2367	-2.3871
H	-5.2127	-3.7771	1.9896	H	-2.5293	-4.8587	-1.9773
H	-4.4041	-4.1493	-0.2547	H	-4.7428	-4.1286	-1.3541
H	-3.0811	-4.3895	0.8651	H	-4.3682	-3.4891	-2.9391
H	-6.1614	-0.0329	4.059	H	1.3815	-3.6374	-0.673
H	-8.1285	-0.7579	3.0658	H	0.7454	-5.273	0.8372
H	-8.1604	-1.7356	1.5014	H	-1.0166	-5.5986	1.275
H	-1.0599	-1.4017	0.1557	H	-3.9282	0.0703	-2.1261
H	-2.2456	-1.4213	1.4505	H	-2.5676	-1.0377	-2.1961
H	-1.2701	-2.8479	1.1142	H	-3.8909	-1.1805	-3.3476
H	6.8298	-4.2617	-0.4637	H	6.8316	-3.6962	-0.3019
H	7.2329	-4.0695	1.2432	H	7.6547	-2.6253	0.8345
H	4.2337	-4.5523	-0.9587	H	4.7767	-2.7386	3.2952
H	3.1822	-5.0227	0.3649	H	6.2931	-1.9346	2.9383
H	4.0603	-0.1597	1.1651	H	4.4786	1.1319	0.1311
H	5.3871	0.1751	0.0877	H	4.6749	0.3546	-1.4092
H	4.0724	-0.3981	-1.8924	H	2.7434	-1.1002	-1.0648
H	1.6835	-0.7563	-0.0027	H	2.1904	0.4018	1.5451
H	1.6598	-0.8433	-1.7551	H	1.2321	-0.8808	0.8427
H	1.7297	-3.0938	-0.7328	H	2.6906	-1.685	2.6838
H	3.0946	-2.776	-1.7914	H	2.9834	-2.515	1.1643
H	3.5717	1.9219	-3.0502	H	1.2376	-0.0427	-2.9287
H	2.0622	-3.4295	1.7463	H	4.4828	-0.1318	3.6785
H	3.591	-2.9882	2.5184	H	5.8492	0.3783	2.6751
H	2.5382	-1.7391	1.8684	H	4.2207	0.9372	2.3073
H	7.2033	-0.4926	0.4201	H	6.3157	-0.4901	-2.1102
H	-5.3382	-1.4938	-2.2498	H	-4.6137	-2.7616	1.8148
H	5.0576	-4.6626	1.979	H	6.3205	-4.2246	2.0801
H	5.4817	-5.8233	0.7305	H	4.8921	-3.921	1.0968
4c-9	X axis(Å)	Y axis(Å)	Z axis(Å)	4c-10	X axis(Å)	Y axis(Å)	Z axis(Å)
C	2.0172	5.7582	0.076	C	-3.7691	-4.0215	2.2957
C	1.8688	4.864	-1.1552	C	-4.2728	-3.7697	0.8746
C	1.2301	3.5041	-0.8277	C	-3.3716	-2.8131	0.0811
C	-0.1156	3.6767	-0.0651	C	-1.8799	-3.2643	0.1125
C	0.081	4.5236	1.2463	C	-1.3663	-3.4205	1.5916
C	0.7168	5.8917	0.8745	C	-2.2901	-4.4181	2.3417
C	-0.8427	2.3482	0.2517	C	-0.9367	-2.3379	-0.6837

C	-2.2087	2.5895	0.9351	C	0.5303	-2.8176	-0.6595
C	-2.0692	3.4801	2.1829	C	1.0407	-3.1174	0.7589
C	-1.3085	4.7774	1.8936	C	0.0772	-3.9951	1.5617
C	0.9777	3.844	2.3149	C	-1.3252	-2.0938	2.3976
C	1.0519	2.7091	-2.1015	C	-3.8835	-2.6912	-1.3355
O	0.2556	2.9537	-2.9972	O	-3.8907	-3.5796	-2.1762
O	-1.0128	4.4403	-0.9144	O	-1.7828	-4.5746	-0.5012
C	-2.9314	1.2841	1.1861	C	1.416	-1.8	-1.3324
O	-3.2918	0.5781	0.0369	O	1.4188	-0.5221	-0.7805
C	-3.3062	0.7627	2.3531	C	2.1862	-2.0132	-2.3962
C	-5.86	-0.1865	-1.4612	C	0.9923	2.4721	-1.3636
C	-5.6279	-0.0985	0.0471	C	1.4845	1.3741	-2.3062
C	-4.19	-0.4768	0.4455	C	2.3028	0.2898	-1.5856
C	-3.7997	-1.8736	-0.1188	C	3.4571	0.9083	-0.7451
C	-3.9676	-1.9233	-1.683	C	2.9079	1.9675	0.2806
C	-5.4261	-1.532	-2.0495	C	2.1077	3.053	-0.4901
C	-2.3881	-2.3562	0.2895	C	4.3365	-0.1362	-0.0195
C	-2.1015	-3.7815	-0.2402	C	5.5135	0.5155	0.7463
C	-2.3329	-3.9066	-1.7556	C	5.0212	1.6277	1.6946
C	-3.706	-3.3743	-2.1766	C	4.1134	2.6425	0.9921
C	-0.7417	-4.3008	0.1766	C	6.3654	-0.5499	1.4201
C	0.5012	-3.6789	-0.3494	C	7.2987	-1.3222	0.5461
C	-0.578	-5.3325	1.0215	C	6.3983	-0.8544	2.7281
O	0.5165	-2.6338	-0.9888	O	7.3613	-1.1634	-0.6667
C	-3.0013	-0.9846	-2.4527	C	1.9855	1.3733	1.3788
C	-4.0513	-0.4189	1.9488	C	2.81	-0.7147	-2.598
O	-4.4934	-1.2348	2.7461	O	3.6396	-0.5056	-3.4713
C	4.9572	-3.5387	1.7549	C	-2.1876	4.9435	1.6751
C	3.9395	-2.532	1.2738	C	-2.1769	3.4567	1.4008
C	4.1513	-1.6771	0.2445	C	-2.8111	2.8811	0.349
C	5.5121	-1.6095	-0.4767	C	-3.6462	3.7205	-0.6392
C	6.6224	-2.3628	0.3071	C	-3.9246	5.1525	-0.105
C	3.1046	-0.7362	-0.3365	C	-2.7718	1.3977	0.0092
C	3.6038	0.7156	-0.3915	C	-4.173	0.7815	-0.1815
C	4.9151	0.8109	-1.1824	C	-4.9576	1.5719	-1.2386
C	5.9729	-0.1313	-0.6049	C	-5.0292	3.0541	-0.8726
C	2.5574	1.65	-0.9439	C	-4.0369	-0.6942	-0.483
C	1.9519	1.5681	-2.1276	C	-4.3168	-1.3321	-1.6179
O	2.1791	2.6915	-0.1019	O	-3.5365	-1.4623	0.5677
C	5.3836	-2.244	-1.8816	C	-2.8834	3.8357	-1.9804
C	2.6533	-2.5777	2.034	C	-1.3762	2.6891	2.4075
O	2.3326	-3.5344	2.7313	O	-0.8223	3.2255	3.3616
O	-4.7346	-2.8452	0.4261	O	4.3283	1.6303	-1.6517
C	6.1483	-3.7137	0.82	C	-2.6887	5.7875	0.5104
H	2.815	5.368	0.7175	H	-3.9399	-3.1291	2.9078
H	2.347	6.7547	-0.2416	H	-4.3682	-4.8182	2.7528
H	1.2673	5.3919	-1.9064	H	-4.3488	-4.7326	0.3531

H	2.8625	4.7215	-1.5988	H	-5.2924	-3.368	0.9356
H	0.008	6.4862	0.2833	H	-2.1867	-5.4222	1.9101
H	0.9142	6.4754	1.7828	H	-1.9774	-4.5072	3.3899
H	-1.029	1.8047	-0.6837	H	-1.2498	-2.3059	-1.7358
H	-0.217	1.6939	0.8695	H	-1.0107	-1.3104	-0.3103
H	-2.8439	3.1434	0.2285	H	0.5835	-3.7553	-1.2304
H	-3.0648	3.7387	2.5659	H	2.013	-3.6236	0.6981
H	-1.5638	2.9349	2.9888	H	1.2272	-2.1863	1.3082
H	-1.1947	5.3405	2.8288	H	0.463	-4.1053	2.5833
H	-1.9247	5.4079	1.2398	H	0.0784	-5.0052	1.1326
H	2.027	3.7814	2.0201	H	-2.3159	-1.6902	2.6149
H	0.9599	4.4176	3.2498	H	-0.8419	-2.2525	3.3694
H	0.6521	2.829	2.5566	H	-0.7652	-1.3052	1.888
H	-1.0758	3.99	-1.7836	H	-2.2508	-4.558	-1.3623
H	-3.1691	1.1005	3.362	H	2.3535	-2.8972	-2.9808
H	-5.3309	0.632	-1.9618	H	0.19	2.0773	-0.7325
H	-6.9249	-0.0299	-1.6706	H	0.542	3.2783	-1.9546
H	-6.346	-0.7532	0.5575	H	2.0867	1.834	-3.1003
H	-5.8591	0.9245	0.3706	H	0.6112	0.927	-2.7985
H	-5.5456	-1.4998	-3.14	H	1.6704	3.7717	0.2149
H	-6.1212	-2.3037	-1.6935	H	2.7836	3.6332	-1.1316
H	-1.6289	-1.6443	-0.0491	H	3.7347	-0.7477	0.6629
H	-2.3102	-2.3929	1.3838	H	4.7553	-0.828	-0.7605
H	-2.8459	-4.4422	0.2287	H	6.1602	1.0182	0.0127
H	-1.5542	-3.3801	-2.3178	H	4.4783	1.2028	2.5459
H	-2.2575	-4.9603	-2.0538	H	5.884	2.1589	2.1164
H	-4.4779	-4.0522	-1.7898	H	4.7129	3.2143	0.2722
H	-3.7877	-3.4242	-3.27	H	3.7574	3.3729	1.73
H	1.4378	-4.2133	-0.1159	H	7.9373	-2.0623	1.0575
H	0.4007	-5.6907	1.3305	H	7.0503	-1.6238	3.1323
H	-1.4335	-5.8441	1.4539	H	5.7697	-0.3476	3.4527
H	-3.2185	0.0744	-2.3008	H	1.0232	1.03	0.9943
H	-1.9545	-1.1397	-2.1791	H	2.4384	0.5271	1.9017
H	-3.0789	-1.1584	-3.533	H	1.7576	2.1325	2.1366
H	5.3188	-3.2158	2.7397	H	-2.8225	5.1269	2.5516
H	4.4923	-4.5225	1.8916	H	-1.1796	5.2934	1.9298
H	6.9499	-1.7659	1.1694	H	-4.7117	5.1253	0.6611
H	7.5101	-2.4999	-0.3231	H	-4.3052	5.794	-0.9098
H	2.8514	-1.0886	-1.3445	H	-2.1848	1.2683	-0.9098
H	2.1622	-0.7562	0.2148	H	-2.2418	0.816	0.7647
H	3.8159	1.029	0.6415	H	-4.7205	0.8665	0.7684
H	4.7499	0.578	-2.2413	H	-4.5015	1.4606	-2.2294
H	5.2977	1.8391	-1.1492	H	-5.9783	1.1771	-1.3186
H	6.8783	-0.0723	-1.2226	H	-5.5745	3.589	-1.6609
H	6.2532	0.2525	0.386	H	-5.6394	3.1442	0.0369
H	2.0535	0.8582	-2.9261	H	-4.6942	-0.9799	-2.5587
H	6.3534	-2.2653	-2.392	H	-1.8946	4.2874	-1.8461

H	5.0139	-3.2739	-1.8287	H	-2.724	2.8646	-2.4593
H	4.6952	-1.6936	-2.5303	H	-3.437	4.4572	-2.6937
H	1.9882	-1.7086	1.9412	H	-1.2983	1.6044	2.2683
H	-4.7302	-2.7607	1.4033	H	4.6714	1.002	-2.3222
H	5.8754	-4.3672	-0.0164	H	-1.8982	5.8984	-0.2405
H	6.9619	-4.2175	1.3547	H	-2.9242	6.7977	0.865
4c-11	X axis(Å)	Y axis(Å)	Z axis(Å)	4c-12	X axis(Å)	Y axis(Å)	Z axis(Å)
C	2.7546	5.04	-1.0531	C	2.2613	5.367	-0.3754
C	2.1572	4.1366	-2.1342	C	1.8705	4.5098	-1.5795
C	1.4376	2.9118	-1.5502	C	1.1784	3.1968	-1.1719
C	0.3816	3.3309	-0.4863	C	-0.0333	3.4672	-0.2347
C	1.0455	4.1673	0.6701	C	0.4067	4.2741	1.0427
C	1.7525	5.4037	0.0491	C	1.099	5.5917	0.5963
C	-0.4295	2.1519	0.0937	C	-0.8246	2.2019	0.17
C	-1.5005	2.6247	1.1007	C	-2.0657	2.5534	1.0254
C	-0.8956	3.497	2.212	C	-1.6834	3.4001	2.2521
C	-0.0654	4.6538	1.6434	C	-0.8568	4.6324	1.8733
C	2.0869	3.3818	1.5121	C	1.3782	3.5049	1.977
C	0.8153	2.094	-2.6582	C	0.7761	2.4328	-2.4123
O	-0.1055	2.4504	-3.38	O	-0.1406	2.7209	-3.1692
O	-0.5802	4.207	-1.1296	O	-0.9667	4.3164	-0.9545
C	-2.2886	1.4357	1.5942	C	-2.8681	1.3143	1.3534
O	-3.2621	0.9791	0.7081	O	-3.4214	0.6655	0.2497
C	-2.1724	0.7894	2.7524	C	-3.1433	0.804	2.5524
C	-6.3021	0.5347	0.4947	C	-6.1427	-0.0528	-0.9845
C	-5.3994	0.3944	1.7199	C	-5.7583	0.0337	0.4929
C	-3.9822	-0.0851	1.3636	C	-4.2964	-0.3692	0.7475
C	-4.0182	-1.3885	0.5137	C	-3.9831	-1.7692	0.1451
C	-4.8805	-1.1885	-0.7893	C	-4.301	-1.8095	-1.3957
C	-6.305	-0.7178	-0.3863	C	-5.7844	-1.4024	-1.6148
C	-2.6215	-1.9511	0.1565	C	-2.5437	-2.263	0.4139
C	-2.7231	-3.2701	-0.6456	C	-2.3109	-3.6826	-0.1531
C	-3.6344	-3.1503	-1.8784	C	-2.6929	-3.8002	-1.6378
C	-4.9985	-2.5473	-1.5333	C	-4.0992	-3.2602	-1.9172
C	-1.3736	-3.8574	-1.0065	C	-0.9121	-4.1938	0.1237
C	-0.4477	-3.1306	-1.9161	C	0.272	-3.5064	-0.457
C	-0.9533	-5.0519	-0.5566	C	-0.665	-5.269	0.8909
O	-0.6124	-1.9711	-2.2733	O	0.2005	-2.4982	-1.1488
C	-4.2908	-0.1585	-1.7899	C	-3.4061	-0.8759	-2.2536
C	-3.1783	-0.2548	2.6318	C	-4.005	-0.3219	2.2292
O	-3.3128	-1.1502	3.4547	O	-4.4087	-1.116	3.068
C	5.7978	-2.6022	2.2328	C	5.8796	-2.5242	2.0988
C	4.8075	-1.5701	1.742	C	4.7504	-1.6077	1.685
C	4.083	-1.7044	0.6033	C	4.3318	-1.4594	0.4033
C	4.2595	-2.9299	-0.3173	C	5.0248	-2.2083	-0.7563
C	5.5273	-3.7556	0.036	C	6.3866	-2.8208	-0.327
C	3.0434	-0.7084	0.1026	C	3.1691	-0.5785	-0.0406

C	3.3189	-0.2551	-1.3446	C	3.5596	0.3885	-1.1715
C	3.3658	-1.4777	-2.2715	C	4.1274	-0.3921	-2.3649
C	4.4184	-2.4797	-1.7958	C	5.3236	-1.2393	-1.9322
C	2.3373	0.8157	-1.7619	C	2.4063	1.2999	-1.5193
C	1.4371	0.7808	-2.7431	C	1.6385	1.2779	-2.6076
O	2.4157	1.9921	-1.0189	O	2.1552	2.3072	-0.5875
C	3.0226	-3.8467	-0.1773	C	4.105	-3.3509	-1.2461
C	4.7057	-0.3869	2.6554	C	4.1332	-0.89	2.8461
O	5.3841	-0.2757	3.6714	O	4.5325	-1.0302	3.9976
O	-4.6825	-2.416	1.2975	O	-4.8683	-2.7345	0.7756
C	5.6888	-3.9513	1.5342	C	6.3058	-3.5142	1.0226
H	3.6327	4.5524	-0.6154	H	3.1044	4.9014	0.147
H	3.1242	5.9611	-1.5194	H	2.626	6.3386	-0.7294
H	1.4629	4.7267	-2.7459	H	1.2131	5.0952	-2.2352
H	2.9666	3.8186	-2.8038	H	2.7779	4.2998	-2.1603
H	1.0063	6.0882	-0.375	H	0.3685	6.2534	0.1127
H	2.2726	5.9728	0.8302	H	1.4674	6.1403	1.4726
H	-0.9488	1.6292	-0.7205	H	-1.1758	1.6889	-0.7346
H	0.2331	1.4143	0.5616	H	-0.1835	1.4879	0.6998
H	-2.2164	3.264	0.5639	H	-2.7317	3.1775	0.412
H	-1.6994	3.9114	2.8339	H	-2.592	3.7359	2.7683
H	-0.2708	2.8961	2.8826	H	-1.125	2.7956	2.9767
H	0.3774	5.2177	2.4743	H	-0.5709	5.1657	2.7891
H	-0.7392	5.3542	1.1333	H	-1.4971	5.3258	1.3129
H	3.0072	3.1635	0.9669	H	2.37	3.3623	1.5437
H	2.3894	3.9669	2.3893	H	1.5329	4.0613	2.9096
H	1.6994	2.4286	1.881	H	1.0041	2.5157	2.2535
H	-0.9326	3.7525	-1.9239	H	-1.1909	3.8772	-1.8027
H	-1.5106	0.9331	3.584	H	-2.8568	1.1105	3.5396
H	-5.9918	1.4072	-0.0907	H	-5.659	0.7607	-1.5365
H	-7.3266	0.7433	0.8253	H	-7.2217	0.1149	-1.0852
H	-5.8662	-0.3044	2.426	H	-6.4332	-0.6076	1.0743
H	-5.3573	1.3661	2.2286	H	-5.9369	1.0612	0.8352
H	-6.9056	-0.521	-1.2835	H	-6.0113	-1.3663	-2.688
H	-6.8253	-1.5193	0.1543	H	-6.4489	-2.1675	-1.1925
H	-2.0388	-1.1998	-0.3846	H	-1.8178	-1.549	0.0132
H	-2.0639	-2.1705	1.0764	H	-2.3636	-2.3113	1.4958
H	-3.2159	-3.9954	0.0191	H	-3.0026	-4.3477	0.3853
H	-3.1581	-2.5494	-2.6609	H	-1.9711	-3.2758	-2.2731
H	-3.7913	-4.1438	-2.3182	H	-2.6528	-4.8531	-1.9455
H	-5.5579	-3.2682	-0.9233	H	-4.8321	-3.9352	-1.4566
H	-5.5787	-2.4261	-2.4571	H	-4.2906	-3.3059	-2.997
H	0.4341	-3.7022	-2.2519	H	1.2485	-3.9606	-0.2197
H	0.0102	-5.4773	-0.8204	H	0.3378	-5.6349	1.0902
H	-1.5763	-5.6494	0.1044	H	-1.4781	-5.8246	1.3512
H	-4.3313	0.8694	-1.4246	H	-3.6025	0.1845	-2.0839
H	-3.2485	-0.3663	-2.045	H	-2.339	-1.0359	-2.0788

H	-4.8588	-0.1686	-2.7283	H	-3.5855	-1.0499	-3.3216
H	6.8102	-2.2032	2.0881	H	6.7411	-1.9034	2.3771
H	5.6712	-2.7737	3.3088	H	5.5991	-3.1009	2.9887
H	6.427	-3.2491	-0.34	H	7.152	-2.0351	-0.2619
H	5.4982	-4.7332	-0.4614	H	6.7429	-3.5309	-1.0839
H	2.0501	-1.1722	0.1656	H	2.3521	-1.2277	-0.3738
H	2.9799	0.1753	0.7388	H	2.7508	0.0068	0.78
H	4.3142	0.2129	-1.3708	H	4.3669	1.0376	-0.8003
H	2.3862	-1.9656	-2.3217	H	3.3608	-1.0338	-2.8147
H	3.614	-1.1659	-3.2939	H	4.4525	0.3041	-3.1484
H	4.4016	-3.3548	-2.4582	H	5.6931	-1.8027	-2.7988
H	5.4039	-2.0129	-1.9326	H	6.1327	-0.5527	-1.6469
H	1.1722	0.0086	-3.4404	H	1.6222	0.6186	-3.4539
H	3.1233	-4.7423	-0.8011	H	4.5942	-3.9402	-2.0303
H	2.876	-4.1773	0.8566	H	3.8416	-4.0362	-0.4332
H	2.0998	-3.3462	-0.4805	H	3.1657	-2.9797	-1.6665
H	3.9931	0.4006	2.3829	H	3.2936	-0.2174	2.6347
H	-4.2518	-2.4607	2.1772	H	-4.7884	-2.6379	1.7481
H	4.8442	-4.5184	1.9417	H	5.6012	-4.3526	0.9829
H	6.5882	-4.5435	1.7394	H	7.2815	-3.9407	1.2833
4d-1	X axis(Å)	Y axis(Å)	Z axis(Å)	4d-2	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-2.7674	5.0924	-0.2394	C	-0.605	5.3162	0.9965
C	-2.2045	4.375	-1.4689	C	-0.5231	4.929	-0.4789
C	-1.415	3.1103	-1.1015	C	0.0448	3.5184	-0.7003
C	-0.3128	3.4206	-0.0473	C	1.3951	3.311	0.0498
C	-0.9298	4.0611	1.2497	C	1.2572	3.6407	1.5787
C	-1.7149	5.3408	0.8483	C	0.7133	5.0857	1.7398
C	0.5713	2.2081	0.3155	C	1.9891	1.9005	-0.1327
C	1.6987	2.5899	1.3009	C	3.3571	1.7076	0.571
C	1.1372	3.2702	2.56	C	3.3265	2.1923	2.0354
C	0.2243	4.454	2.2158	C	2.6655	3.5595	2.2255
C	-1.8896	3.1251	2.0315	C	0.3197	2.679	2.3574
C	-0.824	2.4765	-2.3421	C	0.1825	3.2712	-2.1847
O	0.0449	2.9635	-3.052	O	0.9781	3.8187	-2.9358
O	0.5783	4.4176	-0.6142	O	2.3657	4.2454	-0.4883
C	2.5797	1.391	1.5623	C	3.8187	0.263	0.4554
O	3.2862	0.9443	0.4475	O	3.3255	-0.4511	-0.6359
C	2.7775	0.735	2.7037	C	4.5941	-0.4077	1.3066
C	6.1299	0.5284	-0.61	C	3.7283	-2.4333	-2.953
C	5.6178	0.3714	0.8223	C	4.5597	-2.2696	-1.6792
C	4.1611	-0.1176	0.8784	C	3.7175	-1.8303	-0.4739
C	3.9703	-1.4204	0.0491	C	2.4919	-2.7714	-0.2604
C	4.4141	-1.2054	-1.4475	C	1.5977	-2.8306	-1.5548
C	5.889	-0.7166	-1.4699	C	2.4766	-3.2951	-2.7487
C	2.542	-2.0122	0.1113	C	1.6334	-2.4195	0.9782
C	2.4383	-3.3327	-0.6881	C	0.4498	-3.396	1.1658
C	2.9295	-3.185	-2.1366	C	-0.4022	-3.5425	-0.105

C	4.3262	-2.5597	-2.2049	C	0.4542	-3.8611	-1.3361
C	1.0666	-3.9693	-0.6192	C	-0.3882	-3.068	2.3862
C	-0.1308	-3.2742	-1.1622	C	-1.0897	-1.7596	2.5005
C	0.8557	-5.1806	-0.0771	C	-0.5415	-3.9171	3.4164
O	-0.1217	-2.1174	-1.5668	O	-1.0397	-0.8905	1.6381
C	3.5471	-0.1811	-2.2283	C	0.9364	-1.4799	-1.9338
C	3.7356	-0.2911	2.3179	C	4.576	-1.758	0.7661
O	4.11	-1.1737	3.0778	O	5.1364	-2.7008	1.308
C	-4.5353	-4.0676	1.4059	C	-5.6012	-1.7213	1.4057
C	-3.5993	-2.9217	1.1082	C	-4.6629	-0.5652	1.1519
C	-3.9756	-1.7754	0.4921	C	-4.3671	-0.0966	-0.0854
C	-5.4378	-1.5458	0.0585	C	-4.9171	-0.7784	-1.3545
C	-6.273	-2.8566	0.0848	C	-5.6	-2.1415	-1.0493
C	-3.0372	-0.6179	0.1705	C	-3.4571	1.0911	-0.3775
C	-3.1412	-0.1489	-1.2941	C	-2.2831	0.7016	-1.2952
C	-4.5909	0.188	-1.6582	C	-2.8267	0.1092	-2.6064
C	-5.504	-1.0061	-1.3944	C	-3.7538	-1.0763	-2.3385
C	-2.2531	1.0384	-1.5602	C	-1.3123	1.8474	-1.4916
C	-1.3976	1.1604	-2.5728	C	-0.7388	2.2387	-2.6284
O	-2.3349	2.0907	-0.6553	O	-0.9378	2.5264	-0.3311
C	-6.0881	-0.5269	1.0246	C	-5.9555	0.1485	-2.0276
C	-2.2076	-3.1597	1.5931	C	-4.0836	0.0012	2.4105
O	-1.7861	-4.2834	1.8454	O	-4.2455	-0.5299	3.5061
O	4.8534	-2.4324	0.6035	O	2.9891	-4.118	-0.0387
C	-6.0088	-3.6899	1.3286	C	-6.4599	-2.0875	0.2021
H	-3.1955	6.0531	-0.5496	H	-0.8809	6.3746	1.0752
H	-3.6005	4.5113	0.1713	H	-1.4151	4.7578	1.4782
H	-3.0404	4.1217	-2.1335	H	-1.5286	5.0064	-0.912
H	-1.5657	5.0719	-2.0262	H	0.098	5.6685	-1.001
H	-2.2071	5.7731	1.7289	H	0.5693	5.319	2.8025
H	-1.0193	6.1087	0.4858	H	1.4518	5.8088	1.3699
H	-0.0314	1.3889	0.7248	H	1.2794	1.1385	0.2102
H	1.0431	1.819	-0.596	H	2.1447	1.7198	-1.2046
H	2.3457	3.3306	0.8089	H	4.0927	2.3191	0.0305
H	0.5853	2.5488	3.1739	H	2.8107	1.4556	2.6643
H	1.9637	3.6345	3.1834	H	4.3514	2.2532	2.4238
H	0.8352	5.2516	1.7736	H	3.3254	4.3305	1.8076
H	-0.1838	4.872	3.1449	H	2.6011	3.7761	3.2998
H	-1.4466	2.1489	2.2452	H	0.6023	1.6289	2.2473
H	-2.1598	3.5731	2.9957	H	0.3475	2.9054	3.4303
H	-2.8324	2.9427	1.512	H	-0.7264	2.7588	2.0553
H	0.8997	4.09	-1.481	H	2.3728	4.163	-1.4652
H	2.3664	0.8738	3.6846	H	5.077	-0.1041	2.2153
H	5.6579	1.4021	-1.0731	H	3.4461	-1.4452	-3.3331
H	7.2046	0.7449	-0.5854	H	4.3521	-2.887	-3.7325
H	6.2715	-0.3273	1.3601	H	5.0635	-3.22	-1.4613
H	5.7155	1.3395	1.3302	H	5.3524	-1.5363	-1.8758

H	6.5531	-1.515	-1.114	H	2.794	-4.3351	-2.5978
H	6.2003	-0.5037	-2.5005	H	1.8871	-3.292	-3.6745
H	2.2789	-2.2391	1.1527	H	2.2499	-2.4803	1.8846
H	1.8122	-1.2758	-0.2382	H	1.2831	-1.3858	0.9113
H	3.1345	-4.037	-0.2086	H	0.8943	-4.3869	1.3431
H	2.9626	-4.1709	-2.6179	H	-1.1335	-4.3493	0.0329
H	2.2287	-2.5852	-2.7279	H	-0.9885	-2.6362	-0.2918
H	5.0513	-3.2733	-1.7927	H	0.8691	-4.8711	-1.2246
H	4.6061	-2.426	-3.2577	H	-0.195	-3.9019	-2.2202
H	-1.0626	-3.8656	-1.1692	H	-1.6681	-1.6068	3.4278
H	-0.13	-5.6335	-0.0092	H	-1.144	-3.6804	4.2891
H	1.6738	-5.7568	0.3461	H	-0.0632	-4.8928	3.4136
H	3.6904	0.8485	-1.8949	H	1.6451	-0.7416	-2.3135
H	3.8092	-0.1914	-3.2935	H	0.1962	-1.624	-2.7301
H	2.4772	-0.3948	-2.1601	H	0.418	-1.0205	-1.0901
H	-4.3301	-4.876	0.6924	H	-5.0052	-2.5932	1.705
H	-4.343	-4.4686	2.4087	H	-6.2752	-1.49	2.2397
H	-6.0363	-3.4731	-0.7934	H	-4.8416	-2.9236	-0.9057
H	-7.3443	-2.6287	0.0166	H	-6.21	-2.4649	-1.9021
H	-3.2727	0.2059	0.8565	H	-4.0491	1.8891	-0.8437
H	-1.9895	-0.868	0.3558	H	-3.0604	1.5366	0.5352
H	-2.8155	-0.9797	-1.9366	H	-1.7173	-0.09	-0.7874
H	-4.9419	1.0627	-1.0973	H	-3.3582	0.8762	-3.1829
H	-4.6576	0.4573	-2.7202	H	-1.9998	-0.2405	-3.2369
H	-6.5357	-0.7281	-1.6454	H	-4.154	-1.4388	-3.2942
H	-5.2227	-1.8033	-2.0966	H	-3.1348	-1.8918	-1.9384
H	-1.1513	0.485	-3.3696	H	-0.8257	1.871	-3.6325
H	-7.1408	-0.3602	0.7686	H	-5.5182	1.0915	-2.3698
H	-6.0512	-0.8728	2.0634	H	-6.3994	-0.3327	-2.9068
H	-5.5931	0.4491	0.9995	H	-6.7716	0.404	-1.3426
H	-1.5625	-2.2782	1.712	H	-3.4812	0.9135	2.3248
H	4.6782	-2.5007	1.5657	H	3.6736	-4.0872	0.662
H	-6.304	-3.1398	2.2293	H	-7.2705	-1.3598	0.0808
H	-6.6194	-4.6	1.3053	H	-6.9346	-3.0606	0.3729
4d-3	X axis(Å)	Y axis(Å)	Z axis(Å)	4d-4	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-2.7942	5.0535	-0.3643	C	2.5226	5.165	-0.6268
C	-2.2462	4.2799	-1.5662	C	2.2077	4.6656	0.7826
C	-1.4516	3.0335	-1.1499	C	1.3202	3.4074	0.7791
C	-0.3363	3.3937	-0.1261	C	0.0284	3.63	-0.0593
C	-0.9377	4.092	1.1484	C	0.3689	4.0748	-1.5276
C	-1.7292	5.3516	0.6987	C	1.2657	5.3427	-1.4824
C	0.5557	2.2009	0.2795	C	-0.9385	2.4248	-0.0753
C	1.6941	2.6305	1.2315	C	-2.255	2.7441	-0.8318
C	1.1464	3.362	2.4672	C	-1.9708	3.2867	-2.2462
C	0.2276	4.5287	2.0819	C	-0.9529	4.43	-2.2603
C	-1.8869	3.1921	1.984	C	1.0973	2.9916	-2.3658
C	-0.8772	2.3397	-2.3659	C	1.0106	3.012	2.2063

O	-0.0178	2.7913	-3.1099	O	0.2262	3.5754	2.9571
O	0.5447	4.365	-0.7504	O	-0.7024	4.7324	0.5432
C	2.5849	1.4482	1.5299	C	-3.218	1.5713	-0.8262
O	3.304	0.9822	0.4315	O	-3.1754	0.7492	0.2986
C	2.7807	0.8221	2.6883	C	-4.1082	1.2551	-1.766
C	6.1639	0.5874	-0.5872	C	-4.8123	-0.3576	2.6383
C	5.6394	0.4522	0.843	C	-5.2932	0.0144	1.2346
C	4.1894	-0.0568	0.8948	C	-4.2222	-0.2363	0.1623
C	4.0265	-1.3794	0.0915	C	-3.6915	-1.6985	0.2249
C	4.4814	-1.1878	-1.4052	C	-3.1139	-2.0298	1.6504
C	5.9492	-0.678	-1.4238	C	-4.2179	-1.7684	2.7125
C	2.6069	-1.9928	0.1529	C	-2.66	-2.041	-0.8739
C	2.5326	-3.3306	-0.6207	C	-2.2028	-3.5162	-0.7975
C	3.0323	-3.2019	-2.0679	C	-1.7154	-3.9135	0.6049
C	4.4202	-2.5578	-2.1365	C	-2.7184	-3.5323	1.6982
C	1.174	-3.9946	-0.5526	C	-1.1944	-3.8755	-1.8709
C	-0.0357	-3.3311	-1.1083	C	0.1178	-3.1774	-1.9397
C	0.9871	-5.2071	-0.0045	C	-1.4175	-4.8249	-2.7951
O	-0.0541	-2.1735	-1.5108	O	0.4262	-2.2483	-1.2027
C	3.6071	-0.1923	-2.2147	C	-1.8573	-1.2041	2.0369
C	3.7511	-0.2038	2.3335	C	-4.7694	0.0876	-1.2071
O	4.1259	-1.0667	3.1156	O	-5.6289	-0.5435	-1.8071
C	-4.6489	-4.1301	1.1953	C	4.6149	-4.2211	-0.0422
C	-3.6885	-2.971	1.1051	C	3.6183	-3.1326	0.2828
C	-4.0451	-1.742	0.6637	C	3.8657	-1.81	0.1158
C	-5.5146	-1.3852	0.3617	C	5.2438	-1.3089	-0.3632
C	-6.4992	-2.5507	0.6622	C	6.3241	-2.4251	-0.3194
C	-3.0663	-0.6275	0.3198	C	2.8536	-0.6908	0.3419
C	-3.1926	-0.2224	-1.166	C	3.3897	0.3981	1.285
C	-4.6443	0.1057	-1.5507	C	4.73	0.9518	0.781
C	-5.6136	-1.0056	-1.1373	C	5.7442	-0.1693	0.5644
C	-2.299	0.9439	-1.4984	C	2.3929	1.5149	1.4598
C	-1.4554	1.0147	-2.5256	C	1.7856	1.8454	2.5973
O	-2.366	2.0378	-0.6431	O	2.101	2.2775	0.3308
C	-5.9802	-0.198	1.2404	C	5.1272	-0.7954	-1.8178
C	-2.2911	-3.3027	1.5085	C	2.3181	-3.6677	0.7961
O	-1.8883	-4.4561	1.6119	O	2.0727	-4.8694	0.8483
O	4.9199	-2.3654	0.6754	O	-4.8179	-2.5927	0.0161
C	-5.9052	-3.916	0.3591	C	5.8073	-3.7465	-0.8628
H	-3.2263	5.9991	-0.7134	H	3.0494	6.1243	-0.559
H	-3.6223	4.4922	0.0827	H	3.2175	4.4727	-1.115
H	-3.0901	3.9959	-2.2079	H	3.1573	4.4638	1.2948
H	-1.6146	4.95	-2.1632	H	1.7182	5.4709	1.3453
H	-2.2115	5.8231	1.5644	H	1.5633	5.6314	-2.4986
H	-1.0388	6.1028	0.2935	H	0.6948	6.1915	-1.0838
H	-0.0394	1.3999	0.7336	H	-0.4574	1.536	-0.4996
H	1.0172	1.7715	-0.6192	H	-1.2024	2.1699	0.959

H	2.3302	3.3529	0.6997	H	-2.7657	3.5414	-0.2731
H	0.6029	2.6668	3.1177	H	-1.62	2.4754	-2.896
H	1.9793	3.7538	3.0648	H	-2.8997	3.659	-2.6967
H	0.8318	5.3063	1.5969	H	-1.4158	5.3141	-1.803
H	-0.1697	4.9874	2.9964	H	-0.7461	4.7095	-3.3014
H	-1.4412	2.2258	2.2337	H	0.5596	2.0402	-2.3865
H	-2.143	3.6822	2.9314	H	1.2027	3.3211	-3.4068
H	-2.8372	2.9885	1.4868	H	2.1079	2.7807	-2.0107
H	0.8566	3.9972	-1.6044	H	-0.8479	4.5236	1.4907
H	2.3602	0.98	3.6623	H	-4.3437	1.7158	-2.7058
H	5.6845	1.4447	-1.0726	H	-4.0756	0.3785	2.9789
H	7.2351	0.8196	-0.5564	H	-5.6545	-0.2861	3.337
H	6.2976	-0.2255	1.4016	H	-6.2007	-0.5585	1.005
H	5.7181	1.4319	1.3316	H	-5.5875	1.0718	1.2398
H	6.6214	-1.4593	-1.0457	H	-5.0338	-2.4927	2.5899
H	6.2672	-0.4813	-2.4557	H	-3.8179	-1.9342	3.721
H	2.3375	-2.2028	1.1962	H	-3.1081	-1.8928	-1.865
H	1.8693	-1.2754	-0.2185	H	-1.8114	-1.3538	-0.8144
H	3.2382	-4.0121	-0.1221	H	-3.0988	-4.1261	-0.9867
H	3.0839	-4.1957	-2.5313	H	-1.5464	-4.9973	0.6439
H	2.3266	-2.6233	-2.6745	H	-0.7487	-3.4513	0.8257
H	5.152	-3.2523	-1.7037	H	-3.6096	-4.1645	1.5937
H	4.7077	-2.4407	-3.1892	H	-2.2901	-3.7816	2.6775
H	-0.9505	-3.9481	-1.1279	H	0.8152	-3.5415	-2.7134
H	0.0112	-5.682	0.0582	H	-0.692	-5.0854	-3.5599
H	1.8155	-5.7637	0.4249	H	-2.3495	-5.3838	-2.807
H	3.7342	0.8461	-1.9029	H	-2.0739	-0.1495	2.2175
H	3.8777	-0.222	-3.2773	H	-1.4201	-1.5858	2.9677
H	2.5396	-0.4188	-2.15	H	-1.0737	-1.245	1.2757
H	-4.1759	-5.0563	0.8484	H	4.9753	-4.6504	0.9016
H	-4.9217	-4.281	2.2472	H	4.1304	-5.0322	-0.5994
H	-7.4304	-2.4208	0.0966	H	6.6594	-2.589	0.7141
H	-6.7868	-2.5381	1.7229	H	7.2146	-2.1188	-0.8826
H	-3.2495	0.2248	0.9843	H	2.5971	-0.2559	-0.6329
H	-2.0251	-0.9112	0.4939	H	1.9069	-1.0498	0.7493
H	-2.8789	-1.0858	-1.7709	H	3.5676	-0.0662	2.2661
H	-4.9578	1.0559	-1.1011	H	4.5963	1.5126	-0.1521
H	-4.7154	0.2494	-2.6367	H	5.1366	1.6643	1.5102
H	-6.6355	-0.6869	-1.3798	H	6.6711	0.2613	0.164
H	-5.4109	-1.887	-1.76	H	5.9993	-0.5825	1.5502
H	-1.2214	0.3023	-3.2935	H	1.8402	1.416	3.5788
H	-5.4138	0.7207	1.0637	H	4.4557	0.0639	-1.909
H	-7.0346	0.0354	1.0506	H	6.1041	-0.4782	-2.2008
H	-5.8789	-0.4357	2.3062	H	4.7431	-1.5701	-2.4905
H	-1.623	-2.4558	1.7202	H	1.5801	-2.9374	1.148
H	4.7357	-2.4165	1.637	H	-5.2799	-2.3227	-0.8053
H	-6.6359	-4.7006	0.5869	H	5.5222	-3.6442	-1.916

H	-5.6695	-4.002	-0.7083	H	6.6006	-4.5022	-0.827
4d-5	X axis(Å)	Y axis(Å)	Z axis(Å)	4d-6	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-0.5958	5.3378	1.041	C	-3.1639	-4.4084	-1.8723
C	-0.5473	4.9508	-0.436	C	-3.6481	-4.1388	-0.4481
C	0.0064	3.5365	-0.6687	C	-2.8169	-3.0656	0.2729
C	1.3719	3.3219	0.0514	C	-1.2947	-3.3861	0.2193
C	1.2695	3.6516	1.583	C	-0.8076	-3.5648	-1.2669
C	0.7365	5.0994	1.7564	C	-1.6573	-4.6727	-1.9469
C	1.9565	1.9092	-0.1452	C	-0.4147	-2.35	0.9514
C	3.3403	1.713	0.5261	C	1.0844	-2.7192	0.9074
C	3.3427	2.1937	1.9921	C	1.5816	-3.0208	-0.5155
C	2.6914	3.5633	2.1989	C	0.6803	-4.0101	-1.2569
C	0.3448	2.6942	2.3818	C	-0.9049	-2.2771	-2.1296
C	0.1112	3.2862	-2.1554	C	-3.3124	-2.9196	1.6946
O	0.8926	3.8293	-2.9245	O	-3.1618	-3.7323	2.5963
O	2.3344	4.2527	-0.5077	O	-1.0732	-4.6558	0.886
C	3.7996	0.269	0.3952	C	1.9265	-1.6318	1.5234
O	3.2826	-0.4416	-0.6872	O	1.7484	-0.349	1.0161
C	4.5956	-0.4038	1.2255	C	2.8374	-1.7959	2.4797
C	3.6317	-2.4151	-3.0207	C	1.2066	2.6016	1.7055
C	4.4937	-2.2545	-1.7669	C	1.9	1.5347	2.5517
C	3.6802	-1.8209	-0.54	C	2.677	0.5164	1.7037
C	2.4614	-2.7646	-0.3006	C	3.6601	1.2198	0.722
C	1.5361	-2.8202	-1.5729	C	2.9003	2.2444	-0.2012
C	2.3867	-3.2798	-2.7891	C	2.1459	3.2651	0.6941
C	1.6332	-2.4179	0.9591	C	4.4961	0.2407	-0.1325
C	0.4549	-3.3955	1.1723	C	5.4813	0.9766	-1.0692
C	-0.4281	-3.5382	-0.0776	C	4.8075	2.0723	-1.9125
C	0.3986	-3.8521	-1.3301	C	3.9401	3.0094	-1.0664
C	-0.3531	-3.0705	2.4134	C	6.2885	0.0168	-1.9221
C	-1.038	-1.7559	2.5533	C	5.6093	-0.8675	-2.9102
C	-0.4913	-3.926	3.4403	C	7.6252	-0.0896	-1.8384
O	-1.007	-0.8855	1.6912	O	4.3956	-0.8924	-3.0713
C	0.8643	-1.4693	-1.9322	C	1.8742	1.5943	-1.1685
C	4.5678	-1.7518	0.6797	C	3.3923	-0.4585	2.6128
O	5.1433	-2.6956	1.2039	O	4.3394	-0.1989	3.3424
C	-5.3171	-1.9344	1.3731	C	-3.4529	5.2127	-0.0289
C	-4.6019	-0.619	1.1805	C	-3.0877	3.8224	0.4394
C	-4.431	-0.0419	-0.0342	C	-3.4445	2.6903	-0.2162
C	-5.0363	-0.6493	-1.3154	C	-4.332	2.742	-1.4789
C	-5.9233	-1.8953	-1.0405	C	-4.9615	4.1454	-1.7021
C	-3.5366	1.1595	-0.3112	C	-3.0347	1.2771	0.179
C	-2.3525	0.7367	-1.2078	C	-4.2468	0.3415	0.3367
C	-2.8641	0.0846	-2.5083	C	-5.0967	0.3281	-0.9408
C	-3.8563	-1.0535	-2.2372	C	-5.5134	1.743	-1.3386
C	-1.3778	1.8738	-1.4283	C	-3.7982	-1.0488	0.7053
C	-0.8234	2.2566	-2.5773	C	-3.9781	-1.6406	1.8837

O	-0.9753	2.5522	-0.277	O	-3.1182	-1.7631	-0.2756
C	-5.9499	0.3685	-2.0404	C	-3.4804	2.3841	-2.7199
C	-4.0382	-0.0557	2.4475	C	-2.2823	3.829	1.7006
O	-4.1157	-0.6411	3.5243	O	-1.983	4.8614	2.291
O	2.9653	-4.1113	-0.0958	O	4.6077	1.9907	1.5068
C	-5.3939	-2.7566	0.0928	C	-3.9656	5.2673	-1.4621
H	-0.864	6.3976	1.126	H	-3.7006	-5.2753	-2.276
H	-1.3986	4.7836	1.5395	H	-3.4318	-3.5633	-2.516
H	-1.5612	5.0348	-0.848	H	-4.7024	-3.8371	-0.4943
H	0.0675	5.6863	-0.971	H	-3.6191	-5.0787	0.1183
H	0.6161	5.3326	2.822	H	-1.3657	-4.7795	-2.9996
H	1.471	5.8189	1.3716	H	-1.4521	-5.6436	-1.4776
H	1.2528	1.1492	0.214	H	-0.5813	-1.3496	0.5357
H	2.0865	1.7284	-1.2205	H	-0.7055	-2.2956	2.0089
H	4.0638	2.3258	-0.0291	H	1.2189	-3.6344	1.5013
H	2.8373	1.4573	2.6296	H	1.6666	-2.0954	-1.0986
H	4.3758	2.25	2.3589	H	2.597	-3.4359	-0.4694
H	3.3451	4.3322	1.7678	H	0.7809	-4.9981	-0.7897
H	2.6514	3.7783	3.2746	H	1.0489	-4.1275	-2.2841
H	0.6195	1.6428	2.2646	H	-0.4099	-1.419	-1.6673
H	0.3978	2.9197	3.454	H	-0.4285	-2.4343	-3.1051
H	-0.7073	2.7799	2.1034	H	-1.9327	-1.9758	-2.3408
H	2.3206	4.1695	-1.4844	H	-1.5009	-4.6258	1.7677
H	5.0995	-0.1029	2.1237	H	3.1597	-2.6765	3.0008
H	3.3385	-1.4262	-3.3902	H	0.3509	2.1558	1.1872
H	4.237	-2.865	-3.8167	H	0.7928	3.3709	2.368
H	5.0041	-3.2048	-1.5646	H	2.5769	2.0294	3.26
H	5.2801	-1.5191	-1.98	H	1.138	1.0248	3.1551
H	2.7093	-4.3198	-2.649	H	2.8655	3.885	1.2446
H	1.7752	-3.2749	-3.7004	H	1.566	3.958	0.071
H	2.2712	-2.4811	1.8503	H	5.0936	-0.4056	0.524
H	1.2815	-1.384	0.9031	H	3.8348	-0.4232	-0.6967
H	0.9038	-4.3866	1.3362	H	6.1933	1.5009	-0.4142
H	-1.1552	-4.3462	0.0753	H	5.5767	2.6684	-2.4205
H	-1.0199	-2.6319	-0.2466	H	4.1957	1.6365	-2.7095
H	0.8168	-4.8623	-1.2321	H	4.5958	3.6152	-0.4277
H	-0.2717	-3.8904	-2.1985	H	3.4321	3.7208	-1.7302
H	-1.584	-1.6	3.4994	H	6.2723	-1.5203	-3.5031
H	-1.0724	-3.6903	4.3276	H	8.2011	-0.7775	-2.4501
H	-0.0226	-4.9061	3.4195	H	8.1911	0.5229	-1.1413
H	1.5639	-0.726	-2.3187	H	1.0021	1.1795	-0.6591
H	0.1135	-1.6124	-2.7184	H	1.4861	2.3412	-1.872
H	0.3559	-1.0166	-1.0784	H	2.3085	0.7883	-1.7653
H	-4.8076	-2.5498	2.1243	H	-4.2212	5.6133	0.645
H	-6.3274	-1.734	1.751	H	-2.5852	5.8803	0.0398
H	-6.0213	-2.5029	-1.949	H	-5.8115	4.2933	-1.0217
H	-6.9426	-1.5808	-0.7757	H	-5.3687	4.2258	-2.7179

H	-4.116	1.9603	-0.785	H	-2.351	0.888	-0.5869
H	-3.1473	1.6055	0.6049	H	-2.4597	1.2474	1.1067
H	-1.7925	-0.0361	-0.6646	H	-4.8719	0.7337	1.1521
H	-3.3357	0.8379	-3.1509	H	-4.5523	-0.1407	-1.7695
H	-2.0219	-0.3243	-3.08	H	-5.9971	-0.2791	-0.7829
H	-4.2373	-1.4227	-3.198	H	-6.0794	1.6968	-2.2779
H	-3.3	-1.8869	-1.7881	H	-6.2151	2.109	-0.5761
H	-0.9329	1.886	-3.5781	H	-4.4487	-1.2944	2.7837
H	-5.4168	1.2546	-2.3953	H	-3.0865	1.3638	-2.6808
H	-6.4208	-0.0894	-2.9185	H	-4.0743	2.4608	-3.638
H	-6.7509	0.7175	-1.3778	H	-2.6193	3.0531	-2.8253
H	-3.5466	0.923	2.388	H	-1.9694	2.8578	2.1015
H	3.6662	-4.0822	0.5886	H	4.99	1.4078	2.1959
H	-6.0547	-3.6171	0.2482	H	-3.1277	5.1952	-2.165
H	-4.4051	-3.158	-0.1594	H	-4.4429	6.2372	-1.6437
4d-7	X axis(Å)	Y axis(Å)	Z axis(Å)	4d-8	X axis(Å)	Y axis(Å)	Z axis(Å)
C	3.6154	-4.0006	1.9246	C	2.6886	5.1034	-0.5966
C	3.9308	-3.7986	0.4421	C	2.3838	4.5888	0.8096
C	2.9183	-2.8801	-0.2607	C	1.4562	3.3606	0.8016
C	1.4577	-3.3673	-0.036	C	0.1575	3.637	-0.0099
C	1.13	-3.4672	1.5009	C	0.4868	4.0955	-1.4765
C	2.1613	-4.4138	2.1744	C	1.4228	5.3346	-1.426
C	0.3938	-2.515	-0.7614	C	-0.8449	2.461	-0.0287
C	-1.0366	-3.06	-0.5436	C	-2.1632	2.8294	-0.7588
C	-1.3637	-3.2557	0.9449	C	-1.8866	3.3893	-2.168
C	-0.2914	-4.068	1.6748	C	-0.8358	4.5026	-2.1799
C	1.1537	-2.1071	2.2502	C	1.1674	3.0051	-2.3453
C	3.2593	-2.7774	-1.7306	C	1.158	2.951	2.2271
O	3.1235	-3.6623	-2.5641	O	0.4148	3.5339	3.0044
O	1.34	-4.7094	-0.5766	O	-0.5295	4.7503	0.6229
C	-2.0815	-2.1822	-1.1851	C	-3.1587	1.6837	-0.7598
O	-1.8716	-0.8087	-1.1294	O	-3.1041	0.8198	0.3334
C	-3.1969	-2.6117	-1.7713	C	-4.0877	1.4273	-1.6801
C	-1.7355	1.776	-2.8134	C	-4.7228	-0.27	2.6951
C	-2.5553	0.5121	-3.0651	C	-5.2252	0.156	1.3147
C	-3.0034	-0.1767	-1.7664	C	-4.1964	-0.1166	0.2065
C	-3.7283	0.8148	-0.8104	C	-3.7308	-1.6022	0.2208
C	-2.8181	2.0605	-0.4942	C	-3.1333	-1.9956	1.622
C	-2.4118	2.7376	-1.8316	C	-4.1949	-1.7085	2.7201
C	-4.2264	0.1643	0.4996	C	-2.7436	-1.964	-0.912
C	-4.9654	1.1726	1.4088	C	-2.3569	-3.4612	-0.8841
C	-4.1661	2.4637	1.6537	C	-1.8576	-3.9202	0.4953
C	-3.6324	3.0757	0.3548	C	-2.8107	-3.5163	1.6243
C	-5.4351	0.5398	2.7046	C	-1.3923	-3.838	-1.9914
C	-4.4483	-0.0075	3.6776	C	-0.0448	-3.211	-2.065
C	-6.7319	0.4381	3.0412	C	-1.6872	-4.7397	-2.9429
O	-3.2387	-0.0058	3.4859	O	0.3322	-2.3341	-1.297

C	-1.5226	1.7246	0.2939	C	-1.8288	-1.2401	1.9926
C	-3.8689	-1.3683	-2.1105	C	-4.7688	0.2636	-1.138
O	-4.9991	-1.3258	-2.5767	O	-5.6639	-0.3224	-1.7317
C	2.7901	5.4158	-0.101	C	4.5709	-4.2874	0.138
C	2.4748	3.989	-0.488	C	3.5099	-3.2224	0.2692
C	3.0744	2.907	0.0677	C	3.7258	-1.9216	-0.0431
C	4.186	3.0669	1.1275	C	5.0627	-1.443	-0.6467
C	4.705	4.5286	1.2258	C	6.0657	-2.6002	-0.9144
C	2.7427	1.454	-0.2542	C	2.7529	-0.7804	0.2212
C	3.9894	0.6348	-0.6373	C	3.3743	0.2357	1.1985
C	5.0659	0.7312	0.4514	C	4.7581	0.719	0.7273
C	5.41	2.1873	0.7554	C	5.6881	-0.4434	0.3607
C	3.6304	-0.8055	-0.8982	C	2.4537	1.4071	1.4227
C	3.7557	-1.449	-2.0564	C	1.8814	1.7394	2.5776
O	3.1164	-1.5184	0.1793	O	2.1897	2.2139	0.3185
C	3.6349	2.6482	2.5112	C	4.844	-0.7513	-2.0153
C	1.4158	3.896	-1.5402	C	2.2183	-3.7354	0.8221
O	0.9349	4.8831	-2.0866	O	2.0161	-4.9284	1.0283
O	-4.906	1.3212	-1.4913	O	-4.9019	-2.4393	0.0209
C	3.5756	5.5442	1.1974	C	5.98	-3.7084	0.1202
H	4.282	-4.7702	2.3319	H	3.2459	6.0447	-0.522
H	3.8458	-3.0819	2.4753	H	3.353	4.3991	-1.1093
H	4.9437	-3.3838	0.3593	H	3.3355	4.3468	1.3
H	3.9561	-4.7784	-0.0519	H	1.9314	5.3993	1.3954
H	1.9838	-4.4568	3.2566	H	1.7112	5.6318	-2.4423
H	2.0251	-5.439	1.8061	H	0.8854	6.1932	-1.0026
H	0.4665	-1.4698	-0.4401	H	-0.3967	1.5655	-0.4744
H	0.5832	-2.521	-1.8427	H	-1.1003	2.1976	1.0057
H	-1.0913	-4.0469	-1.0248	H	-2.6426	3.6301	-0.1777
H	-1.4956	-2.2846	1.4382	H	-1.5711	2.58	-2.8381
H	-2.3252	-3.7756	1.0474	H	-2.8113	3.797	-2.5959
H	-0.3174	-5.1006	1.3035	H	-1.2646	5.3917	-1.6996
H	-0.5518	-4.1276	2.7394	H	-0.6382	4.7943	-3.2195
H	0.5357	-1.3464	1.7659	H	0.6013	2.0704	-2.3711
H	0.7728	-2.2269	3.2719	H	1.2638	3.3485	-3.3826
H	2.1563	-1.6872	2.3517	H	2.1775	2.7585	-2.0125
H	1.6701	-4.7026	-1.4998	H	-0.6604	4.5333	1.5706
H	-3.5793	-3.6041	-1.9126	H	-4.3395	1.9282	-2.5947
H	-0.7434	1.494	-2.4463	H	-3.9423	0.4224	3.0298
H	-1.5687	2.2934	-3.7656	H	-5.5404	-0.1754	3.4197
H	-3.4309	0.7745	-3.6729	H	-6.1635	-0.3705	1.0984
H	-1.9514	-0.1751	-3.6715	H	-5.4714	1.225	1.3523
H	-3.2974	3.1648	-2.3199	H	-5.0475	-2.3901	2.6034
H	-1.7396	3.5826	-1.6374	H	-3.7765	-1.9176	3.713
H	-4.9336	-0.6424	0.2658	H	-3.2079	-1.7685	-1.8873
H	-3.3903	-0.3043	1.0265	H	-1.8611	-1.3203	-0.8576
H	-5.8659	1.4804	0.8563	H	-3.2855	-4.0223	-1.0674

H	-4.8071	3.2021	2.1527	H	-1.7454	-5.0121	0.5025
H	-3.3301	2.2861	2.3386	H	-0.8626	-3.5161	0.7031
H	-4.479	3.4653	-0.2249	H	-3.7344	-4.1018	1.5305
H	-3.0135	3.9483	0.6002	H	-2.3692	-3.8095	2.5854
H	-4.8737	-0.4304	4.6036	H	0.6126	-3.5789	-2.8711
H	-7.0661	-0.0153	3.9696	H	-0.9937	-5.012	-3.7328
H	-7.5102	0.8151	2.3829	H	-2.6496	-5.2446	-2.9538
H	-0.7972	1.154	-0.2893	H	-1.9886	-0.1796	2.1964
H	-1.0093	2.6456	0.5964	H	-1.3895	-1.6605	2.9056
H	-1.7188	1.1536	1.2049	H	-1.066	-1.3054	1.2123
H	3.3623	5.8763	-0.9167	H	4.5179	-4.9936	0.9754
H	1.8658	5.9959	0.0106	H	4.3875	-4.8593	-0.7801
H	5.3815	4.7484	0.3883	H	7.0922	-2.215	-0.9566
H	5.2984	4.664	2.1388	H	5.8709	-3.0468	-1.8996
H	2.2504	1.0125	0.6223	H	2.4823	-0.3027	-0.7278
H	2.0181	1.3556	-1.065	H	1.8042	-1.1153	0.6446
H	4.404	1.0649	-1.5606	H	3.5206	-0.2791	2.1598
H	4.7405	0.2291	1.3706	H	4.6614	1.391	-0.1343
H	5.975	0.2107	0.1237	H	5.2298	1.3141	1.5199
H	6.1527	2.2164	1.5632	H	6.6206	-0.031	-0.0453
H	5.9063	2.6043	-0.132	H	5.9613	-0.968	1.2858
H	4.1103	-1.1186	-3.0136	H	1.9231	1.2789	3.5456
H	3.3372	1.5955	2.5451	H	4.236	0.1554	-1.9534
H	4.3894	2.7915	3.2933	H	5.8029	-0.459	-2.4597
H	2.7532	3.2358	2.7897	H	4.343	-1.4265	-2.7194
H	1.0789	2.893	-1.823	H	1.4381	-2.9975	1.0408
H	-5.42	0.5603	-1.8343	H	-5.3717	-2.1287	-0.7817
H	2.9095	5.4035	2.0562	H	6.6994	-4.4997	-0.1196
H	3.9821	6.5588	1.2808	H	6.2467	-3.3266	1.1129
4d-9	X axis(Å)	Y axis(Å)	Z axis(Å)	4d-10	X axis(Å)	Y axis(Å)	Z axis(Å)
C	2.2856	4.8993	0.166	C	-2.7772	4.9066	-0.4927
C	1.9157	4.1053	1.4185	C	-2.2065	4.1018	-1.6629
C	1.0155	2.8966	1.1115	C	-1.4201	2.8661	-1.1981
C	-0.2383	3.3143	0.2896	C	-0.321	3.2566	-0.1682
C	0.1676	4.0574	-1.0345	C	-0.9454	3.9892	1.0766
C	1.0646	5.2749	-0.6787	C	-1.7316	5.2346	0.5802
C	-1.205	2.1506	-0.0228	C	0.5707	2.0799	0.2832
C	-2.4797	2.6306	-0.7606	C	1.6876	2.5414	1.2462
C	-2.1303	3.456	-2.0135	C	1.1143	3.3021	2.4521
C	-1.1213	4.573	-1.7317	C	0.2021	4.4558	2.0174
C	0.9323	3.1709	-2.0528	C	-1.9065	3.1096	1.9202
C	0.6352	2.2139	2.4049	C	-0.8303	2.1407	-2.387
O	-0.1336	2.6498	3.2508	O	0.0489	2.5698	-3.1216
O	-0.9907	4.2719	1.0815	O	0.5665	4.2139	-0.806
C	-3.4131	1.4685	-1.0347	C	2.5733	1.3706	1.5969
O	-3.6906	0.6576	0.0652	O	3.4355	0.9758	0.5765
C	-4.0035	1.1443	-2.184	C	2.638	0.6926	2.7406

C	-5.9058	-0.5048	1.843	C	6.39	0.5218	-0.1465
C	-5.9698	-0.1344	0.3605	C	5.7014	0.3521	1.2081
C	-4.6304	-0.3523	-0.3591	C	4.2411	-0.1099	1.0786
C	-4.0983	-1.7998	-0.1417	C	4.1252	-1.3886	0.1987
C	-3.952	-2.1266	1.3904	C	4.756	-1.1543	-1.225
C	-5.3238	-1.9017	2.085	C	6.2326	-0.7031	-1.053
C	-2.78	-2.1042	-0.8885	C	2.6846	-1.9327	0.0683
C	-2.324	-3.5674	-0.683	C	2.63	-3.2245	-0.7801
C	-2.2586	-3.9683	0.8002	C	3.3196	-3.0743	-2.1453
C	-3.5469	-3.6189	1.5527	C	4.7304	-2.4914	-2.0171
C	-1.0367	-3.8788	-1.4207	C	1.2251	-3.7747	-0.9065
C	0.2216	-3.1666	-1.0701	C	0.1478	-2.968	-1.5461
C	-0.9592	-4.787	-2.4078	C	0.8752	-4.9893	-0.4506
O	0.2873	-2.3058	-0.2016	O	0.3339	-1.863	-2.0432
C	-2.8856	-1.2709	2.1251	C	4.0174	-0.0917	-2.0825
C	-4.7748	-0.0357	-1.8288	C	3.65	-0.3133	2.4551
O	-5.415	-0.6849	-2.6449	O	3.9399	-1.2071	3.2391
C	6.75	-1.9677	-1.6248	C	-5.0614	-3.9135	1.7356
C	5.8424	-0.8668	-1.1249	C	-4.0139	-2.926	1.2961
C	5.1326	-0.9429	0.0284	C	-4.2725	-1.7809	0.6238
C	5.1677	-2.2108	0.9075	C	-5.7022	-1.4213	0.1864
C	5.8175	-3.4185	0.1766	C	-6.6738	-2.6282	0.3209
C	4.243	0.163	0.5855	C	-3.2216	-0.736	0.2649
C	2.8106	-0.3238	0.8843	C	-3.2578	-0.3387	-1.2239
C	2.8593	-1.5196	1.8485	C	-4.6752	0.0741	-1.65
C	3.7255	-2.6441	1.2838	C	-5.7016	-1.0034	-1.3063
C	1.948	0.822	1.3657	C	-2.3024	0.7879	-1.5309
C	1.2994	0.9272	2.5245	C	-1.4385	0.8289	-2.5432
O	1.7956	1.8715	0.4578	O	-2.3476	1.8881	-0.6808
C	5.9813	-1.9177	2.1903	C	-6.2332	-0.2627	1.0628
C	5.8218	0.3229	-2.0346	C	-2.6358	-3.3251	1.6944
O	6.4127	0.3416	-3.1097	O	-1.6944	-3.3533	0.9126
O	-5.0867	-2.7253	-0.6697	O	4.9045	-2.4391	0.8316
C	7.0759	-3.0255	-0.5786	C	-6.4854	-3.3804	1.6309
H	2.8115	5.8145	0.4632	H	-3.2039	5.8417	-0.8748
H	2.9986	4.3243	-0.4352	H	-3.6126	4.3562	-0.0455
H	2.8437	3.7766	1.9038	H	-3.0384	3.8011	-2.3127
H	1.4158	4.7765	2.1287	H	-1.5637	4.7559	-2.2656
H	1.4044	5.7742	-1.595	H	-2.2296	5.7276	1.4248
H	0.4801	6.0231	-0.1275	H	-1.0356	5.9764	0.1673
H	-0.7034	1.3647	-0.5995	H	-0.0295	1.2875	0.7456
H	-1.5196	1.6867	0.9207	H	1.0538	1.6299	-0.594
H	-3.0278	3.2973	-0.0798	H	2.3308	3.2539	0.7096
H	-1.7355	2.8024	-2.8009	H	0.558	2.6243	3.1098
H	-3.0419	3.9103	-2.4226	H	1.935	3.71	3.0558
H	-1.6091	5.3385	-1.1146	H	0.8139	5.2201	1.5209
H	-0.8679	5.0708	-2.6766	H	-0.2121	4.9398	2.9111

H	0.3995	2.2475	-2.2938	H	-1.4649	2.149	2.1981
H	1.0779	3.7116	-2.996	H	-2.1752	3.6217	2.8523
H	1.9287	2.8844	-1.7108	H	-2.8502	2.8949	1.4151
H	-1.1712	3.8738	1.9596	H	0.8972	3.8173	-1.6402
H	-3.9615	1.5946	-3.1568	H	2.091	0.7922	3.6576
H	-5.3176	0.246	2.3822	H	5.9971	1.4137	-0.647
H	-6.9154	-0.4585	2.2684	H	7.4575	0.7136	0.0151
H	-6.7583	-0.7273	-0.1205	H	6.2723	-0.368	1.8083
H	-6.279	0.9156	0.2803	H	5.7523	1.3096	1.7423
H	-6.0498	-2.6441	1.7287	H	6.8283	-1.5235	-0.6319
H	-5.2308	-2.0669	3.166	H	6.676	-0.4813	-2.0321
H	-2.9223	-1.958	-1.9673	H	2.2902	-2.179	1.0629
H	-2.0027	-1.3976	-0.5827	H	2.0261	-1.1607	-0.3408
H	-3.1065	-4.1999	-1.1284	H	3.2175	-3.9759	-0.2313
H	-2.0862	-5.0493	0.8809	H	3.3877	-4.0554	-2.6328
H	-1.4079	-3.4929	1.3001	H	2.7262	-2.4471	-2.8192
H	-4.3518	-4.273	1.1934	H	5.3754	-3.2344	-1.5306
H	-3.4169	-3.8639	2.6147	H	5.1487	-2.3465	-3.0215
H	1.1153	-3.4581	-1.6478	H	-0.8518	-3.4341	-1.5664
H	-0.0363	-5.0073	-2.936	H	-0.1392	-5.3698	-0.5265
H	-1.8367	-5.3469	-2.7209	H	1.5998	-5.6365	0.0342
H	-3.1695	-0.2215	2.2248	H	4.1343	0.9255	-1.7039
H	-2.7353	-1.6416	3.1464	H	4.4157	-0.081	-3.1045
H	-1.9111	-1.2937	1.6304	H	2.9439	-0.2828	-2.1597
H	6.2669	-2.4485	-2.4853	H	-4.9674	-4.8132	1.1139
H	7.6992	-1.5493	-1.9818	H	-4.8843	-4.2239	2.7725
H	5.1098	-3.852	-0.5435	H	-6.5149	-3.336	-0.5044
H	6.0518	-4.2178	0.891	H	-7.7149	-2.292	0.237
H	4.7028	0.5546	1.5024	H	-3.4036	0.1437	0.896
H	4.182	1.0197	-0.0873	H	-2.2065	-1.0557	0.5167
H	2.3713	-0.6715	-0.0611	H	-2.9679	-1.2197	-1.8142
H	3.245	-1.2122	2.8281	H	-4.9617	1.0227	-1.1791
H	1.8484	-1.9086	2.0217	H	-4.7001	0.2528	-2.7328
H	3.7582	-3.4669	2.0095	H	-6.6993	-0.6508	-1.5979
H	3.217	-3.0413	0.3944	H	-5.4902	-1.8797	-1.9349
H	1.2287	0.2612	3.3626	H	-1.2142	0.1093	-3.3073
H	5.5254	-1.1382	2.8084	H	-7.2657	-0.0105	0.7946
H	6.0631	-2.8141	2.8159	H	-6.2213	-0.5221	2.1271
H	6.9979	-1.5829	1.9569	H	-5.6426	0.6524	0.955
H	5.2463	1.1974	-1.7083	H	-2.5313	-3.6496	2.7433
H	-5.3087	-2.4539	-1.5853	H	4.6124	-2.5198	1.7637
H	7.8381	-2.6488	0.113	H	-6.7048	-2.7269	2.4829
H	7.5081	-3.9052	-1.0694	H	-7.194	-4.2148	1.6883
4d-11	X axis(Å)	Y axis(Å)	Z axis(Å)	4d-12	X axis(Å)	Y axis(Å)	Z axis(Å)
C	2.6209	5.1036	0.5025	C	-4.0516	-4.3576	0.3278
C	2.1326	4.2406	1.667	C	-3.3265	-3.8152	1.5606
C	1.3827	2.9826	1.1997	C	-2.2798	-2.7475	1.2146

C	0.2325	3.3433	0.2154	C	-1.2929	-3.2461	0.1141
C	0.7801	4.1423	-1.0251	C	-2.0674	-3.6981	-1.1782
C	1.5196	5.4111	-0.518	C	-3.0949	-4.7954	-0.7872
C	-0.6058	2.1312	-0.2473	C	-0.1907	-2.2264	-0.2482
C	-1.7673	2.5497	-1.1777	C	0.7941	-2.7632	-1.3075
C	-1.2765	3.3924	-2.3661	C	0.0659	-3.3023	-2.5506
C	-0.4186	4.5789	-1.9139	C	-1.0479	-4.2924	-2.1905
C	1.7561	3.3357	-1.9234	C	-2.8291	-2.5555	-1.902
C	0.8764	2.2127	2.4001	C	-1.5394	-2.3206	2.4636
O	-0.0547	2.5377	3.1239	O	-0.8534	-3.0427	3.1737
O	-0.6865	4.2302	0.9051	O	-0.6114	-4.4243	0.6187
C	-2.5666	1.3301	-1.5703	C	1.8359	-1.7067	-1.6005
O	-3.5113	0.9209	-0.6303	O	2.7754	-1.5182	-0.5867
C	-2.4752	0.6158	-2.6902	C	1.9593	-0.9487	-2.6889
C	-6.5156	0.2644	-0.2256	C	5.7888	-1.6335	-0.0096
C	-5.6577	0.1217	-1.4821	C	5.0805	-1.2456	-1.3074
C	-4.1942	-0.2304	-1.1737	C	3.7322	-0.5481	-1.0601
C	-4.0833	-1.4669	-0.2339	C	3.8911	0.6672	-0.0988
C	-4.9036	-1.2494	1.0917	C	4.5459	0.2312	1.2645
C	-6.378	-0.9281	0.7252	C	5.904	-0.4657	0.9743
C	-2.6278	-1.8617	0.1004	C	2.5832	1.4521	0.1567
C	-2.5478	-3.1107	1.0087	C	2.8187	2.6795	1.069
C	-3.4426	-3.0111	2.2556	C	3.5466	2.3213	2.3756
C	-4.8685	-2.5613	1.9244	C	4.8126	1.4964	2.1271
C	-1.1119	-3.4288	1.3721	C	1.554	3.477	1.3212
C	-0.3011	-2.3931	2.074	C	0.4156	2.8722	2.0634
C	-0.5131	-4.5921	1.0728	C	1.3971	4.7485	0.915
O	0.9237	-2.3504	2.0451	O	0.4093	1.7195	2.4756
C	-4.3663	-0.1063	1.9943	C	3.6706	-0.7344	2.1069
C	-3.4483	-0.4418	-2.4712	C	3.1276	-0.1393	-2.3832
O	-3.5916	-1.3846	-3.2372	O	3.5408	0.7531	-3.1124
C	4.8561	-4.1031	-1.3483	C	-2.2975	4.7753	-1.7918
C	3.8268	-3.0829	-0.9195	C	-1.9357	3.3892	-1.3255
C	4.1315	-1.8095	-0.567	C	-2.7706	2.5797	-0.6311
C	5.5945	-1.3187	-0.5216	C	-4.2213	2.9918	-0.3295
C	6.6122	-2.4893	-0.6177	C	-4.4245	4.5238	-0.4879
C	3.1172	-0.7367	-0.1893	C	-2.3871	1.1908	-0.1457
C	3.4305	-0.0921	1.172	C	-2.8212	0.8937	1.3041
C	4.8534	0.4807	1.1851	C	-4.3095	1.1787	1.5079
C	5.8769	-0.5941	0.823	C	-4.6244	2.6242	1.123
C	2.4257	0.9777	1.5132	C	-2.4679	-0.5228	1.6745
C	1.6261	0.9803	2.577	C	-1.6819	-0.8904	2.6841
O	2.3233	2.0462	0.6282	O	-2.9431	-1.5226	0.8318
C	5.8455	-0.3517	-1.7029	C	-5.1545	2.2577	-1.3231
C	2.4308	-3.6233	-0.9366	C	-0.571	2.9684	-1.7778
O	2.1721	-4.7764	-1.2684	O	-0.2702	1.8258	-2.098
O	-4.6766	-2.6067	-0.9041	O	4.8123	1.6084	-0.7171

C	6.2198	-3.5079	-1.6745	C	-3.7929	5.0686	-1.7619
H	3.0178	6.0468	0.8966	H	-4.6716	-5.2124	0.6238
H	3.4632	4.6067	0.0086	H	-4.747	-3.5996	-0.0491
H	3.0018	3.9625	2.2768	H	-4.0753	-3.4026	2.2487
H	1.4841	4.8478	2.3116	H	-2.8504	-4.6532	2.0857
H	1.9591	5.9552	-1.3639	H	-3.6829	-5.0919	-1.6653
H	0.8032	6.1025	-0.0554	H	-2.5696	-5.7011	-0.4574
H	0.0281	1.3844	-0.7399	H	-0.6313	-1.2862	-0.5962
H	-1.0457	1.6338	0.6273	H	0.3907	-1.9843	0.6512
H	-2.4493	3.1941	-0.6043	H	1.3334	-3.6158	-0.8703
H	-0.7027	2.7786	-3.0697	H	-0.3593	-2.4811	-3.1388
H	-2.1389	3.7733	-2.9279	H	0.7861	-3.8053	-3.2084
H	-1.0563	5.2894	-1.3723	H	-0.5925	-5.2045	-1.784
H	-0.0583	5.117	-2.8	H	-1.562	-4.6001	-3.1101
H	1.3502	2.3663	-2.2239	H	-2.1921	-1.6942	-2.1188
H	1.9768	3.891	-2.8433	H	-3.2272	-2.9093	-2.861
H	2.7211	3.1448	-1.4498	H	-3.6872	-2.1837	-1.3389
H	-0.9578	3.8049	1.746	H	-0.2161	-4.2079	1.4889
H	-1.8366	0.714	-3.5466	H	1.3667	-0.8822	-3.5804
H	-6.2544	1.1936	0.2925	H	5.2614	-2.4713	0.4595
H	-7.567	0.3696	-0.519	H	6.7935	-2.0041	-0.2456
H	-6.1009	-0.6507	-2.1241	H	5.7419	-0.593	-1.8917
H	-5.7125	1.0621	-2.0453	H	4.936	-2.1547	-1.9052
H	-6.847	-1.8024	0.2555	H	6.6176	0.2612	0.5647
H	-6.9582	-0.7275	1.6349	H	6.3487	-0.8297	1.9093
H	-2.0873	-2.098	-0.8259	H	2.1908	1.8281	-0.7962
H	-2.1012	-1.0156	0.5549	H	1.8148	0.7907	0.5688
H	-2.9363	-3.9536	0.4182	H	3.5045	3.3424	0.5202
H	-3.488	-3.9894	2.7515	H	3.825	3.2416	2.9052
H	-3.0128	-2.3258	2.9945	H	2.8875	1.7731	3.0571
H	-5.3771	-3.3704	1.3847	H	5.5597	2.1376	1.6417
H	-5.427	-2.4317	2.8604	H	5.2481	1.2123	3.0937
H	-0.8823	-1.6297	2.616	H	-0.4533	3.5328	2.2254
H	0.5239	-4.7913	1.3332	H	0.4963	5.3229	1.1085
H	-1.037	-5.3837	0.5457	H	2.1903	5.2622	0.3775
H	-4.4944	0.8853	1.5562	H	3.5694	-1.725	1.6594
H	-4.9052	-0.089	2.9496	H	4.1187	-0.8926	3.0955
H	-3.3044	-0.2155	2.2292	H	2.6596	-0.353	2.2718
H	4.9676	-4.8399	-0.5423	H	-1.7767	5.4974	-1.1497
H	4.5106	-4.6477	-2.2356	H	-1.9346	4.9408	-2.8138
H	6.684	-3.0101	0.3471	H	-3.9794	5.0519	0.3667
H	7.6179	-2.1062	-0.8315	H	-5.494	4.7694	-0.4768
H	3.1162	0.0259	-0.9792	H	-2.8309	0.4627	-0.8361
H	2.0921	-1.1096	-0.1623	H	-1.3047	1.0379	-0.1823
H	3.3781	-0.8782	1.939	H	-2.2666	1.5733	1.9651
H	4.9412	1.3262	0.4919	H	-4.9267	0.4846	0.9255
H	5.0884	0.8753	2.1819	H	-4.5796	1.0231	2.5601

H	6.8768	-0.1417	0.8031	H	-5.6963	2.8069	1.2729
H	5.8899	-1.3286	1.6403	H	-4.1002	3.2835	1.8287
H	1.5173	0.2668	3.3714	H	-1.1706	-0.306	3.4255
H	5.2313	0.5522	-1.6444	H	-4.9009	2.4838	-2.3645
H	6.8916	-0.0251	-1.7268	H	-5.1013	1.1691	-1.2187
H	5.6239	-0.8241	-2.6662	H	-6.1997	2.5482	-1.1666
H	1.6251	-2.9431	-0.638	H	0.1609	3.7909	-1.847
H	-4.2929	-2.6811	-1.8037	H	4.5081	1.775	-1.6347
H	6.2004	-3.0442	-2.6674	H	-4.2763	4.6341	-2.6442
H	6.9676	-4.3082	-1.719	H	-3.9542	6.1512	-1.8242

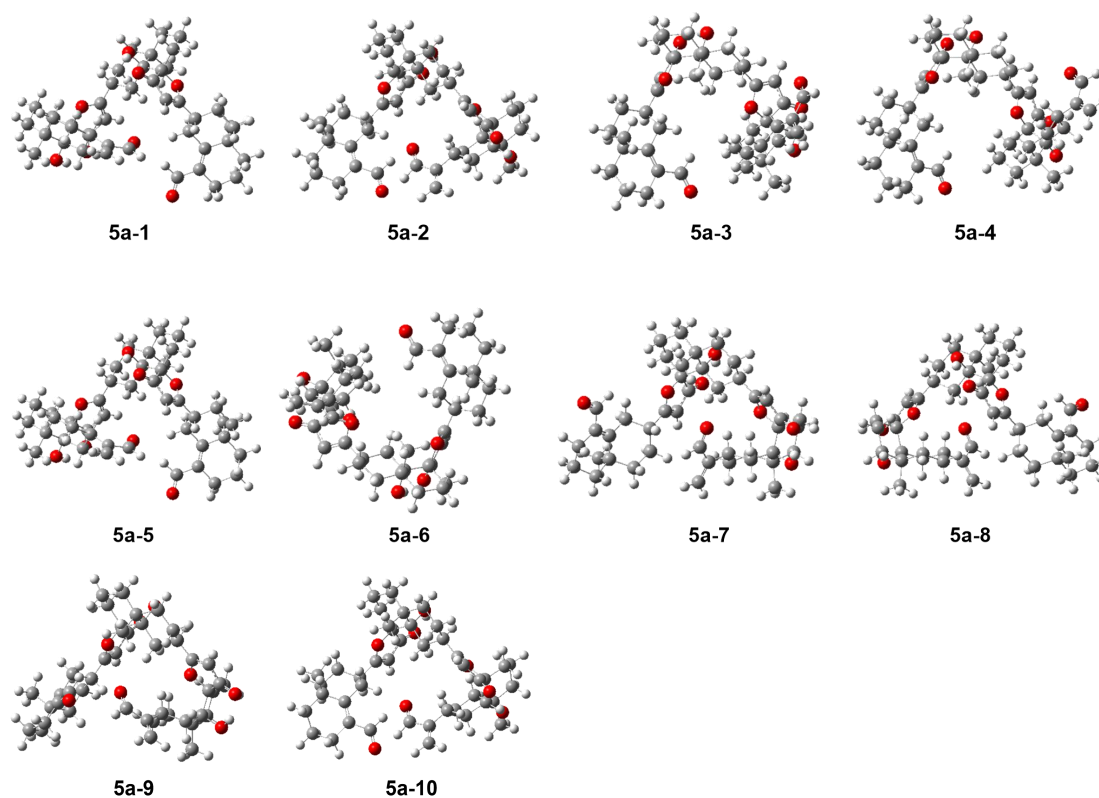
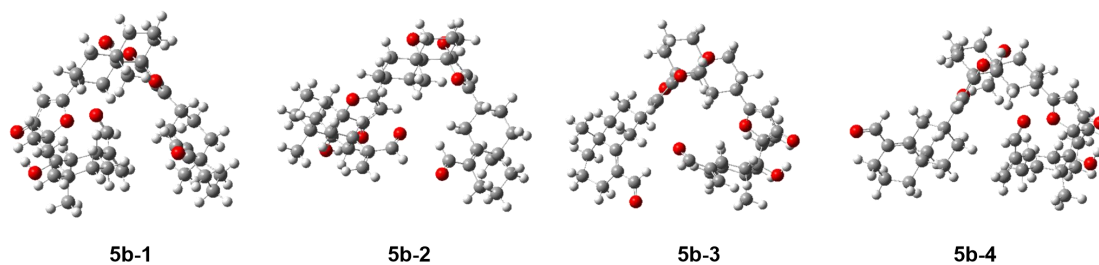


Figure S26. Optimized geometries of predominant conformers for **5a** at the B3LYP/6-31G (d,p) level



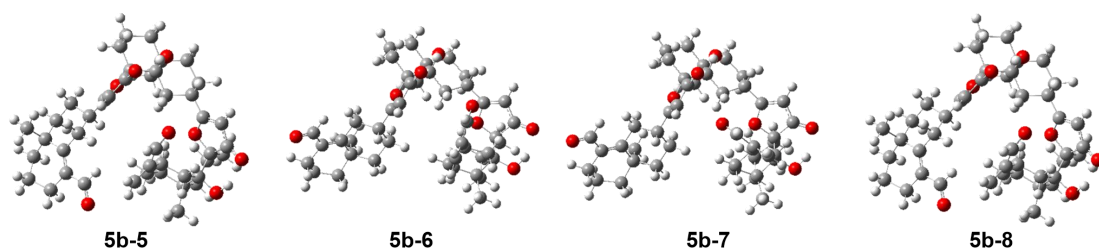


Figure S27. Optimized geometries of predominant conformers for **5b** at the B3LYP/6-31G (d,p) level

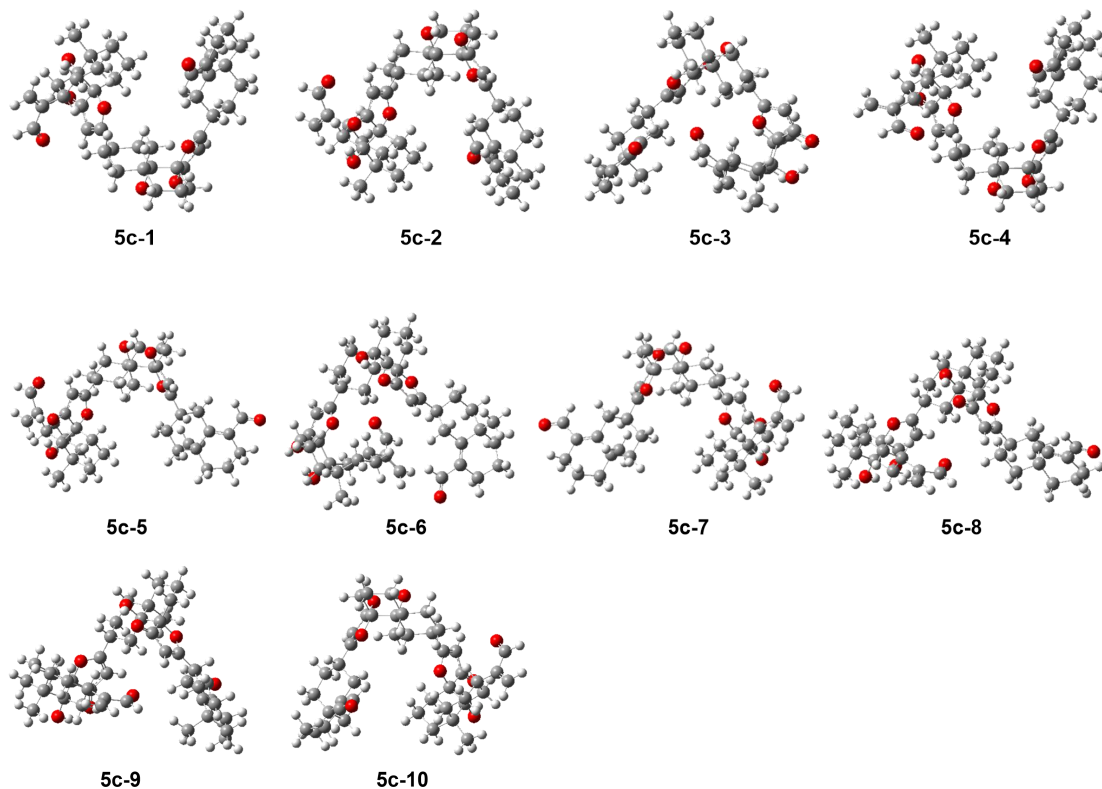
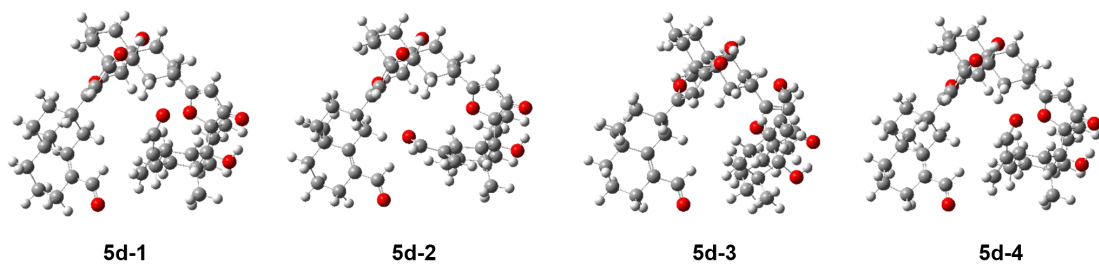


Figure S28. Optimized geometries of predominant conformers for **5c** at the B3LYP/6-31G (d,p) level



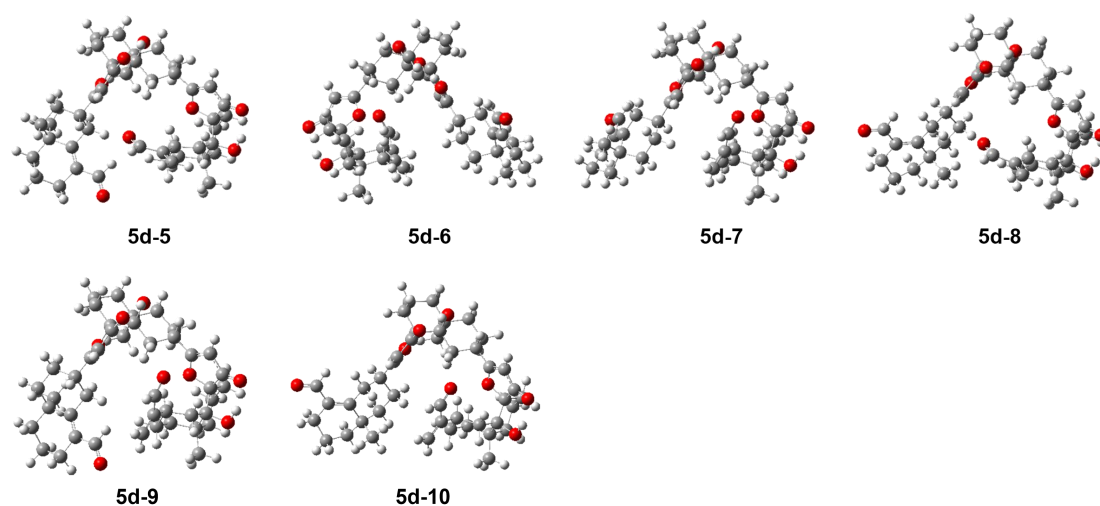


Figure S29. Optimized geometries of predominant conformers for **5d** at the B3LYP/6-31G (d,p) level

Table S10. Conformational analysis of the optimized **5a-5d** at the B3LYP/6-31G(d,p) level in the gas phase

	<i>Conformers</i>	G (Hartree)	ΔG (Kcal/mol)	Population
5a	5a-1	-2273.32755	0	26.11%
	5a-2	-2273.32296	2.88215343	0.20%
	5a-3	-2273.32577	1.11571278	3.97%
	5a-4	-2273.32732	0.14369979	20.49%
	5a-5	-2273.32569	1.16905113	3.63%
	5a-6	-2273.32610	0.9098895	5.62%
	5a-7	-2273.32719	0.22464858	17.87%
	5a-8	-2273.32721	0.21147087	18.27%
	5a-9	-2273.32573	1.13955816	3.81%
	5a-10	-2273.32151	3.78953289	0.04%
	<i>Conformers</i>	G (Hartree)	ΔG (Kcal/mol)	Population
5b	5b-1	-2273.32493	1.72188744	1.77%
	5b-2	-2273.32768	0	32.35%
	5b-3	-2273.32663	0.65951301	10.62%
	5b-4	-2273.32671	0.6086847	11.57%
	5b-5	-2273.32621	0.91867464	6.86%
	5b-6	-2273.32710	0.36521082	17.46%
	5b-7	-2273.32679	0.55911141	12.58%

	5b-8	-2273.32621	0.92369472	6.80%
	<i>Conformers</i>	G (Hartree)	ΔG (Kcal/mol)	Population
5c	5c-1	-2273.32758	0.39282126	0.12888
	5c-2	-2273.32759	0.38968371	0.12956
	5c-3	-2273.32541	1.75514547	0.01291
	5c-4	-2273.32730	0.56852406	0.09579
	5c-5	-2273.32820	0.00376506	0.2486
	5c-6	-2273.32636	1.15712844	0.03545
	5c-7	-2273.32821	0	0.25019
	5c-8	-2273.32672	0.93624492	0.05148
	5c-9	-2273.32610	1.32467361	0.02672
	5c-10	-2273.32584	1.48406115	0.02041
	<i>Conformers</i>	G (Hartree)	ΔG (Kcal/mol)	Population
5d	5d-1	-2273.32413	1.72753503	0.01842
	5d-2	-2273.32519	1.06551198	0.05633
	5d-3	-2273.32572	0.73355919	0.09866
	5d-4	-2273.32341	2.18436231	0.00852
	5d-5	-2273.32368	2.00991453	0.01143
	5d-6	-2273.32689	0.00062751	0.34015
	5d-7	-2273.32689	0	0.34051
	5d-8	-2273.32471	1.36420674	0.03401
	5d-9	-2273.32413	1.72816254	0.0184
	5d-10	-2273.32544	0.90737946	0.07357

Functional		Solvent?		Basis Set			Type of Data
mPW1PW91		PCM		6-311+G(d, p)			Unscaled Shifts
		DP4+	0.00%	100.00%	0.00%	0.00%	-
Nuclei	sp2?	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
C		18.3	21.55607	21.82157	21.94932	21.59465	
C		31.3	36.246	36.36782	36.04792	36.33177	
C		92	98.69048	98.46936	98.69253	98.6618	
C		75.4	81.87816	81.95582	81.72346	81.84974	
C		37.6	42.64005	42.60591	42.62287	42.52195	
C		34.1	36.55098	36.69831	36.57469	36.82871	
C		31.3	35.23173	32.78495	35.5436	32.88309	
C		36.1	41.33967	41.56197	41.61825	41.6875	
C		24.9	27.26463	29.04145	26.99847	29.74543	
C		36.2	38.03185	38.57211	38.00868	38.52104	
C		20.5	21.05673	21.05256	21.12924	21.01376	
C	x	209.5	219.76383	219.72898	219.76727	219.45918	
C	x	196.4	210.24603	209.64999	209.04615	209.1008	
C	x	102.3	108.81501	108.79838	109.23918	109.63201	
C		18.5	21.93447	22.0267	22.22221	21.84011	
C		33	37.49785	37.12982	37.48782	37.51751	
C		93.2	100.6201	101.02182	100.59036	101.50714	
C		74.9	81.06317	81.09058	81.2752	81.19902	
C		37.9	43.10681	43.01961	42.79934	43.04095	
C		36.5	38.55219	38.64146	38.80975	38.67102	
C		39.2	42.31939	42.32394	42.02892	43.00614	
C		32.8	37.00575	36.32004	37.07622	36.5374	
C		26.1	26.57447	27.46567	26.52118	26.94698	
C		33	34.98498	35.35867	35.16265	35.16356	
C	x	155.1	163.65337	163.78709	163.51283	163.88008	
C	x	194.9	205.95272	206.73378	205.90891	205.56136	
C	x	133.6	146.92233	146.59425	146.42563	146.68358	
C		23.6	23.4849	23.48257	23.49751	23.48049	
C	x	210.6	219.90321	219.86677	220.43652	220.24413	
C		24.7	27.35717	27.42038	27.48137	27.42022	
C	x	134.4	141.97974	141.99707	141.82783	141.85327	
C	x	160.1	178.20808	178.10343	178.24145	178.29149	
C		36.9	43.02426	42.97189	43.12577	43.10683	
C		39.7	41.53099	41.72881	41.55168	41.59056	
C		26.9	30.72313	31.34156	31.05132	31.09181	
C		41.6	46.98801	47.25335	47.11677	46.55886	
C		26.1	28.11746	28.39491	27.77094	27.61689	
C		40.9	43.93483	44.147	43.96939	43.79322	
C	x	196.4	207.46617	207.69633	207.56607	207.62454	
C	x	102.3	108.30978	108.30034	108.43877	107.70642	
C		25	26.48507	26.46756	26.42021	26.51846	
C	x	190.8	199.79571	200.245	198.82542	198.95854	
C		18.3	21.07971	20.97377	20.93372	20.93665	
H	x	9.5	9.63468	9.84476	9.70147	9.62404	
H		1.96	1.57484	1.9384	1.59529	1.99945	
H		1.56	2.0164	1.63356	2.01212	1.5941	
H		2.5	1.46262	2.30154	1.45585	2.27433	
H		1.5	2.26127	1.44309	2.29886	1.40482	
H		2.14	1.19166	2.09986	1.16997	2.13617	
H		1.14	2.12863	1.15192	2.10519	1.18695	
H		1.79	1.97342	1.43671	2.05902	1.38791	
H		2.22	1.34408	2.15866	1.11719	1.90461	
H		3.64	3.39684	3.57022	3.55441	3.6924	
H		1.98	1.9706	1.76344	2.00091	1.58432	
H		2.02	1.72863	2.01206	1.76049	2.05487	
H		1.2	2.11941	1.19481	2.08436	1.20027	
H		2.27	1.20109	2.15654	1.16345	2.13385	

H		1.42	1.5839	1.60003	1.63142	1.54777	
H		1.42	0.47362	1.96915	0.5032	1.9687	
H		1.42	1.92821	0.39009	2.03633	0.46695	
H		5.24	4.8984	4.9081	4.90316	4.89227	
H	x	5.74	5.70356	5.6275	5.73213	5.71453	
H		1.83	1.88986	1.98435	1.43943	1.94755	
H		1.56	1.53744	1.52061	1.8815	1.48732	
H		2.29	2.14289	2.13646	2.11571	2.1256	
H		1.33	1.30652	1.32149	1.24577	1.33791	
H		2.02	1.98452	1.97591	1.93378	1.98504	
H		1.25	1.30024	1.2617	1.22323	1.29603	
H		1.71	1.38511	1.36224	1.25829	1.27601	
H		1.6	1.29397	1.28027	1.48585	1.36607	
H		2.99	2.75067	2.82806	2.91025	2.69781	
H		1.53	1.82851	1.34833	1.38359	1.85306	
H		1.59	1.30857	1.73839	1.86893	1.27287	
H		1.12	1.14175	1.13083	1.2081	1.14943	
H		2.4	2.36607	2.40206	2.48979	2.40394	
H	x	5.88	6.45586	6.49801	6.47015	6.44683	
H	x	6.19	6.84392	6.88861	6.81846	6.86401	
H		1.18	1.49322	1.54028	1.55131	1.51194	
H		1.18	0.35268	0.34361	0.34874	0.33855	
H		1.18	1.34657	1.34929	1.33877	1.33493	
H		2.19	2.01937	1.98929	2.62692	2.60937	
H		2.5	2.60517	2.59746	2.04159	2.00589	
H		1.29	1.37991	1.39516	1.39131	1.3919	
H		1.48	1.62179	1.65183	1.65306	1.61981	
H		2.38	2.50754	2.60865	3.15069	3.99974	
H		3.83	4.05595	3.7875	3.25812	2.33497	
H		2.7	2.66896	2.75839	2.83003	2.6065	
H		1.97	2.12741	2.16738	1.85221	1.65013	
H		1.85	1.68276	1.80986	2.19939	1.94362	
H		1.66	1.85623	1.90267	1.55862	1.48696	
H		1.48	1.49759	1.51911	1.93012	1.82907	
H	x	5.86	5.5186	5.62859	5.60933	5.40767	
H		1.14	1.89697	0.8077	1.43727	0.76142	
H		1.14	0.7803	1.36536	1.46906	1.80592	
H		1.14	1.32353	1.88044	1.11942	1.32941	
H	x	10.45	10.64428	10.65019	10.58051	10.59033	
H		5.67	5.54863	5.59871	5.53503	5.65398	
H		1.46	1.62177	1.6557	1.61281	1.64723	
H		1.46	1.68433	1.69788	1.71081	1.71599	

Functional mPW1PW91	Solvent? PCM		Basis Set 6-311+G(d,p)		Type of Data Unscaled Shifts	
	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	0.00%	100.00%	0.00%	0.00%	–	–
sDP4+ (C data)	10.69%	68.40%	16.60%	4.31%	–	–
sDP4+ (all data)	0.00%	100.00%	0.00%	0.00%	–	–
uDP4+ (H data)	0.00%	100.00%	0.00%	0.00%	–	–
uDP4+ (C data)	9.73%	25.41%	48.71%	16.15%	–	–
uDP4+ (all data)	0.00%	100.00%	0.00%	0.00%	–	–
DP4+ (H data)	0.00%	100.00%	0.00%	0.00%	–	–
DP4+ (C data)	3.82%	63.89%	29.73%	2.56%	–	–
DP4+ (all data)	0.00%	100.00%	0.00%	0.00%	–	–

Figure S30. DP4+ analysis of experimental NMR data of **5** and unscaled shifts of **5a-5d** (Isomer 1-4)

Table S11. The Cartesian coordinates of the lowest energy conformers for **5a–5d** in the gas phase at the B3LYP/6-31G(d,p) level

5a-1	X axis(Å)	Y axis(Å)	Z axis(Å)	5a-2	X axis(Å)	Y axis(Å)	Z axis(Å)
C	2.9406	4.9869	-0.0584	C	-2.7287	5.059	-0.1256
C	2.5401	4.2711	1.2315	C	-2.2703	4.313	-1.3785
C	1.8056	2.946	0.9742	C	-1.5434	2.9987	-1.0502
C	0.5994	3.1379	0.0093	C	-0.3693	3.2291	-0.0547
C	1.0579	3.7904	-1.3472	C	-0.8797	3.92	1.2648
C	1.7768	5.1335	-1.0436	C	-1.6047	5.2448	0.898
C	-0.1997	1.8433	-0.258	C	0.455	1.9583	0.279
C	-1.4102	2.0831	-1.1836	C	1.651	2.2857	1.2022
C	-1.03	2.8206	-2.4789	C	1.1983	3.0266	2.4744
C	-0.1988	4.079	-2.2145	C	0.3423	4.2561	2.1619
C	2.0153	2.9048	-2.1893	C	-1.8511	3.0485	2.1048
C	1.3765	2.3419	2.2933	C	-1.0674	2.3496	-2.3299
O	0.5133	2.7785	3.0423	O	-0.1825	2.771	-3.062
O	-0.3246	4.0729	0.6243	O	0.5572	4.1627	-0.6725
C	-2.1405	0.7913	-1.4616	C	2.5173	1.0754	1.4799
O	-3.3546	0.6257	-0.7952	O	3.2096	0.5647	0.3759
C	-1.7507	-0.1927	-2.2705	C	2.7768	0.5088	2.6578
C	-6.2443	0.5194	-1.4533	C	5.9897	0.9488	-0.5588
C	-5.1176	-0.1182	-2.2564	C	5.5631	0.665	0.8766
C	-3.9743	-0.5647	-1.335	C	4.3064	-0.2201	0.9025
C	-4.4682	-1.5771	-0.2432	C	4.5581	-1.5806	0.1693
C	-5.7013	-1.0206	0.5631	C	5.0966	-1.3759	-1.2949
C	-6.7789	-0.4403	-0.3977	C	6.2604	-0.343	-1.3201
C	-3.3505	-2.0359	0.7285	C	3.3377	-2.5315	0.1609
C	-2.9326	-1.0052	1.7949	C	2.2045	-2.1631	-0.8164
C	-4.1584	-0.4319	2.5289	C	2.7507	-1.8713	-2.2251
C	-5.246	0.0635	1.5729	C	3.9498	-0.9195	-2.2298
C	-1.879	-1.6103	2.7124	C	1.1022	-3.2143	-0.8932
C	-0.4893	-1.7143	2.1786	C	-0.2121	-2.7944	-1.4564
C	-2.0535	-2.0493	3.9701	C	1.1595	-4.4916	-0.4791
C	-6.4219	-2.1511	1.3557	C	5.6999	-2.6886	-1.8764
C	-2.8522	-1.1356	-2.1732	C	3.8504	-0.4173	2.3301
O	-2.8406	-2.2334	-2.7127	O	4.3112	-1.2156	3.1342
C	4.589	-4.6	-0.8549	C	-4.7684	-4.2175	1.1903
C	3.692	-3.4278	-0.5351	C	-3.8279	-3.0718	0.9141
C	4.1396	-2.1562	-0.3938	C	-4.2277	-1.8458	0.5003
C	5.6379	-1.8092	-0.5248	C	-5.7192	-1.5193	0.2804
C	6.5379	-3.0766	-0.5284	C	-6.6065	-2.7964	0.2755
C	3.2582	-0.9554	-0.0832	C	-3.2854	-0.6895	0.1918
C	3.7478	-0.1903	1.1584	C	-3.5266	-0.1076	-1.2131
C	5.1998	0.2626	0.9701	C	-4.9831	0.3452	-1.3595
C	6.1023	-0.9353	0.6739	C	-5.935	-0.8195	-1.0896

C	2.8423	0.9728	1.462	C	-2.5808	1.0249	-1.5096
C	2.1066	1.1147	2.5619	C	-1.791	1.1154	-2.5778
O	2.7432	1.9596	0.4872	O	-2.5031	2.0378	-0.5608
C	5.8639	-1.0422	-1.8491	C	-6.1991	-0.5907	1.4207
C	2.2509	-3.8137	-0.4063	C	-2.3956	-3.4067	1.1648
O	1.8939	-4.9819	-0.2903	O	-1.9751	-4.5586	1.1445
O	-4.9362	-2.7702	-0.9202	O	5.6053	-2.2808	0.89
C	5.9604	-4.1949	-1.3808	C	-6.2175	-3.7811	1.3676
O	-0.1582	-1.282	1.0805	O	-0.4782	-1.6297	-1.7282
H	0.2455	-2.2035	2.8405	H	-0.9555	-3.597	-1.6018
H	3.3286	5.9823	0.189	H	-3.117	6.0428	-0.4149
H	3.7704	4.4505	-0.5318	H	-3.57	4.5259	0.331
H	3.4473	4.0945	1.8235	H	-3.1512	4.1152	-2.0029
H	1.9074	4.9424	1.8265	H	-1.6164	4.9709	-1.9652
H	2.1511	5.58	-1.9737	H	-2.0186	5.711	1.8013
H	1.0618	5.8563	-0.6294	H	-0.8838	5.9659	0.491
H	0.4523	1.0657	-0.672	H	-0.176	1.184	0.7298
H	-0.5884	1.4519	0.6907	H	0.8575	1.5302	-0.6482
H	-2.1115	2.739	-0.6479	H	2.3062	2.9834	0.6599
H	-0.4772	2.1598	-3.1567	H	0.6387	2.3508	3.1321
H	-1.9423	3.1067	-3.0184	H	2.0767	3.3534	3.0458
H	-0.8367	4.8272	-1.7268	H	0.9753	5.011	1.6778
H	0.0959	4.5201	-3.1754	H	0.0091	4.7082	3.1049
H	1.6218	1.8991	-2.3587	H	-1.4531	2.0516	2.3114
H	2.1827	3.3542	-3.1758	H	-2.049	3.5221	3.0742
H	3.0032	2.7886	-1.7394	H	-2.826	2.9124	1.6327
H	-0.546	3.7473	1.5219	H	0.8061	3.8124	-1.5544
H	-0.8677	-0.3087	-2.8679	H	2.4136	0.7165	3.6456
H	-5.8993	1.4473	-0.9837	H	5.2233	1.5388	-1.0742
H	-7.0582	0.8004	-2.1319	H	6.8988	1.5615	-0.5518
H	-5.5048	-0.9687	-2.8313	H	6.3847	0.1873	1.4247
H	-4.7597	0.6167	-2.989	H	5.3761	1.6254	1.3739
H	-7.2802	-1.2646	-0.9234	H	7.1604	-0.7991	-0.8852
H	-7.5613	0.0681	0.1805	H	6.5198	-0.096	-2.3576
H	-2.475	-2.3575	0.1503	H	3.712	-3.5376	-0.068
H	-3.676	-2.9582	1.2306	H	2.9281	-2.628	1.1747
H	-2.4555	-0.1531	1.3007	H	1.7398	-1.2462	-0.4354
H	-4.5993	-1.1783	3.1981	H	1.9632	-1.4292	-2.8485
H	-3.844	0.4018	3.1699	H	3.0268	-2.8097	-2.722
H	-6.1044	0.4001	2.1691	H	4.3207	-0.8358	-3.2599
H	-4.8835	0.9583	1.0584	H	3.6026	0.0844	-1.9671
H	-1.2437	-2.4642	4.564	H	0.309	-5.1671	-0.5454
H	-3.0206	-2.0211	4.4612	H	2.0516	-4.9234	-0.0387
H	-5.753	-2.6871	2.0339	H	4.9879	-3.5178	-1.8834
H	-7.2391	-1.7403	1.9606	H	6.0313	-2.5374	-2.9108
H	-6.8643	-2.897	0.6859	H	6.5747	-3.0202	-1.3059
H	4.7124	-5.201	0.0552	H	-4.702	-4.9305	0.3586

H	4.1196	-5.2468	-1.6063	H	-4.4624	-4.7529	2.0975
H	6.6591	-3.4584	0.4948	H	-6.5212	-3.3124	-0.6908
H	7.547	-2.8289	-0.8811	H	-7.6647	-2.5274	0.3835
H	3.2422	-0.2963	-0.9608	H	-3.4249	0.0826	0.9593
H	2.2184	-1.2348	0.0849	H	-2.2342	-0.9781	0.2562
H	3.719	-0.8817	2.0136	H	-3.3467	-0.9085	-1.9453
H	5.2784	0.9982	0.1603	H	-5.2035	1.1772	-0.6796
H	5.5574	0.7636	1.8785	H	-5.16	0.7208	-2.3753
H	7.1259	-0.5775	0.5038	H	-6.9694	-0.4613	-1.1699
H	6.1415	-1.5516	1.5829	H	-5.8014	-1.55	-1.8997
H	2.0009	0.4872	3.425	H	-1.6519	0.4479	-3.4062
H	5.3332	-0.0853	-1.8754	H	-5.673	0.3692	1.4281
H	6.9273	-0.8215	-1.998	H	-7.2682	-0.3691	1.3228
H	5.5216	-1.6202	-2.7145	H	-6.0446	-1.0458	2.4053
H	1.5105	-3.0035	-0.4174	H	-1.7179	-2.5652	1.3665
H	-4.2196	-3.0969	-1.5049	H	5.3286	-2.3676	1.827
H	5.8845	-3.8798	-2.4278	H	-6.3568	-3.3309	2.3572
H	6.6301	-5.0625	-1.3632	H	-6.8718	-4.6597	1.3289
5a-3	X axis(Å)	Y axis(Å)	Z axis(Å)	5a-4	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-2.8425	4.6512	1.4157	C	-2.6313	4.7521	1.4904
C	-3.0211	4.3874	-0.0798	C	-2.9144	4.4817	0.0126
C	-2.1394	3.2351	-0.5881	C	-2.1119	3.2917	-0.5392
C	-0.6465	3.4534	-0.2089	C	-0.5906	3.4509	-0.255
C	-0.4802	3.6229	1.3476	C	-0.321	3.6306	1.2857
C	-1.3733	4.8015	1.8237	C	-1.1345	4.8491	1.8014
C	0.3036	2.3561	-0.737	C	0.2771	2.3071	-0.8238
C	1.7795	2.6452	-0.3774	C	1.7839	2.5303	-0.5563
C	1.9714	2.9014	1.1233	C	2.0801	2.8056	0.924
C	1.0035	3.9586	1.6617	C	1.1916	3.91	1.502
C	-0.8557	2.3617	2.172	C	-0.6949	2.3942	2.1478
C	-2.3243	3.0719	-2.0804	C	-2.3986	3.1313	-2.0157
O	-1.9149	3.8344	-2.9446	O	-2.0047	3.8666	-2.9102
O	-0.2082	4.6984	-0.8126	O	-0.1377	4.6685	-0.9014
C	2.7015	1.5553	-0.8667	C	2.6058	1.3749	-1.0717
O	2.2436	0.2392	-0.7891	O	2.1703	0.0891	-0.7495
C	3.9146	1.7537	-1.3793	C	3.704	1.4814	-1.8173
C	1.4356	-1.9253	-2.6639	C	0.9956	-2.233	-2.154
C	2.6052	-0.9665	-2.8431	C	2.1246	-1.3536	-2.6742
C	3.2128	-0.5804	-1.4864	C	2.985	-0.8307	-1.5152
C	3.6861	-1.8409	-0.6785	C	3.5942	-2.0058	-0.6715
C	2.5467	-2.9204	-0.5446	C	2.4891	-3.0171	-0.183
C	1.8697	-3.1815	-1.9199	C	1.5379	-3.408	-1.3503
C	4.2691	-1.4997	0.7161	C	4.454	-1.5291	0.526
C	3.23	-1.1155	1.7866	C	3.6591	-0.9806	1.7251
C	2.1013	-2.1589	1.867	C	2.5574	-1.9635	2.1589
C	1.4907	-2.4733	0.4986	C	1.6755	-2.4125	0.9902
C	3.9195	-0.8254	3.1116	C	4.6059	-0.5567	2.8375

C	4.6473	0.4751	3.2199	C	5.3448	0.7264	2.6367
C	3.9246	-1.5967	4.2112	C	4.832	-1.1932	3.9984
C	3.1154	-4.2997	-0.0979	C	3.1164	-4.357	0.3033
C	4.3379	0.4053	-1.715	C	4.0504	0.0919	-2.0657
O	5.4555	0.1373	-2.1345	O	5.0652	-0.2529	-2.6558
C	-3.8425	-4.8414	0.2279	C	-4.1389	-4.7385	0.2089
C	-3.173	-3.5596	-0.2132	C	-3.4663	-3.4771	-0.2835
C	-3.5996	-2.3238	0.1469	C	-3.7511	-2.2382	0.1885
C	-4.8627	-2.1374	1.0156	C	-4.8629	-2.019	1.2374
C	-5.6957	-3.4437	1.1374	C	-5.7497	-3.2805	1.4317
C	-2.9168	-1.0131	-0.2277	C	-3.0407	-0.9534	-0.2217
C	-3.8861	-0.0055	-0.8732	C	-4.022	0.1341	-0.6942
C	-5.1044	0.2388	0.0264	C	-5.0923	0.4077	0.3713
C	-5.7981	-1.0746	0.379	C	-5.8099	-0.8785	0.7751
C	-3.1922	1.2967	-1.1783	C	-3.2905	1.4031	-1.0487
C	-3.0477	1.8461	-2.3818	C	-3.2052	1.9457	-2.261
O	-2.6562	1.9803	-0.0921	O	-2.6459	2.0594	-0.005
C	-4.4428	-1.6891	2.4356	C	-4.2216	-1.6566	2.5978
C	-1.9764	-3.8006	-1.0778	C	-2.4448	-3.742	-1.3441
O	-1.6284	-4.923	-1.4284	O	-2.183	-4.8705	-1.7462
O	4.7539	-2.4755	-1.4248	O	4.4798	-2.7617	-1.5341
C	-4.8227	-4.663	1.3797	C	-4.9276	-4.5563	1.499
O	4.7031	1.2828	2.3004	O	5.2152	1.4163	1.6325
H	5.1399	0.6744	4.1867	H	6.0243	1.0258	3.4527
H	-3.3852	5.5648	1.6865	H	-3.1202	5.6886	1.7842
H	-3.3113	3.8428	1.9877	H	-3.0932	3.968	2.1004
H	-4.0804	4.1682	-0.2662	H	-3.9911	4.303	-0.1039
H	-2.7936	5.3079	-0.6326	H	-2.687	5.3879	-0.5635
H	-1.3148	4.9025	2.915	H	-1.002	4.9602	2.8852
H	-0.9958	5.7471	1.4134	H	-0.7477	5.7742	1.3545
H	0.2389	2.3017	-1.8316	H	-0.0517	1.3436	-0.4177
H	-0.0041	1.3744	-0.3591	H	0.1445	2.245	-1.9119
H	2.066	3.5692	-0.9005	H	2.086	3.4267	-1.1169
H	1.852	1.9711	1.6894	H	1.9586	1.8925	1.5167
H	2.9973	3.2423	1.3113	H	3.1289	3.1057	1.0398
H	1.2728	4.9331	1.2343	H	1.473	4.8661	1.0422
H	1.1501	4.0578	2.7449	H	1.4089	4.0189	2.5724
H	-0.3471	1.4599	1.8211	H	-0.2423	1.4694	1.7804
H	-0.5785	2.4969	3.2247	H	-0.3515	2.5308	3.1806
H	-1.926	2.1469	2.169	H	-1.7709	2.2204	2.2092
H	-0.4107	4.6683	-1.7714	H	-0.4018	4.638	-1.8451
H	4.4782	2.6551	-1.5229	H	4.2324	2.3449	-2.1722
H	0.6151	-1.4297	-2.1332	H	0.3049	-1.6411	-1.5432
H	1.0427	-2.2055	-3.6482	H	0.4131	-2.6126	-3.0016
H	3.3651	-1.4238	-3.4893	H	2.7382	-1.9167	-3.3885
H	2.2408	-0.0762	-3.3716	H	1.6801	-0.5203	-3.2336
H	2.5652	-3.729	-2.5708	H	2.07	-4.0686	-2.0485

H	1.0017	-3.8388	-1.7911	H	0.6948	-3.9951	-0.9644
H	4.855	-2.3569	1.0772	H	5.0861	-2.3619	0.8657
H	5.0194	-0.7066	0.6092	H	5.1808	-0.7856	0.1762
H	2.7452	-0.1812	1.4921	H	3.137	-0.072	1.4165
H	2.4629	-3.0918	2.3128	H	2.9905	-2.8507	2.6336
H	1.3081	-1.7914	2.5309	H	1.9219	-1.4909	2.9189
H	0.7376	-3.2617	0.6277	H	0.9543	-3.1516	1.3632
H	0.9351	-1.597	0.1507	H	1.0713	-1.563	0.6572
H	4.4367	-1.3076	5.1248	H	5.521	-0.8133	4.7478
H	3.4226	-2.5581	4.2421	H	4.3426	-2.1294	4.2457
H	3.6749	-4.245	0.8395	H	3.8546	-4.217	1.097
H	2.3052	-5.0242	0.0478	H	2.3422	-5.0288	0.693
H	3.7905	-4.7228	-0.8502	H	3.6192	-4.8887	-0.5124
H	-4.3717	-5.2683	-0.6339	H	-4.8134	-5.0994	-0.5783
H	-3.0924	-5.5779	0.5413	H	-3.396	-5.5267	0.382
H	-6.2711	-3.6143	0.2169	H	-6.4609	-3.3769	0.5997
H	-6.4337	-3.3537	1.9444	H	-6.3571	-3.1858	2.3406
H	-2.4735	-0.5871	0.6819	H	-2.459	-0.5933	0.6371
H	-2.0777	-1.1534	-0.9121	H	-2.3035	-1.1105	-1.0114
H	-4.2451	-0.441	-1.8171	H	-4.531	-0.2395	-1.5945
H	-4.8144	0.7625	0.9454	H	-4.651	0.8767	1.2591
H	-5.8208	0.8938	-0.4858	H	-5.8302	1.1215	-0.0169
H	-6.6393	-0.8635	1.0518	H	-6.5347	-0.6484	1.5667
H	-6.2378	-1.4773	-0.5441	H	-6.3978	-1.2167	-0.0895
H	-3.3604	1.5138	-3.3529	H	-3.6	1.6289	-3.207
H	-3.9315	-0.7214	2.4378	H	-3.6608	-0.7175	2.5627
H	-5.3167	-1.5896	3.0897	H	-4.9874	-1.5412	3.3736
H	-3.7605	-2.4086	2.9015	H	-3.5231	-2.4307	2.9341
H	-1.407	-2.9222	-1.4023	H	-1.9337	-2.8737	-1.7743
H	5.4433	-1.8034	-1.613	H	5.1289	-2.1419	-1.9304
H	-4.2783	-4.565	2.3258	H	-4.246	-4.5302	2.3568
H	-5.4477	-5.5589	1.471	H	-5.5866	-5.419	1.6505
5a-5	X axis(Å)	Y axis(Å)	Z axis(Å)	5a-6	X axis(Å)	Y axis(Å)	Z axis(Å)
C	2.9082	4.9839	0.171	C	3.2598	-4.4323	1.2789
C	2.5217	4.1859	1.4164	C	3.3882	-4.112	-0.2104
C	1.7855	2.8796	1.081	C	2.3786	-3.0524	-0.6812
C	0.5677	3.1329	0.1451	C	0.9233	-3.4379	-0.2889
C	1.0107	3.8719	-1.1717	C	0.801	-3.663	1.2644
C	1.7338	5.1929	-0.7904	C	1.8211	-4.7511	1.6979
C	-0.238	1.859	-0.195	C	-0.1445	-2.4327	-0.7742
C	-1.4608	2.1623	-1.085	C	-1.5757	-2.8834	-0.4025
C	-1.0923	2.977	-2.3371	C	-1.7164	-3.2014	1.0926
C	-0.256	4.2157	-2.0039	C	-0.6334	-4.1621	1.5897
C	1.9576	3.0427	-2.0804	C	1.0558	-2.3895	2.1152
C	1.3696	2.1887	2.3609	C	2.5255	-2.8424	-2.1719
O	0.52	2.5785	3.1501	O	2.1893	-3.629	-3.0462
O	-0.3472	4.0274	0.8304	O	0.606	-4.706	-0.9211

C	-2.2067	0.8944	-1.4258	C	-2.6206	-1.8836	-0.8345
O	-3.3754	0.6655	-0.6986	O	-2.2764	-0.5317	-0.8022
C	-1.8758	-0.0108	-2.3454	C	-3.8485	-2.1939	-1.2455
C	-6.2989	0.6482	-1.1993	C	-1.8548	1.6821	-2.7741
C	-5.2275	0.0812	-2.122	C	-2.934	0.6096	-2.8254
C	-4.0412	-0.4621	-1.3134	C	-3.3696	0.1939	-1.4129
C	-4.489	-1.5709	-0.2984	C	-3.872	1.4161	-0.5666
C	-5.6686	-1.0854	0.6253	C	-2.8405	2.6075	-0.5658
C	-6.7887	-0.4047	-0.2131	C	-2.3404	2.905	-2.0074
C	-3.3267	-2.1317	0.5603	C	-4.2626	1.0494	0.8894
C	-2.8387	-1.215	1.6985	C	-3.0818	0.8005	1.8532
C	-4.0144	-0.7061	2.5516	C	-2.0603	1.9473	1.7921
C	-5.1441	-0.1093	1.709	C	-1.6414	2.2917	0.3618
C	-1.7468	-1.9196	2.4916	C	-3.4935	0.535	3.2953
C	-0.3872	-1.9699	1.879	C	-2.5098	-0.1807	4.163
C	-1.8631	-2.494	3.7004	C	-4.6645	0.8461	3.8759
C	-6.3608	-2.2819	1.3429	C	-3.494	3.9329	-0.0744
C	-2.975	-0.9581	-2.2645	C	-4.4204	-0.8891	-1.5276
O	-3.0032	-2.0033	-2.8996	O	-5.6	-0.7253	-1.8073
C	4.7167	-4.5185	-0.8048	C	3.046	5.203	-0.0253
C	3.7554	-3.3605	-0.7	C	2.5661	3.8404	-0.4703
C	4.1575	-2.0678	-0.6544	C	3.0878	2.6738	-0.0174
C	5.6365	-1.6634	-0.8195	C	4.2826	2.6587	0.961
C	6.5622	-2.8728	-1.1292	C	4.9477	4.056	1.1058
C	3.2548	-0.8959	-0.3066	C	2.5888	1.2822	-0.3885
C	3.7138	-0.2686	1.0251	C	3.7156	0.3814	-0.9258
C	5.1869	0.1641	0.9565	C	4.8781	0.3029	0.073
C	6.0949	-0.987	0.5014	C	5.3841	1.6965	0.4392
C	2.8194	0.8747	1.4198	C	3.1938	-0.9953	-1.2461
C	2.0917	0.9397	2.5322	C	3.1047	-1.5387	-2.4577
O	2.7193	1.9298	0.5198	O	2.7598	-1.7576	-0.1674
C	5.8127	-0.6784	-2.0011	C	3.7962	2.201	2.3564
C	2.3199	-3.768	-0.589	C	1.4441	3.9153	-1.4563
O	1.9761	-4.9174	-0.3341	O	1.0161	4.9784	-1.8933
O	-5.0097	-2.6886	-1.0607	O	-5.0728	1.9309	-1.195
C	6.1387	-4.1406	-0.4057	C	3.9233	5.1721	1.2192
O	-0.1064	-1.4063	0.8274	O	-1.4122	-0.5497	3.7639
H	0.3726	-2.5433	2.4371	H	-2.8287	-0.3654	5.2029
H	3.2988	5.9615	0.4778	H	3.9013	-5.2888	1.5186
H	3.7327	4.4797	-0.345	H	3.647	-3.5935	1.8677
H	3.4353	3.9722	1.986	H	4.4144	-3.7728	-0.4019
H	1.8953	4.8166	2.0603	H	3.2559	-5.0381	-0.7844
H	2.0982	5.6981	-1.6939	H	1.7886	-4.8869	2.7864
H	1.0237	5.8875	-0.323	H	1.5416	-5.7205	1.2651
H	0.4054	1.1098	-0.6703	H	0.0651	-1.4342	-0.374
H	-0.6133	1.4054	0.7311	H	-0.1037	-2.3439	-1.8677
H	-2.1499	2.7895	-0.5011	H	-1.7754	-3.8153	-0.9513

H	-0.547	2.3586	-3.0593	H	-1.6883	-2.2789	1.681
H	-2.0093	3.297	-2.8486	H	-2.6987	-3.6513	1.2866
H	-0.8868	4.9322	-1.4623	H	-0.8048	-5.1489	1.1407
H	0.028	4.7163	-2.9386	H	-0.7508	-4.3026	2.6719
H	1.5625	2.0493	-2.3082	H	0.4517	-1.538	1.7918
H	2.1123	3.554	-3.0384	H	0.8101	-2.5774	3.1676
H	2.9513	2.8997	-1.6514	H	2.0976	-2.0634	2.1038
H	-0.5584	3.6448	1.7078	H	0.8088	-4.6358	-1.8777
H	-1.0361	-0.0703	-3.0098	H	-4.3401	-3.1429	-1.3397
H	-5.9151	1.5228	-0.6623	H	-0.9414	1.2814	-2.3208
H	-7.1447	1.0014	-1.8009	H	-1.5892	1.9778	-3.7958
H	-5.6578	-0.7067	-2.753	H	-3.794	0.977	-3.3996
H	-4.9008	0.8801	-2.8001	H	-2.5353	-0.2517	-3.3769
H	-7.3299	-1.1693	-0.7872	H	-3.1528	3.3623	-2.5889
H	-7.531	0.0521	0.4542	H	-1.5373	3.651	-1.9789
H	-3.6366	-3.0968	0.9861	H	-4.8922	1.8602	1.2778
H	-2.4873	-2.4006	-0.0935	H	-4.9261	0.1748	0.8883
H	-2.3775	-0.3222	1.2646	H	-2.5807	-0.1089	1.5117
H	-4.4295	-1.5104	3.1682	H	-2.4647	2.8391	2.2864
H	-3.6539	0.0577	3.2526	H	-1.1571	1.6813	2.3553
H	-5.9643	0.1759	2.381	H	-0.9618	3.1529	0.3987
H	-4.7962	0.8278	1.2642	H	-1.0425	1.4658	-0.035
H	-1.0286	-2.9752	4.2032	H	-4.8838	0.6087	4.9134
H	-2.8049	-2.5174	4.2387	H	-5.4559	1.3603	3.3405
H	-5.6633	-2.8879	1.9269	H	-3.9367	3.8443	0.921
H	-7.1376	-1.9253	2.0299	H	-2.7508	4.738	-0.0294
H	-6.8499	-2.9545	0.6293	H	-4.2876	4.2691	-0.7511
H	4.4038	-5.3472	-0.1589	H	3.6065	5.6589	-0.8517
H	4.7055	-4.8919	-1.8364	H	2.1929	5.8597	0.1854
H	7.602	-2.6334	-0.8732	H	5.5845	4.2659	0.2354
H	6.5573	-3.0843	-2.2077	H	5.6118	4.0759	1.9791
H	3.2679	-0.1617	-1.1205	H	2.1312	0.8308	0.5017
H	2.209	-1.1849	-0.206	H	1.7906	1.3035	-1.1333
H	3.6368	-1.045	1.8013	H	4.0974	0.8348	-1.8521
H	5.3068	1.0187	0.2795	H	4.5779	-0.2298	0.9835
H	5.5194	0.5092	1.9438	H	5.7041	-0.2745	-0.3615
H	7.1186	-0.6059	0.3948	H	6.1831	1.6004	1.1857
H	6.1277	-1.7316	1.3077	H	5.8526	2.1259	-0.4573
H	1.9879	0.2515	3.348	H	3.3591	-1.1529	-3.4259
H	5.2925	0.2721	-1.8537	H	3.4045	1.1791	2.3521
H	6.8722	-0.4396	-2.1526	H	4.6156	2.2246	3.0842
H	5.4333	-1.1127	-2.9338	H	2.9964	2.8458	2.7368
H	1.5676	-2.9856	-0.7589	H	1.0089	2.9679	-1.7941
H	-4.3294	-2.9639	-1.7116	H	-5.7051	1.1918	-1.3206
H	6.8207	-4.9604	-0.6591	H	3.3043	5.0372	2.1136
H	6.2021	-4.0003	0.6799	H	4.4313	6.1367	1.3335
5a-7	X axis(Å)	Y axis(Å)	Z axis(Å)	5a-8	X axis(Å)	Y axis(Å)	Z axis(Å)

C	-1.8952	5.1212	0.183	C	2.1467	4.7502	0.5425
C	-1.6153	4.4754	-1.1728	C	1.8057	3.845	1.726
C	-0.822	3.1632	-1.0645	C	0.9364	2.6413	1.3259
C	0.4642	3.3309	-0.2033	C	-0.3289	3.0879	0.5377
C	0.129	3.9172	1.2152	C	0.055	3.9428	-0.723
C	-0.6359	5.2572	1.0428	C	0.9126	5.1555	-0.2693
C	1.2847	2.0314	-0.059	C	-1.2525	1.9211	0.1318
C	2.5949	2.2307	0.7397	C	-2.5398	2.4009	-0.5787
C	2.3404	2.9433	2.0842	C	-2.2182	3.3406	-1.7573
C	1.462	4.1915	1.961	C	-1.2501	4.467	-1.3821
C	-0.7297	2.9821	2.1078	C	0.8496	3.1641	-1.8049
C	-0.5065	2.666	-2.4562	C	0.5755	1.851	2.5629
O	0.2781	3.1739	-3.2453	O	-0.2063	2.1942	3.4387
O	1.3226	4.3002	-0.8577	O	-1.1103	3.9549	1.4011
C	3.3625	0.9273	0.8917	C	-3.4278	1.2296	-0.9553
O	3.3292	0.0549	-0.2024	O	-3.6549	0.2918	0.0571
C	4.0576	0.5255	1.9556	C	-4.0169	0.9993	-2.1281
C	5.1048	-1.0905	-2.269	C	-5.8188	-0.7313	1.7832
C	5.4666	-0.8585	-0.8068	C	-5.9504	-0.3656	0.3092
C	4.235	-1.0356	0.0894	C	-4.6399	-0.6453	-0.4359
C	3.606	-2.4678	-0.0656	C	-4.2161	-2.1532	-0.3158
C	3.3055	-2.8279	-1.5696	C	-4.1571	-2.6357	1.1826
C	4.5207	-2.4824	-2.4783	C	-5.433	-2.1955	1.9577
C	2.3422	-2.6878	0.806	C	-2.8869	-2.4839	-1.0411
C	1.063	-2.0072	0.2868	C	-1.6137	-2.0037	-0.3238
C	0.8094	-2.3578	-1.1887	C	-1.5933	-2.4543	1.1461
C	2.0366	-2.0887	-2.0651	C	-2.8859	-2.0901	1.8837
C	-0.099	-2.2914	1.226	C	-0.3855	-2.3947	-1.1291
C	-0.156	-1.4833	2.483	C	-0.0327	-1.5162	-2.2855
C	-1.0931	-3.1753	1.0432	C	0.4265	-3.4406	-0.9066
C	3.0748	-4.3575	-1.755	C	-4.1313	-4.1901	1.281
C	4.6051	-0.7488	1.5258	C	-4.7702	-0.2181	-1.8794
O	5.2694	-1.4728	2.2552	O	-5.4098	-0.7996	-2.7455
C	-5.4345	-2.7073	1.8033	C	6.8492	-1.8348	-1.7019
C	-4.6587	-1.4651	1.44	C	5.8951	-0.8041	-1.1414
C	-4.5572	-0.9808	0.179	C	5.1678	-0.9885	-0.0114
C	-5.2022	-1.7114	-1.0144	C	5.2349	-2.3137	0.7754
C	-5.7346	-3.1228	-0.6341	C	5.9424	-3.4423	-0.0252
C	-3.7802	0.2705	-0.2096	C	4.2331	0.0445	0.6068
C	-2.7028	-0.0267	-1.2725	C	2.8141	-0.5072	0.8536
C	-3.3561	-0.6693	-2.5078	C	2.8855	-1.7761	1.7172
C	-4.149	-1.9213	-2.1339	C	3.8027	-2.8227	1.0871
C	-1.8583	1.188	-1.5991	C	1.9193	0.5729	1.4206
C	-1.2393	1.4461	-2.7501	C	1.2735	0.576	2.5853
O	-1.6754	2.1077	-0.5665	O	1.739	1.6843	0.5967
C	-6.3843	-0.8711	-1.5493	C	6.0122	-2.0855	2.0932
C	-4.0051	-0.8183	2.617	C	5.8548	0.4496	-1.9606

O	-3.744	-1.4434	3.6396	O	6.4553	0.5607	-3.0244
O	4.5851	-3.4372	0.3869	O	-5.238	-2.9577	-0.9566
C	-6.4184	-3.1385	0.7234	C	7.1976	-2.9511	-0.7262
O	0.6471	-0.5897	2.7264	O	-0.6832	-0.5223	-2.5855
H	-0.9704	-1.7324	3.1843	H	0.8591	-1.8128	-2.8632
H	-2.3302	6.1153	0.0243	H	2.6446	5.6541	0.9135
H	-2.6574	4.5416	0.7151	H	2.876	4.249	-0.1034
H	-2.5752	4.2995	-1.6752	H	2.7449	3.5034	2.1798
H	-1.0662	5.1937	-1.7955	H	1.2915	4.442	2.4904
H	-0.9156	5.6617	2.0239	H	1.2349	5.738	-1.1419
H	0.0197	6.0083	0.5832	H	0.3058	5.8377	0.3403
H	0.6768	1.2478	0.4036	H	-0.7126	1.2095	-0.5001
H	1.5557	1.668	-1.0586	H	-1.5529	1.3722	1.0334
H	3.2415	2.8888	0.142	H	-3.1187	2.9879	0.1487
H	1.8807	2.2482	2.7975	H	-1.7998	2.7687	-2.5945
H	3.2976	3.2452	2.5288	H	-3.1451	3.7944	-2.1312
H	2.0345	4.9741	1.4467	H	-1.7658	5.1628	-0.7078
H	1.26	4.5843	2.9659	H	-1.013	5.0475	-2.283
H	-0.2879	1.9909	2.2305	H	0.3451	2.2491	-2.1248
H	-0.8396	3.4086	3.1124	H	0.9839	3.7841	-2.6998
H	-1.7419	2.8328	1.7273	H	1.8521	2.8783	-1.4807
H	1.4581	4.0233	-1.7881	H	-1.2867	3.4815	2.2413
H	4.2252	0.9866	2.9096	H	-3.996	1.5436	-3.0523
H	4.3979	-0.327	-2.6128	H	-5.0811	-0.0846	2.2717
H	6.0042	-0.9796	-2.886	H	-6.7742	-0.5467	2.2881
H	6.2674	-1.5456	-0.5064	H	-6.7802	-0.9239	-0.142
H	5.8725	0.1566	-0.7093	H	-6.2146	0.6975	0.2403
H	5.3265	-3.2077	-2.2997	H	-6.287	-2.8024	1.6269
H	4.2427	-2.5958	-3.5341	H	-5.3115	-2.4054	3.0282
H	2.1597	-3.7676	0.9018	H	-2.8255	-3.5711	-1.1922
H	2.549	-2.3726	1.8364	H	-2.9182	-2.087	-2.0637
H	1.2079	-0.9259	0.3047	H	-1.6191	-0.913	-0.2893
H	0.5133	-3.4066	-1.2979	H	-1.4329	-3.5347	1.2247
H	-0.0287	-1.7646	-1.5722	H	-0.7474	-1.9832	1.6626
H	1.8032	-2.3957	-3.093	H	-2.8252	-2.4859	2.906
H	2.2045	-1.0083	-2.1153	H	-2.9338	-1.0027	1.9967
H	-1.8897	-3.3113	1.7709	H	1.2891	-3.6526	-1.5325
H	-1.1431	-3.8111	0.1659	H	0.2503	-4.1412	-0.097
H	2.2788	-4.7473	-1.1153	H	-3.3053	-4.6371	0.7218
H	2.8017	-4.5857	-2.7922	H	-4.0302	-4.511	2.3246
H	3.9786	-4.9345	-1.5291	H	-5.0561	-4.6363	0.8982
H	-4.7234	-3.5209	1.9954	H	6.3963	-2.2704	-2.602
H	-5.9983	-2.5464	2.7305	H	7.7879	-1.3597	-2.0123
H	-4.9076	-3.8456	-0.6033	H	5.2641	-3.8495	-0.7878
H	-6.4284	-3.4907	-1.4005	H	6.1945	-4.281	0.6359
H	-4.4797	1.0303	-0.58	H	4.6691	0.3883	1.554
H	-3.2933	0.7218	0.6566	H	4.149	0.9419	-0.0082

H	-2.0154	-0.7619	-0.8336	H	2.3867	-0.7919	-0.1185
H	-4.0095	0.0524	-3.013	H	3.2383	-1.5385	2.728
H	-2.5903	-0.9625	-3.2363	H	1.8843	-2.2102	1.8303
H	-4.6334	-2.3186	-3.0352	H	3.8506	-3.6977	1.7481
H	-3.424	-2.684	-1.8163	H	3.3276	-3.1669	0.1588
H	-1.191	0.8994	-3.672	H	1.2252	-0.1469	3.3766
H	-6.0678	0.1057	-1.928	H	5.5166	-1.3686	2.7551
H	-6.8884	-1.3846	-2.3763	H	6.1142	-3.021	2.6554
H	-7.1319	-0.6861	-0.7699	H	7.0204	-1.6997	1.9065
H	-3.7491	0.2461	2.5266	H	5.2562	1.2843	-1.5763
H	4.8786	-3.185	1.2885	H	-5.3813	-2.6128	-1.8638
H	-7.292	-2.4764	0.7212	H	7.933	-2.5965	0.0049
H	-6.7878	-4.1464	0.945	H	7.6711	-3.7775	-1.2689
5a-9	X axis(Å)	Y axis(Å)	Z axis(Å)	5a-10	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-1.8397	5.069	0.6834	C	-2.7566	5.0351	-0.2491
C	-1.6313	4.6128	-0.7597	C	-2.3153	4.2385	-1.4768
C	-0.815	3.315	-0.8682	C	-1.5807	2.9402	-1.1057
C	0.5196	3.4008	-0.0706	C	-0.3927	3.2128	-0.1376
C	0.2638	3.7923	1.4304	C	-0.8859	3.9561	1.16
C	-0.5326	5.1241	1.4785	C	-1.6184	5.264	0.7497
C	1.3745	2.1169	-0.1474	C	0.4389	1.9578	0.2356
C	2.7268	2.2552	0.5937	C	1.646	2.3233	1.1294
C	2.5408	2.7691	2.0351	C	1.2091	3.1144	2.3766
C	1.6338	3.9996	2.1288	C	0.3479	4.3298	2.0256
C	-0.5194	2.7303	2.2454	C	-1.844	3.1184	2.0483
C	-0.5813	3.0008	-2.3273	C	-1.1222	2.2394	-2.3643
O	0.1406	3.6258	-3.0924	O	-0.2535	2.6348	-3.1296
O	1.3212	4.4678	-0.6429	O	0.5229	4.1218	-0.8061
C	3.5469	0.9785	0.5451	C	2.5164	1.1254	1.4443
O	3.1289	-0.0189	-0.3408	O	3.216	0.5884	0.3576
C	4.6327	0.7184	1.2726	C	2.7738	0.5923	2.6382
C	4.0823	-1.2703	-2.8608	C	5.9978	0.9724	-0.5714
C	4.9438	-0.8841	-1.6655	C	5.5658	0.7207	0.8684
C	4.1582	-1.0352	-0.3563	C	4.3159	-0.1737	0.91
C	3.6235	-2.4974	-0.1608	C	4.583	-1.55	0.2126
C	2.8197	-3.0143	-1.4138	C	5.1255	-1.3763	-1.2543
C	3.5813	-2.7032	-2.7342	C	6.2816	-0.3355	-1.2997
C	2.7856	-2.6888	1.1322	C	3.3721	-2.5128	0.2226
C	1.3484	-2.1255	1.0863	C	2.2399	-2.1788	-0.7678
C	0.6107	-2.6215	-0.1673	C	2.7867	-1.9107	-2.1809
C	1.4066	-2.3829	-1.4514	C	3.9789	-0.9507	-2.2039
C	0.5217	-2.4084	2.3345	C	1.1512	-3.2446	-0.8297
C	-0.6879	-1.5598	2.5594	C	-0.1749	-2.8423	-1.3779
C	0.7726	-3.3226	3.2865	C	1.2314	-4.5214	-0.4183
C	2.6548	-4.5633	-1.3894	C	5.7408	-2.6979	-1.802
C	5.0262	-0.5977	0.8012	C	3.8532	-0.3372	2.3396
O	5.9365	-1.241	1.3053	O	4.3134	-1.1128	3.166

C	-5.4325	-2.7464	1.5213	C	-4.8191	-4.2434	1.0287
C	-4.6777	-1.4711	1.229	C	-3.8529	-3.0896	0.9531
C	-4.5106	-0.9683	-0.0191	C	-4.2316	-1.8172	0.6883
C	-5.0235	-1.7198	-1.2635	C	-5.7159	-1.4148	0.5814
C	-5.4993	-3.1629	-0.9336	C	-6.6846	-2.5957	0.8726
C	-3.7905	0.3342	-0.3483	C	-3.2719	-0.6877	0.3431
C	-2.6209	0.1169	-1.3289	C	-3.5373	-0.1866	-1.0928
C	-3.138	-0.5553	-2.612	C	-5.0044	0.2302	-1.2786
C	-3.8785	-1.8566	-2.3024	C	-5.9682	-0.8848	-0.8547
C	-1.84	1.3909	-1.5766	C	-2.6108	0.941	-1.4605
C	-1.303	1.803	-2.7238	C	-1.8391	0.9896	-2.5445
O	-1.6203	2.1916	-0.4562	O	-2.5304	1.9987	-0.5622
C	-6.2098	-0.9441	-1.8814	C	-6.0604	-0.3147	1.615
C	-4.1285	-0.8247	2.4631	C	-2.4225	-3.4682	1.1423
O	-4.1442	-1.3805	3.5583	O	-2.0109	-4.6144	0.9996
O	4.7702	-3.377	-0.0364	O	5.6334	-2.2219	0.9551
C	-6.2938	-3.226	0.36	C	-6.1572	-3.9297	0.3685
O	-1.0338	-0.6772	1.7822	O	-0.4644	-1.6791	-1.6315
H	-1.2639	-1.7718	3.4766	H	-0.9038	-3.657	-1.5297
H	-2.3015	6.0636	0.6826	H	-3.1507	6.0058	-0.5731
H	-2.5567	4.4048	1.1784	H	-3.5904	4.5204	0.241
H	-2.6166	4.4825	-1.2254	H	-3.2049	4.0135	-2.0792
H	-1.1303	5.4176	-1.3131	H	-1.6717	4.8726	-2.0999
H	-0.7586	5.3923	2.5184	H	-2.0201	5.7663	1.639
H	0.081	5.9438	1.0827	H	-0.9046	5.9686	0.3032
H	0.8152	1.2574	0.2389	H	-0.1846	1.2013	0.7253
H	1.5978	1.897	-1.1998	H	0.8304	1.4937	-0.6788
H	3.3138	3.0089	0.0495	H	2.2931	2.9995	0.5513
H	3.514	3.0378	2.465	H	0.6587	2.4657	3.0683
H	2.1431	1.9677	2.67	H	2.0948	3.4641	2.9228
H	2.1601	4.8574	1.6905	H	0.9733	5.0645	1.5022
H	1.4858	4.2521	3.1868	H	0.0271	4.8201	2.9537
H	-0.0384	1.7503	2.2268	H	-1.4421	2.1307	2.2884
H	-0.5877	3.0305	3.2982	H	-2.028	3.6302	3.0009
H	-1.5458	2.5904	1.9012	H	-2.8257	2.9634	1.5967
H	1.3779	4.3309	-1.6121	H	0.7593	3.7367	-1.6768
H	5.1448	1.3005	2.0143	H	2.4054	0.8247	3.6185
H	3.2382	-0.5789	-2.9621	H	5.2298	1.544	-1.1048
H	4.6735	-1.1739	-3.779	H	6.9024	1.5918	-0.5749
H	5.8512	-1.5008	-1.6449	H	6.3883	0.2633	1.4324
H	5.2745	0.1536	-1.8014	H	5.3689	1.6916	1.3408
H	4.4529	-3.367	-2.8173	H	7.1831	-0.774	-0.8499
H	2.9439	-2.934	-3.5976	H	6.5439	-0.1119	-2.3418
H	2.7516	-3.7647	1.3485	H	3.7575	-3.5203	0.0207
H	3.3201	-2.2622	1.9908	H	2.9586	-2.5887	1.2366
H	1.4317	-1.0362	1.022	H	1.764	-1.2594	-0.4075
H	0.3712	-3.6872	-0.0672	H	3.0712	-2.8567	-2.6586

H	-0.3546	-2.1149	-0.2673	H	1.9958	-1.4879	-2.8136
H	0.8361	-2.7941	-2.2946	H	4.3531	-0.8891	-3.2344
H	1.4614	-1.3051	-1.6352	H	3.6235	0.0566	-1.9671
H	0.1318	-3.4508	4.1553	H	0.3888	-5.2078	-0.4759
H	1.6266	-3.99	3.2375	H	2.1353	-4.942	0.0082
H	2.1799	-4.9256	-0.4741	H	5.0344	-3.5319	-1.7936
H	2.0394	-4.9011	-2.2318	H	6.0766	-2.5684	-2.8378
H	3.62	-5.0753	-1.4744	H	6.6148	-3.0101	-1.2193
H	-4.7073	-3.5278	1.7826	H	-4.4067	-5.1316	0.536
H	-6.0881	-2.6114	2.3905	H	-4.9754	-4.5029	2.0832
H	-4.6358	-3.8351	-0.8338	H	-7.67	-2.3995	0.4313
H	-6.1024	-3.5661	-1.7567	H	-6.8516	-2.6884	1.9549
H	-4.5111	1.0431	-0.7758	H	-3.3828	0.12	1.076
H	-3.4129	0.8266	0.5481	H	-2.2236	-0.9886	0.4057
H	-1.9178	-0.5773	-0.8514	H	-3.3459	-1.0265	-1.7773
H	-3.7961	0.1272	-3.1634	H	-5.2205	1.1438	-0.7113
H	-2.3007	-0.7926	-3.2801	H	-5.1902	0.4763	-2.332
H	-4.2695	-2.2751	-3.2388	H	-6.9968	-0.5126	-0.9445
H	-3.1341	-2.5766	-1.934	H	-5.8758	-1.7074	-1.5762
H	-1.2969	1.3672	-3.7039	H	-1.705	0.285	-3.3425
H	-5.9223	0.0496	-2.2385	H	-5.5062	0.615	1.4584
H	-6.625	-1.4822	-2.7414	H	-7.1263	-0.0612	1.5717
H	-7.0194	-0.8023	-1.157	H	-5.8402	-0.6518	2.6351
H	-3.6899	0.1752	2.358	H	-1.7344	-2.6584	1.4258
H	5.3585	-3.0285	0.6669	H	5.3527	-2.2884	1.8925
H	-7.2007	-2.6151	0.2846	H	-6.8749	-4.7257	0.5978
H	-6.6228	-4.2545	0.5479	H	-6.0453	-3.9084	-0.722
5b-1	X axis(Å)	Y axis(Å)	Z axis(Å)	5b-2	X axis(Å)	Y axis(Å)	Z axis(Å)
C	2.3922	4.991	1.6494	C	3.1163	4.334	2.2651
C	2.5617	4.6759	0.1641	C	3.4701	4.2931	0.7782
C	1.7443	3.4503	-0.2801	C	2.7438	3.1727	0.0199
C	0.2449	3.5921	0.1131	C	1.2051	3.2158	0.2644
C	0.0876	3.839	1.6611	C	0.8789	3.1464	1.8004
C	0.9228	5.0844	2.0673	C	1.6056	4.3141	2.5216
C	-0.6534	2.4142	-0.3378	C	0.4228	2.1271	-0.5028
C	-2.1344	2.6635	0.019	C	-1.1069	2.1999	-0.2746
C	-2.3316	3.0016	1.5064	C	-1.4512	2.2489	1.2255
C	-1.4061	4.1238	1.9784	C	-0.6528	3.3089	1.9891
C	0.5348	2.6418	2.5421	C	1.2958	1.8168	2.4861
C	1.9236	3.2493	-1.7665	C	3.0786	3.2537	-1.4519
O	1.4743	3.9691	-2.6481	O	2.7504	4.1504	-2.2164
O	-0.2763	4.7777	-0.5466	O	0.704	4.491	-0.2117
C	-3.0293	1.515	-0.3724	C	-1.8663	1.0946	-0.9894
O	-2.8652	0.3086	0.3112	O	-3.2235	0.9796	-0.6733
C	-4.0064	1.5793	-1.2748	C	-1.3859	0.2289	-1.8815
C	-4.3853	-1.08	2.4527	C	-5.9023	1.3137	-1.8692
C	-4.9818	-0.3722	1.2427	C	-4.6811	0.7227	-2.5641

C	-4.0455	-0.4826	0.0298	C	-3.7916	-0.016	-1.557
C	-3.7546	-1.9783	-0.3385	C	-4.5747	-1.1666	-0.8278
C	-3.2315	-2.8051	0.8967	C	-5.9071	-0.6492	-0.1671
C	-4.1144	-2.5488	2.1517	C	-6.7139	0.234	-1.163
C	-2.7983	-2.1456	-1.5454	C	-3.7209	-1.9389	0.2106
C	-1.3098	-1.8951	-1.2458	C	-3.4577	-1.1864	1.526
C	-0.8321	-2.6564	1.00E-04	C	-4.7669	-0.6564	2.136
C	-1.7542	-2.453	1.2031	C	-5.6002	0.1434	1.1293
C	-0.4597	-2.2156	-2.4642	C	-2.6174	-2.0397	2.4617
C	0.2591	-1.1014	-3.1417	C	-1.1491	-2.1057	2.1875
C	-0.3043	-3.4392	-2.9979	C	-3.0462	-2.7257	3.5339
C	-3.3188	-4.3379	0.6354	C	-6.8571	-1.8273	0.2012
C	-4.6401	0.2794	-1.135	C	-2.559	-0.5427	-2.2532
O	-5.5372	-0.1101	-1.87	O	-2.5155	-1.4903	-3.0262
C	3.7886	-3.9311	2.173	C	3.7469	-4.6837	1.0989
C	3.1342	-2.6319	1.7608	C	3.3108	-3.2488	0.9116
C	3.333	-2.0382	0.5575	C	3.6927	-2.4773	-0.1366
C	4.2866	-2.6494	-0.4894	C	4.6567	-3.0099	-1.2162
C	5.198	-3.7496	0.1203	C	5.358	-4.3244	-0.7761
C	2.6543	-0.7562	0.0938	C	3.2224	-1.0515	-0.3869
C	3.6476	0.2969	-0.4294	C	4.3896	-0.0684	-0.6078
C	4.5086	-0.2999	-1.5511	C	5.2759	-0.5554	-1.7623
C	5.2283	-1.5597	-1.0698	C	5.7804	-1.9744	-1.4966
C	2.9053	1.5547	-0.8149	C	3.844	1.3298	-0.7818
C	2.7194	2.0623	-2.0323	C	3.8023	2.0693	-1.8882
O	2.3516	2.2555	0.2561	O	3.3085	1.8918	0.3755
C	3.449	-3.2784	-1.6282	C	3.8623	-3.2855	-2.5151
C	2.2242	-2.0818	2.8165	C	2.3953	-2.7712	1.9971
O	2.0761	-2.6226	3.9077	O	2.0331	-3.4895	2.9249
O	-5.0089	-2.593	-0.7287	O	-4.9738	-2.1381	-1.8278
C	4.4286	-4.6989	1.0236	C	4.3913	-5.3057	-0.1337
O	0.278	0.0439	-2.7084	O	-0.6133	-1.5013	1.2638
H	0.8003	-1.3691	-4.0651	H	-0.5619	-2.737	2.8757
H	2.9078	4.2313	2.2472	H	3.5967	3.4933	2.7777
H	2.8908	5.9413	1.8745	H	3.5435	5.2402	2.7109
H	2.2691	5.5571	-0.4214	H	3.2271	5.2663	0.3323
H	3.6294	4.5143	-0.0331	H	4.557	4.1719	0.6851
H	0.4923	5.9876	1.6154	H	1.186	5.2751	2.1968
H	0.8698	5.2367	3.1529	H	1.4283	4.2585	3.6032
H	-0.5958	2.3048	-1.428	H	0.5996	2.2523	-1.5791
H	-0.3035	1.468	0.09	H	0.7937	1.1313	-0.235
H	-2.4644	3.5435	-0.5519	H	-1.4624	3.1417	-0.7162
H	-3.3718	3.3069	1.6804	H	-2.5194	2.464	1.3573
H	-2.1734	2.1121	2.1285	H	-1.2812	1.2687	1.683
H	-1.5446	4.2706	3.0573	H	-0.9119	3.2508	3.0541
H	-1.724	5.0629	1.5073	H	-0.9774	4.3035	1.6575
H	0.0543	1.7027	2.2554	H	0.9157	0.9346	1.9653

H	1.6124	2.4692	2.5191	H	2.3774	1.6943	2.5695
H	0.2791	2.8242	3.5931	H	0.907	1.7769	3.511
H	-0.0752	4.7094	-1.5044	H	1.0238	4.6359	-1.1265
H	-4.3282	2.3824	-1.9092	H	-0.4011	0.0921	-2.2832
H	-3.4633	-0.5801	2.7702	H	-5.597	2.0862	-1.1543
H	-5.083	-1.0064	3.2952	H	-6.5348	1.8132	-2.6124
H	-5.9667	-0.7962	1.0099	H	-4.9988	0.0487	-3.3693
H	-5.1509	0.6789	1.5097	H	-4.1267	1.5409	-3.0416
H	-5.0861	-3.0446	2.0212	H	-7.157	-0.405	-1.9391
H	-3.6556	-3.0134	3.034	H	-7.5581	0.7067	-0.6445
H	-2.9301	-3.1586	-1.9499	H	-4.213	-2.8956	0.4361
H	-3.1181	-1.497	-2.3715	H	-2.7724	-2.2439	-0.2492
H	-1.1924	-0.8313	-1.0203	H	-2.8591	-0.3006	1.3096
H	0.1739	-2.3199	0.272	H	-4.5374	-0.0126	2.9949
H	-0.7373	-3.7287	-0.2058	H	-5.3778	-1.4774	2.5264
H	-1.386	-3.0728	2.0313	H	-6.5388	0.4413	1.6149
H	-1.6578	-1.4195	1.5501	H	-5.0803	1.0799	0.9055
H	0.3107	-3.627	-3.8732	H	-2.3747	-3.3065	4.1611
H	-0.8006	-4.3056	-2.5687	H	-4.0909	-2.7433	3.8255
H	-2.7809	-4.6459	-0.265	H	-6.387	-2.5618	0.8602
H	-2.8953	-4.8995	1.4767	H	-7.7537	-1.4571	0.7126
H	-4.3563	-4.6711	0.5193	H	-7.1979	-2.3673	-0.6894
H	4.5552	-3.7057	2.9256	H	4.4595	-4.7194	1.9332
H	3.0569	-4.5952	2.6494	H	2.8923	-5.3112	1.3803
H	6.0017	-3.2907	0.7126	H	6.1539	-4.105	-0.051
H	5.6937	-4.3204	-0.675	H	5.85	-4.8012	-1.6332
H	1.9433	-1.0131	-0.6994	H	2.5648	-1.0521	-1.2666
H	2.0513	-0.2985	0.8796	H	2.6021	-0.6702	0.4253
H	4.3255	0.5688	0.393	H	5.0102	-0.0582	0.3002
H	3.8979	-0.536	-2.4306	H	4.7307	-0.53	-2.7132
H	5.2576	0.4323	-1.8781	H	6.1389	0.1121	-1.8787
H	5.814	-1.9741	-1.9005	H	6.3875	-2.3019	-2.3504
H	5.9557	-1.2563	-0.3041	H	6.4622	-1.9297	-0.6359
H	3.0164	1.7146	-3.0023	H	4.1309	1.8702	-2.89
H	4.094	-3.78	-2.3588	H	4.5111	-3.7138	-3.2879
H	2.7389	-4.0207	-1.2476	H	3.0399	-3.9891	-2.3458
H	2.8648	-2.5345	-2.1773	H	3.4192	-2.3782	-2.9371
H	1.6783	-1.1601	2.5821	H	2.0531	-1.7311	1.9456
H	-5.4145	-2.0485	-1.437	H	-4.1769	-2.4133	-2.3286
H	3.6593	-5.2328	0.4541	H	3.6182	-5.6078	-0.8493
H	5.1039	-5.4633	1.4251	H	4.9226	-6.2206	0.1535
5b-3	X axis(Å)	Y axis(Å)	Z axis(Å)	5b-4	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-0.5416	5.703	-0.9438	C	-2.1227	4.6308	-1.5217
C	-0.962	5.0875	0.3887	C	-2.2212	4.3173	-0.0287
C	-0.4937	3.631	0.5517	C	-1.3449	3.123	0.383
C	1.0358	3.4828	0.2986	C	0.1303	3.3161	-0.0743
C	1.4256	4.0526	-1.1175	C	0.2182	3.5563	-1.6272

C	0.952	5.5277	-1.2249	C	-0.6756	4.7702	-2.0038
C	1.5717	2.0392	0.4648	C	1.0831	2.1741	0.3483
C	3.1	1.9572	0.2414	C	2.5401	2.4684	-0.0618
C	3.5432	2.617	-1.0764	C	2.6715	2.7988	-1.558
C	2.9697	4.0205	-1.2629	C	1.69	3.886	-2.0039
C	0.8237	3.2598	-2.309	C	-0.2237	2.3398	-2.4835
C	-0.8896	3.1471	1.9257	C	-1.4404	2.9159	1.8781
O	-0.398	3.5136	2.9847	O	-1.0058	3.6702	2.7374
O	1.7383	4.2941	1.277	O	0.6351	4.5245	0.5563
C	3.6248	0.5424	0.2642	C	3.4706	1.3489	0.3299
O	2.9185	-0.4091	-0.47	O	3.4225	0.1761	-0.4262
C	4.7412	0.1407	0.8687	C	4.362	1.4053	1.3177
C	3.2762	-1.7376	-3.0656	C	5.1992	-1.0727	-2.4613
C	4.3736	-1.5064	-2.0321	C	5.6435	-0.4011	-1.1687
C	3.7915	-1.5539	-0.6123	C	4.5946	-0.5925	-0.0625
C	3.1104	-2.935	-0.325	C	4.3124	-2.1104	0.2121
C	2.02	-3.2921	-1.402	C	3.9512	-2.8961	-1.1053
C	2.5719	-3.0711	-2.8408	C	4.9521	-2.5604	-2.2478
C	2.5157	-3.0617	1.0975	C	3.2358	-2.353	1.3002
C	1.2086	-2.2846	1.341	C	1.7799	-2.1358	0.8524
C	0.1722	-2.5714	0.2416	C	1.4676	-2.8611	-0.4678
C	0.7394	-2.449	-1.1765	C	2.5044	-2.5711	-1.554
C	0.6079	-2.5248	2.7209	C	0.8388	-2.5046	1.9894
C	-0.2924	-1.4702	3.2663	C	0.4106	-1.414	2.9121
C	0.8204	-3.5762	3.5303	C	0.3438	-3.7267	2.2478
C	1.6199	-4.7958	-1.3402	C	4.0618	-4.4359	-0.8987
C	4.866	-1.2322	0.4036	C	5.0519	0.1341	1.1838
O	5.7394	-1.9938	0.7956	O	5.8923	-0.2602	1.9808
C	-5.3134	-3.3385	-0.6899	C	-7.0871	-2.8123	-0.3509
C	-4.4401	-2.3694	0.0727	C	-6.4001	-1.5153	0.0105
C	-4.5224	-1.0216	-0.0546	C	-5.1224	-1.2177	-0.3334
C	-5.5252	-0.3671	-1.0273	C	-4.2527	-2.2212	-1.1227
C	-6.1338	-1.3938	-2.0224	C	-4.8778	-3.6433	-1.1587
C	-3.6751	-0.0182	0.7176	C	-4.4103	0.0906	-0.0067
C	-2.9611	0.9909	-0.2034	C	-3.052	-0.137	0.6804
C	-3.9903	1.7188	-1.0788	C	-2.1602	-1.0409	-0.1761
C	-4.8235	0.7215	-1.8828	C	-2.8545	-2.369	-0.4634
C	-2.083	1.9862	0.5211	C	-2.366	1.1708	0.9733
C	-1.9467	2.1552	1.8356	C	-2.1223	1.669	2.1834
O	-1.2769	2.7707	-0.3041	O	-1.9358	1.9069	-0.1258
C	-6.6753	0.2707	-0.2124	C	-4.0951	-1.7157	-2.5766
C	-3.4881	-3.0528	1.0044	C	-7.2905	-0.5808	0.7688
O	-3.3495	-4.2713	1.0368	O	-8.3925	-0.9157	1.1907
O	4.1321	-3.9598	-0.4246	O	5.5358	-2.7088	0.7099
C	-6.5299	-2.6935	-1.3415	C	-6.372	-3.6108	-1.4328
O	-0.6254	-0.4837	2.6211	O	0.7268	-0.2417	2.7519
H	-0.6611	-1.6305	4.2937	H	-0.228	-1.7211	3.7577

H	-1.1346	5.2655	-1.7543	H	-2.6614	5.5631	-1.7293
H	-0.783	6.7727	-0.9379	H	-2.6376	3.8516	-2.0945
H	-0.5608	5.704	1.2036	H	-1.9357	5.2105	0.5416
H	-2.0554	5.1469	0.4648	H	-3.2734	4.1188	0.2128
H	1.5133	6.1541	-0.5193	H	-0.2568	5.6905	-1.5761
H	1.1756	5.9245	-2.2235	H	-0.6745	4.9166	-3.0915
H	1.3711	1.6829	1.4837	H	1.0687	2.0717	1.4404
H	1.0426	1.3568	-0.2098	H	0.7501	1.2138	-0.061
H	3.5816	2.5089	1.0613	H	2.8617	3.365	0.4877
H	4.639	2.6822	-1.1049	H	3.6939	3.1361	-1.7724
H	3.2623	1.9898	-1.9318	H	2.5186	1.8997	-2.1672
H	3.2669	4.3987	-2.2495	H	1.7823	4.027	-3.0884
H	3.4381	4.6934	-0.5332	H	1.9942	4.8395	-1.5531
H	1.0404	2.1895	-2.2581	H	0.299	1.419	-2.2116
H	-0.2601	3.3611	-2.3905	H	-1.2934	2.1321	-2.4165
H	1.2354	3.6251	-3.2578	H	-0.0164	2.5242	-3.5447
H	1.3984	4.0655	2.1683	H	0.4845	4.4544	1.523
H	5.4514	0.6787	1.4664	H	4.5808	2.1808	2.0258
H	2.5494	-0.9177	-3.0384	H	4.2975	-0.5882	-2.8522
H	3.7167	-1.7263	-4.0695	H	5.9764	-0.941	-3.2232
H	5.1673	-2.254	-2.1523	H	6.614	-0.8047	-0.8535
H	4.8333	-0.5299	-2.232	H	5.8019	0.6655	-1.3741
H	3.2915	-3.8666	-3.079	H	5.9218	-3.0302	-2.0332
H	1.7599	-3.1713	-3.5726	H	4.606	-3.0019	-3.1912
H	2.3569	-4.1298	1.2929	H	3.3481	-3.3786	1.6799
H	3.2622	-2.7669	1.8463	H	3.4483	-1.7297	2.1787
H	1.46	-1.2195	1.2961	H	1.6364	-1.0715	0.6417
H	-0.6703	-1.8746	0.3308	H	0.4811	-2.551	-0.8329
H	-0.2542	-3.5726	0.3804	H	1.4031	-3.9443	-0.3224
H	-0.0389	-2.7572	-1.8873	H	2.2486	-3.1606	-2.4443
H	0.9205	-1.3917	-1.3923	H	2.4103	-1.5252	-1.8618
H	0.3564	-3.6663	4.5089	H	-0.328	-3.9239	3.0785
H	1.4573	-4.407	3.2448	H	0.6099	-4.5885	1.6438
H	1.2375	-5.0941	-0.3606	H	3.4486	-4.7977	-0.0693
H	0.8367	-5.0185	-2.0747	H	3.7419	-4.9722	-1.8
H	2.468	-5.4509	-1.5688	H	5.0931	-4.7442	-0.6929
H	-4.7008	-3.8185	-1.464	H	-7.1668	-3.4246	0.5567
H	-5.6735	-4.1344	-0.0264	H	-8.1094	-2.6206	-0.6995
H	-5.4085	-1.6312	-2.8128	H	-4.7192	-4.1513	-0.1974
H	-7.0067	-0.964	-2.5298	H	-4.3789	-4.2617	-1.9154
H	-4.3267	0.5094	1.4259	H	-4.2765	0.6542	-0.9392
H	-2.9156	-0.5071	1.3265	H	-5.0026	0.7392	0.6421
H	-2.2966	0.4152	-0.865	H	-3.2379	-0.6523	1.6342
H	-3.4847	2.3941	-1.7807	H	-1.8893	-0.5507	-1.1189
H	-4.6427	2.3486	-0.4618	H	-1.2192	-1.2333	0.348
H	-5.5675	1.2728	-2.4722	H	-2.2024	-2.983	-1.0978
H	-4.1536	0.2413	-2.6098	H	-2.9505	-2.9086	0.4891

H	-2.4035	1.6565	2.6682	H	-2.3328	1.286	3.1629
H	-7.4339	0.7019	-0.8759	H	-3.5155	-2.4256	-3.1779
H	-7.1748	-0.4648	0.4276	H	-5.0659	-1.5823	-3.0664
H	-6.3287	1.0766	0.442	H	-3.5781	-0.7526	-2.6328
H	-2.9039	-2.4175	1.6801	H	-6.9207	0.4377	0.9395
H	4.8654	-3.7249	0.1827	H	5.8478	-2.1836	1.4778
H	-7.3072	-2.5125	-0.5904	H	-6.5731	-3.1742	-2.4177
H	-6.9611	-3.384	-2.0756	H	-6.77	-4.6319	-1.4578
5b-5	X axis(Å)	Y axis(Å)	Z axis(Å)	5b-6	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-0.5119	5.5386	-1.227	C	-1.9661	4.832	-0.9368
C	-1.0258	5.0342	0.119	C	-1.8286	4.2643	0.4781
C	-0.5527	3.6074	0.4475	C	-1.0031	2.9695	0.514
C	0.9917	3.4633	0.3178	C	0.379	3.1661	-0.1738
C	1.4861	3.9231	-1.1047	C	0.2069	3.6444	-1.6626
C	1.0018	5.3738	-1.3728	C	-0.625	4.957	-1.6707
C	1.5217	2.0448	0.6342	C	1.2966	1.9281	-0.104
C	3.0607	1.9672	0.5438	C	2.6768	2.1902	-0.7441
C	3.6168	2.5415	-0.7722	C	2.5471	2.7169	-2.1805
C	3.0384	3.9121	-1.1212	C	1.6111	3.9281	-2.2667
C	0.9927	3.0222	-2.2685	C	-0.4938	2.6158	-2.5902
C	-1.0392	3.247	1.8304	C	-0.8581	2.4752	1.9377
O	-0.629	3.7172	2.883	O	-0.2249	3.0143	2.8343
O	1.6118	4.3607	1.2766	O	1.0756	4.2301	0.5256
C	3.5644	0.5569	0.7225	C	3.5739	0.9774	-0.699
O	3.1874	-0.3718	-0.2482	O	2.9964	-0.2676	-0.9518
C	4.3785	0.1341	1.6873	C	4.8705	1.0044	-0.3966
C	4.5766	-1.5977	-2.5547	C	3.093	-2.5466	-2.8347
C	5.1616	-1.4049	-1.1607	C	4.2859	-1.7268	-2.358
C	4.0644	-1.5104	-0.0901	C	4.0688	-1.2412	-0.9202
C	3.3363	-2.8951	-0.1531	C	3.834	-2.4408	0.0711
C	2.7791	-3.2045	-1.5935	C	2.6865	-3.4044	-0.4175
C	3.8663	-2.9406	-2.6752	C	2.851	-3.7463	-1.9267
C	2.2169	-3.0631	0.9015	C	3.5773	-1.9936	1.5351
C	0.9029	-2.3201	0.5995	C	2.1763	-1.4137	1.7995
C	0.4127	-2.5378	-0.8407	C	1.0828	-2.3727	1.304
C	1.516	-2.3538	-1.8849	C	1.2951	-2.7728	-0.1596
C	-0.1669	-2.7031	1.6085	C	2.0345	-0.9758	3.2477
C	-0.7205	-1.649	2.4984	C	2.6807	0.3203	3.6206
C	-0.6617	-3.9415	1.7756	C	1.3614	-1.6082	4.2224
C	2.3968	-4.7058	-1.748	C	2.7374	-4.7742	0.3229
C	4.6586	-1.2327	1.2739	C	5.2457	-0.3947	-0.4864
O	5.3028	-2.0198	1.9536	O	6.3686	-0.8055	-0.2264
C	-5.6986	-3.2537	-0.2713	C	-7.2066	-2.5257	-0.0924
C	-4.9018	-2.1949	0.4506	C	-6.3666	-1.3548	0.3639
C	-4.7683	-0.9175	0.0167	C	-5.1827	-1.0105	-0.2012
C	-5.4703	-0.4333	-1.2669	C	-4.5882	-1.8261	-1.3707
C	-5.9869	-1.6147	-2.1349	C	-5.3032	-3.1926	-1.5607

C	-3.9429	0.1523	0.7211	C	-4.3243	0.1768	0.2207
C	-2.9643	0.8864	-0.2203	C	-2.8651	-0.2247	0.5025
C	-3.7315	1.4754	-1.4127	C	-2.2568	-0.9259	-0.7178
C	-4.4969	0.3825	-2.1561	C	-3.0902	-2.1425	-1.1109
C	-2.1275	1.9468	0.4628	C	-2.0462	0.9734	0.9074
C	-2.0818	2.2386	1.7623	C	-1.5574	1.2122	2.1217
O	-1.2645	2.6564	-0.3743	O	-1.7728	1.9032	-0.0877
C	-6.6752	0.4519	-0.8682	C	-4.732	-1.0094	-2.6771
C	-4.3005	-2.6799	1.7291	C	-6.9939	-0.5978	1.4928
O	-4.1654	-3.8693	1.994	O	-7.9879	-1.0013	2.0873
O	4.3175	-3.9238	0.1322	O	5.0409	-3.2441	0.0958
C	-6.6665	-2.6929	-1.3055	C	-6.8145	-3.0733	-1.4583
O	-0.4735	-0.4573	2.3609	O	3.3159	0.9955	2.819
H	-1.3977	-2.0005	3.2954	H	2.554	0.6409	4.6685
H	-1.0315	5.0172	-2.0383	H	-2.652	4.2034	-1.5157
H	-0.7701	6.5988	-1.3362	H	-2.4382	5.8203	-0.8824
H	-0.6964	5.7283	0.9033	H	-1.37	5.0235	1.1244
H	-2.1226	5.0787	0.1066	H	-2.8353	4.0851	0.877
H	1.4947	6.0681	-0.6799	H	-0.0506	5.7672	-1.2029
H	1.2996	5.6914	-2.3803	H	-0.812	5.2788	-2.7031
H	1.2411	1.7659	1.6582	H	1.4699	1.6681	0.9458
H	1.0567	1.3031	-0.0251	H	0.8095	1.0627	-0.5672
H	3.4693	2.5798	1.3601	H	3.167	2.9782	-0.1541
H	4.7091	2.6283	-0.7007	H	3.5348	3.011	-2.5584
H	3.4304	1.8517	-1.6046	H	2.1938	1.9216	-2.8482
H	3.4099	4.2147	-2.1087	H	1.5189	4.2341	-3.3167
H	3.4352	4.6527	-0.415	H	2.0829	4.774	-1.7503
H	1.2381	1.9672	-2.1218	H	-0.0409	1.6223	-2.5366
H	-0.0859	3.0779	-2.4279	H	-1.5577	2.4962	-2.3765
H	1.4581	3.3299	-3.213	H	-0.4335	2.9405	-3.6363
H	1.2164	4.1924	2.1584	H	1.1622	3.9769	1.4687
H	4.8053	0.6488	2.5261	H	5.5135	1.8234	-0.138
H	3.8864	-0.7808	-2.7938	H	2.195	-1.9205	-2.8844
H	5.3831	-1.5475	-3.2957	H	3.2814	-2.8986	-3.8558
H	5.9502	-2.146	-0.98	H	5.203	-2.3244	-2.4315
H	5.6464	-0.4208	-1.1264	H	4.4121	-0.8741	-3.0376
H	4.6325	-3.7261	-2.6203	H	3.6996	-4.4324	-2.0542
H	3.4251	-3.0202	-3.6772	H	1.9677	-4.2904	-2.2854
H	2.0206	-4.1374	1.0203	H	3.7429	-2.8493	2.2049
H	2.5842	-2.7619	1.8914	H	4.3518	-1.2789	1.8395
H	1.1048	-1.2497	0.7031	H	2.0519	-0.5079	1.2053
H	-0.4009	-1.8333	-1.0582	H	0.1009	-1.8942	1.4042
H	-0.0244	-3.5364	-0.9578	H	1.0441	-3.2762	1.9221
H	1.108	-2.6189	-2.8693	H	0.5044	-3.4786	-0.4455
H	1.7617	-1.29	-1.9542	H	1.1439	-1.8923	-0.7918
H	-1.4326	-4.1794	2.5044	H	1.2996	-1.2184	5.235
H	-0.3164	-4.7738	1.1684	H	0.8558	-2.5528	4.0511

H	1.6624	-5.0347	-1.008	H	2.6973	-4.6706	1.4103
H	1.9677	-4.8965	-2.7389	H	1.8943	-5.4084	0.0238
H	3.2706	-5.3592	-1.6469	H	3.6526	-5.329	0.0876
H	-4.9962	-3.9373	-0.7652	H	-7.1198	-3.3244	0.6555
H	-6.2784	-3.8512	0.4429	H	-8.2656	-2.2429	-0.1384
H	-5.1511	-2.0792	-2.6761	H	-4.9657	-3.9063	-0.7965
H	-6.6814	-1.25	-2.9021	H	-5.0344	-3.6339	-2.5287
H	-4.6321	0.87	1.1846	H	-4.3645	0.9338	-0.5733
H	-3.3516	-0.271	1.5355	H	-4.7075	0.673	1.1148
H	-2.2566	0.14	-0.6104	H	-2.8657	-0.9409	1.3373
H	-4.4164	2.264	-1.0785	H	-2.1785	-0.2389	-1.5689
H	-3.0378	1.9485	-2.119	H	-1.2352	-1.249	-0.4935
H	-5.0438	0.837	-2.9923	H	-2.6445	-2.6081	-1.9994
H	-3.7568	-0.2931	-2.6074	H	-3.0038	-2.8817	-0.3024
H	-2.5946	1.8217	2.6068	H	-1.6246	0.65	3.0329
H	-7.2257	0.7877	-1.7545	H	-4.3563	-1.5759	-3.5371
H	-7.38	-0.0874	-0.2258	H	-5.7772	-0.7525	-2.8811
H	-6.3712	1.3491	-0.3196	H	-4.1754	-0.0674	-2.6469
H	-3.9845	-1.9135	2.4492	H	-6.5283	0.3531	1.7794
H	4.74	-3.7163	0.9928	H	5.8033	-2.6571	0.2875
H	-7.5562	-2.2904	-0.808	H	-7.2038	-2.4234	-2.2503
H	-7.0144	-3.5022	-1.9579	H	-7.2781	-4.0556	-1.6059
5b-7	X axis(Å)	Y axis(Å)	Z axis(Å)	5b-8	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-2.2048	4.8885	-1.0261	C	-0.3451	5.6356	-0.9607
C	-2.1877	4.3865	0.4169	C	-0.7078	5.018	0.3893
C	-1.3087	3.1386	0.6001	C	-0.2773	3.5469	0.5103
C	0.1315	3.365	0.0522	C	1.2276	3.3594	0.1625
C	0.0895	3.7984	-1.4625	C	1.5495	3.9204	-1.2728
C	-0.7992	5.0648	-1.6064	C	1.1214	5.4116	-1.3408
C	1.094	2.1643	0.2469	C	1.721	1.9022	0.2918
C	2.5161	2.4898	-0.2634	C	3.2271	1.7634	-0.0189
C	2.51	2.9982	-1.715	C	3.6116	2.3998	-1.3644
C	1.528	4.1504	-1.927	C	3.0807	3.827	-1.5149
C	-0.4566	2.7069	-2.422	C	0.8465	3.1589	-2.4288
C	-1.2969	2.7457	2.0594	C	-0.6101	3.0438	1.8958
O	-0.7749	3.3783	2.9675	O	-0.0649	3.3752	2.9389
O	0.7185	4.4759	0.7825	O	2.0073	4.146	1.0991
C	3.4832	1.3371	-0.1534	C	3.6789	0.3245	0.0058
O	3.0565	0.0816	-0.5897	O	2.9141	-0.5929	-0.7144
C	4.7428	1.4444	0.2657	C	4.7481	-0.1381	0.65
C	3.5198	-1.5651	-2.9942	C	3.1046	-2.2866	-3.1171
C	4.5806	-0.7709	-2.2409	C	4.22	-2.0485	-2.1055
C	4.2517	-0.7241	-0.7421	C	3.6394	-1.8444	-0.7008
C	4.1662	-2.1659	-0.1301	C	2.7872	-3.0808	-0.2431
C	3.1766	-3.0984	-0.9247	C	1.6724	-3.4556	-1.2914
C	3.4145	-2.9878	-2.4588	C	2.2577	-3.4944	-2.7331
C	3.8286	-2.1831	1.3824	C	2.1683	-2.9172	1.1675

C	2.3564	-1.8932	1.7341	C	0.9523	-1.979	1.244
C	1.4184	-2.8008	0.9228	C	-0.1069	-2.3389	0.1895
C	1.708	-2.7478	-0.5799	C	0.4902	-2.4541	-1.2167
C	2.0432	-1.9944	3.2212	C	0.4346	-1.9291	2.6721
C	0.8088	-1.3072	3.7017	C	1.1023	-0.9632	3.5952
C	2.7735	-2.607	4.1681	C	-0.5529	-2.6734	3.1955
C	3.4047	-4.6012	-0.5821	C	1.108	-4.8849	-1.0367
C	5.2752	0.1229	-0.0167	C	4.7538	-1.5427	0.2778
O	6.4059	-0.2219	0.2982	O	5.5633	-2.349	0.7159
C	-6.833	-2.9936	-0.5051	C	-5.6795	-3.0472	-0.5496
C	-6.2039	-1.7057	-0.025	C	-4.7168	-2.1581	0.2001
C	-4.9761	-1.2774	-0.4105	C	-4.6592	-0.8112	0.0559
C	-4.1037	-2.1131	-1.3741	C	-5.6126	-0.0702	-0.9039
C	-4.6383	-3.5617	-1.5468	C	-6.3366	-1.0394	-1.8799
C	-4.3254	0.0296	0.0313	C	-3.6866	0.101	0.7936
C	-2.9109	-0.1835	0.5964	C	-2.91	1.0389	-0.1532
C	-2.0269	-0.9078	-0.4258	C	-3.893	1.8604	-0.9989
C	-2.6536	-2.2383	-0.8319	C	-4.8323	0.9441	-1.7804
C	-2.2838	1.1215	1.0085	C	-1.9201	1.9472	0.5424
C	-1.9722	1.4749	2.2535	C	-1.6884	2.0685	1.8481
O	-1.9586	2.0056	-0.0137	O	-1.1335	2.7202	-0.3105
C	-4.0865	-1.4261	-2.7606	C	-6.6793	0.6765	-0.0681
C	-7.0916	-0.94	0.9063	C	-3.8485	-2.9098	1.156
O	-8.1532	-1.3889	1.3262	O	-3.7212	-4.1285	1.1259
O	5.4759	-2.7783	-0.2566	O	3.6714	-4.2274	-0.1689
C	-6.1472	-3.6037	-1.7204	C	-6.8409	-2.294	-1.1853
O	0.0488	-0.7064	2.952	O	2.0263	-0.2415	3.2401
H	0.6098	-1.3703	4.785	H	0.7166	-0.9354	4.6283
H	-2.7863	4.1987	-1.6475	H	-1.003	5.23	-1.7372
H	-2.7332	5.8486	-1.0666	H	-0.5469	6.713	-0.9286
H	-1.836	5.1955	1.07	H	-0.241	5.612	1.1857
H	-3.2209	4.1717	0.7188	H	-1.7926	5.1104	0.5293
H	-0.3222	5.916	-1.103	H	1.749	6.0131	-0.6702
H	-0.883	5.3489	-2.6632	H	1.2929	5.8083	-2.3496
H	1.1766	1.9219	1.3143	H	1.5661	1.5537	1.3197
H	0.6995	1.2686	-0.2456	H	1.1286	1.2421	-0.3515
H	2.9081	3.3046	0.3624	H	3.7765	2.3035	0.7653
H	3.5151	3.3433	-1.9912	H	4.705	2.4207	-1.4623
H	2.2756	2.1785	-2.4056	H	3.2509	1.7832	-2.1971
H	1.528	4.4289	-2.9887	H	3.3303	4.1965	-2.5178
H	1.8984	5.0322	-1.3884	H	3.6189	4.4792	-0.815
H	0.0529	1.747	-2.3038	H	1.0213	2.0804	-2.3934
H	-1.5249	2.5192	-2.2987	H	-0.2351	3.3058	-2.4472
H	-0.323	3.0142	-3.4665	H	1.2167	3.5117	-3.3992
H	0.6178	4.3015	1.7424	H	1.7704	3.869	2.0094
H	5.2954	2.2905	0.6264	H	5.4675	0.3627	1.2684
H	2.5482	-1.0624	-2.9287	H	2.4738	-1.3947	-3.2056

H	3.7805	-1.5979	-4.0585	H	3.5443	-2.4537	-4.1074
H	5.5705	-1.2133	-2.408	H	4.9223	-2.8912	-2.1169
H	4.6163	0.2414	-2.6636	H	4.7879	-1.1638	-2.4212
H	4.3472	-3.5064	-2.7202	H	2.8881	-4.3871	-2.8456
H	2.6169	-3.513	-3.0001	H	1.4459	-3.6056	-3.4636
H	4.1148	-3.1678	1.7748	H	1.8821	-3.9092	1.5453
H	4.4804	-1.484	1.9218	H	2.9413	-2.5895	1.8744
H	2.1548	-0.8549	1.4494	H	1.2714	-0.9639	0.9951
H	0.3743	-2.5121	1.0842	H	-0.8889	-1.5699	0.1795
H	1.4912	-3.8347	1.2816	H	-0.6106	-3.2786	0.4388
H	1.0281	-3.4432	-1.0893	H	-0.3056	-2.7641	-1.9067
H	1.4436	-1.7541	-0.9554	H	0.7944	-1.4586	-1.5543
H	2.4823	-2.6192	5.215	H	-0.861	-2.5901	4.234
H	3.6958	-3.1306	3.9383	H	-1.0695	-3.4298	2.6115
H	3.3238	-4.8106	0.4876	H	0.7144	-5.0116	-0.0248
H	2.6681	-5.2317	-1.0944	H	0.2926	-5.11	-1.7345
H	4.3952	-4.9445	-0.9015	H	1.8737	-5.6553	-1.1817
H	-6.8122	-3.7159	0.3212	H	-5.1213	-3.5794	-1.3306
H	-7.8868	-2.8325	-0.7639	H	-6.0995	-3.8082	0.1196
H	-4.3797	-4.1683	-0.668	H	-5.653	-1.3476	-2.6831
H	-4.1563	-4.0478	-2.4044	H	-7.1748	-0.5305	-2.3725
H	-4.9089	0.5536	0.7908	H	-4.2536	0.687	1.5283
H	-4.2932	0.7088	-0.8306	H	-2.9491	-0.4656	1.3657
H	-2.9943	-0.8251	1.4858	H	-2.323	0.4056	-0.8349
H	-1.8636	-0.2879	-1.3156	H	-4.4682	2.545	-0.3637
H	-1.0354	-1.0896	0.002	H	-3.3491	2.489	-1.7154
H	-2.012	-2.7212	-1.5802	H	-5.5345	1.5612	-2.3558
H	-2.6438	-2.8952	0.049	H	-4.2268	0.4015	-2.5197
H	-2.0864	0.9486	3.1814	H	-2.1271	1.5874	2.7004
H	-3.5095	-2.0151	-3.4829	H	-7.4025	1.1833	-0.7174
H	-5.0974	-1.3045	-3.165	H	-7.2388	-0.0076	0.5794
H	-3.637	-0.4287	-2.7297	H	-6.2418	1.4407	0.5821
H	-6.7585	0.0599	1.2096	H	-3.3226	-2.3189	1.9158
H	6.1395	-2.1816	0.151	H	4.4328	-3.9957	0.4044
H	-6.4451	-3.0681	-2.6289	H	-7.5854	-2.0379	-0.4229
H	-6.4805	-4.6403	-1.847	H	-7.3468	-2.944	-1.9086
5c-1	X axis(Å)	Y axis(Å)	Z axis(Å)	5c-2	X axis(Å)	Y axis(Å)	Z axis(Å)
C	3.6721	-4.0411	1.8877	C	2.8629	4.5897	-2.0992
C	3.9862	-3.7364	0.4224	C	3.3873	4.3448	-0.6846
C	2.9621	-2.7907	-0.2216	C	2.6478	3.211	0.0411
C	1.5049	-3.3053	-0.0259	C	1.1033	3.4141	0.0073
C	1.1809	-3.509	1.501	C	0.5859	3.5649	-1.4712
C	2.2229	-4.4876	2.1084	C	1.3394	4.7398	-2.1515
C	0.4335	-2.4116	-0.6876	C	0.3133	2.307	0.7393
C	-0.9973	-2.967	-0.5013	C	-1.2125	2.5497	0.714
C	-1.3168	-3.2785	0.9673	C	-1.7443	2.8256	-0.6999
C	-0.2353	-4.133	1.6341	C	-0.9324	3.8927	-1.4383

C	1.1929	-2.2015	2.3391	C	0.7723	2.295	-2.3457
C	3.2923	-2.5959	-1.6833	C	3.1662	3.0969	1.4564
O	3.2204	-3.4481	-2.5576	O	3.0077	3.9173	2.3497
O	1.3956	-4.6086	-0.6531	O	0.793	4.6582	0.6848
C	-2.0318	-2.0425	-1.0978	C	-1.9277	1.3861	1.3565
O	-1.8021	-0.6696	-0.9931	O	-1.779	0.1391	0.7474
C	-3.1396	-2.4314	-1.7264	C	-2.6759	1.4463	2.456
C	-1.1546	1.5943	-2.8002	C	-0.5092	-2.468	1.2687
C	-2.1411	0.4702	-3.0873	C	-1.2441	-1.6155	2.2958
C	-2.8135	-0.0137	-1.794	C	-2.3857	-0.8342	1.6308
C	-3.557	1.1542	-1.054	C	-3.4107	-1.7979	0.9323
C	-2.6176	2.3962	-0.8142	C	-2.7059	-2.784	-0.074
C	-1.8419	2.7657	-2.1109	C	-1.4541	-3.4412	0.5763
C	-4.2229	0.7196	0.2764	C	-4.58	-1.0606	0.2327
C	-3.2526	0.4927	1.4516	C	-4.2126	-0.363	-1.0891
C	-2.3189	1.7011	1.6402	C	-3.4886	-1.3292	-2.0431
C	-1.6236	2.1148	0.3408	C	-2.3083	-2.0415	-1.3756
C	-4.0167	0.0821	2.7012	C	-5.4326	0.324	-1.6827
C	-4.5474	-1.3141	2.736	C	-5.8644	1.5998	-1.0353
C	-4.2388	0.8247	3.7981	C	-6.1493	-0.0716	-2.7474
C	-3.4364	3.6693	-0.4477	C	-3.6387	-3.9697	-0.4603
C	-3.7373	-1.1666	-2.121	C	-3.0544	0.0569	2.6552
O	-4.834	-1.0793	-2.6562	O	-3.8051	-0.3133	3.5477
C	2.0341	4.8456	1.9942	C	2.783	-4.5962	-1.7945
C	1.9786	3.3793	1.63	C	2.4989	-3.1563	-1.4317
C	2.4393	2.8777	0.4571	C	3.1206	-2.4981	-0.4215
C	3.1188	3.7834	-0.5902	C	4.2075	-3.1833	0.4318
C	3.4852	5.1773	-0.0104	C	4.7147	-4.5016	-0.2143
C	2.3354	1.4212	0.0275	C	2.8246	-1.0657	-0.0014
C	3.6898	0.8244	-0.4046	C	4.0864	-0.1868	0.1025
C	4.3099	1.6808	-1.5182	C	5.1088	-0.8364	1.0444
C	4.445	3.1382	-1.0766	C	5.4435	-2.2552	0.5841
C	3.5133	-0.6334	-0.7649	C	3.6815	1.2165	0.4901
C	3.6626	-1.2151	-1.9534	C	3.8469	1.8281	1.6613
O	3.1403	-1.4542	0.2976	O	3.036	1.935	-0.5149
C	2.1616	3.9856	-1.7886	C	3.6225	-3.5107	1.8266
C	1.3431	2.5406	2.6963	C	1.4388	-2.5411	-2.2936
O	0.8819	3.0179	3.7281	O	0.9111	-3.1414	-3.2243
O	-4.6247	1.6195	-1.9161	O	-4.0083	-2.629	1.9589
C	2.3606	5.7662	0.8252	C	3.5768	-5.3597	-0.7423
O	-4.3904	-2.1065	1.8147	O	-5.2874	2.0813	-0.0672
H	-5.0959	-1.6003	3.6494	H	-6.7442	2.0941	-1.4808
H	4.3479	-4.8282	2.2434	H	3.3267	5.4982	-2.5017
H	3.8915	-3.1588	2.4991	H	3.1847	3.7732	-2.755
H	4.9922	-3.301	0.3684	H	4.4596	4.1195	-0.7483
H	4.027	-4.6817	-0.1339	H	3.2996	5.2767	-0.1111
H	2.0465	-4.6061	3.1852	H	1.0262	4.8329	-3.1993

H	2.0982	-5.4868	1.6713	H	1.0676	5.6885	-1.6706
H	0.5045	-1.39	-0.2979	H	0.5513	1.3247	0.3157
H	0.6186	-2.3459	-1.7679	H	0.6198	2.27	1.7931
H	-1.0511	-3.9172	-1.0522	H	-1.414	3.4476	1.3153
H	-1.4525	-2.3514	1.5348	H	-1.753	1.9056	-1.2952
H	-2.2724	-3.8144	1.0309	H	-2.7885	3.1563	-0.6414
H	-0.2542	-5.1365	1.19	H	-1.1047	4.8642	-0.9577
H	-0.492	-4.2707	2.6923	H	-1.3213	3.9924	-2.4599
H	0.5623	-1.4178	1.9109	H	0.3525	1.397	-1.8848
H	0.8204	-2.3942	3.3528	H	0.2726	2.4216	-3.3139
H	2.1908	-1.7763	2.4617	H	1.8177	2.0765	-2.5716
H	1.7289	-4.5451	-1.5726	H	1.2328	4.6609	1.5607
H	-3.5346	-3.4111	-1.9132	H	-2.9453	2.2771	3.0789
H	-0.7117	1.938	-3.7423	H	0.2895	-3.0293	1.767
H	-0.3267	1.2234	-2.1873	H	-0.0238	-1.8267	0.5263
H	-2.8938	0.8107	-3.8094	H	-1.6267	-2.25	3.1049
H	-1.5945	-0.3504	-3.5697	H	-0.5201	-0.9283	2.7525
H	-2.5355	3.215	-2.8349	H	-1.7762	-4.1781	1.3248
H	-1.0944	3.5382	-1.892	H	-0.8918	-4.0051	-0.1793
H	-4.9668	1.475	0.5669	H	-5.3939	-1.7757	0.0471
H	-4.8283	-0.1779	0.1	H	-5.0276	-0.3446	0.9329
H	-2.598	-0.3496	1.2146	H	-3.4974	0.435	-0.8796
H	-1.5541	1.459	2.3888	H	-3.1185	-0.7757	-2.9156
H	-2.8692	2.5623	2.0347	H	-4.1805	-2.084	-2.4326
H	-1.0227	3.0118	0.5386	H	-1.8823	-2.7535	-2.0944
H	-0.9046	1.3381	0.064	H	-1.516	-1.3105	-1.1879
H	-4.7847	0.4477	4.6585	H	-7.0046	0.4877	-3.1161
H	-3.8845	1.847	3.8827	H	-5.9136	-0.9792	-3.2935
H	-4.0771	3.525	0.4261	H	-4.5895	-3.6406	-0.8871
H	-2.7679	4.5099	-0.2264	H	-3.1556	-4.6173	-1.2018
H	-4.0848	3.9856	-1.2724	H	-3.8759	-4.5978	0.4058
H	1.0763	5.1726	2.417	H	1.846	-5.1409	-1.9641
H	2.7923	4.9764	2.7771	H	3.3374	-4.6085	-2.7418
H	4.3786	5.1013	0.6247	H	5.3903	-4.2777	-1.0514
H	3.7448	5.8721	-0.819	H	5.3053	-5.0791	0.508
H	1.9096	0.7892	0.8079	H	2.3138	-1.0898	0.9703
H	1.6231	1.3559	-0.8044	H	2.1251	-0.5737	-0.6792
H	4.3722	0.859	0.4572	H	4.5498	-0.1258	-0.8929
H	5.3047	1.2961	-1.776	H	6.0306	-0.2414	1.0624
H	3.7077	1.6278	-2.433	H	4.7343	-0.8627	2.0743
H	5.1892	3.1739	-0.2689	H	5.9677	-2.1795	-0.3787
H	4.8648	3.7234	-1.905	H	6.1599	-2.6977	1.2882
H	3.9313	-0.8167	-2.9128	H	4.2896	1.4976	2.581
H	2.603	4.6577	-2.5335	H	2.7362	-4.1505	1.7547
H	1.9268	3.049	-2.3034	H	4.359	-4.0339	2.4473
H	1.2077	4.4218	-1.4741	H	3.3193	-2.6143	2.3764
H	1.3012	1.458	2.5275	H	1.1363	-1.5126	-2.0637

H	-5.184	0.8504	-2.1577	H	-4.3887	-2.0431	2.6475
H	1.4669	5.9244	0.211	H	2.9158	-5.668	0.0757
H	2.6538	6.7514	1.2061	H	3.9761	-6.281	-1.1822
5c-3	X axis(Å)	Y axis(Å)	Z axis(Å)	5c-4	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-3.0944	4.7622	1.2093	C	5.22	-1.7698	1.7013
C	-2.9949	4.4616	-0.2871	C	5.2636	-1.4369	0.2092
C	-2.0188	3.3172	-0.6033	C	3.8763	-1.1309	-0.3732
C	-0.6233	3.5672	0.0403	C	2.8577	-2.265	-0.0517
C	-0.7531	3.7564	1.5971	C	2.7586	-2.507	1.5
C	-1.727	4.9326	1.8811	C	4.1746	-2.8359	2.0473
C	0.4327	2.487	-0.2934	C	1.4531	-2.0341	-0.6524
C	1.8129	2.8169	0.324	C	0.4863	-3.1994	-0.3452
C	1.7064	3.0518	1.839	C	0.4289	-3.5272	1.1531
C	0.6431	4.1005	2.1842	C	1.8211	-3.7178	1.7622
C	-1.2737	2.5031	2.3461	C	2.1952	-1.3016	2.2993
C	-1.9174	3.1324	-2.099	C	3.984	-0.8901	-1.8607
O	-1.4036	3.9133	-2.8882	O	4.2877	-1.7222	-2.7045
O	-0.1018	4.8166	-0.4872	O	3.3514	-3.4989	-0.6362
C	2.8767	1.7948	-0.0094	C	-0.898	-2.9476	-0.8938
O	2.4733	0.5987	-0.6049	O	-1.3461	-1.6265	-0.9419
C	4.1825	1.9611	0.1964	C	-1.7234	-3.8905	-1.344
C	2.7209	-0.6926	-3.2793	C	-2.0107	0.3913	-3.0471
C	3.807	0.0843	-2.5471	C	-2.335	-1.096	-3.078
C	3.6764	-0.0876	-1.0268	C	-2.5999	-1.6343	-1.6645
C	3.7387	-1.5971	-0.6033	C	-3.7564	-0.8545	-0.9442
C	2.7075	-2.4806	-1.402	C	-3.5401	0.707	-0.9807
C	2.7729	-2.1736	-2.9256	C	-3.1445	1.1817	-2.4077
C	3.5714	-1.8279	0.9222	C	-4.0112	-1.3249	0.5137
C	2.1345	-1.6662	1.4578	C	-2.9701	-0.8523	1.5513
C	1.1329	-2.4838	0.6277	C	-2.7505	0.6653	1.4621
C	1.2715	-2.2473	-0.8759	C	-2.4551	1.1312	0.0373
C	1.9662	-1.9969	2.9339	C	-3.2741	-1.2509	2.9879
C	0.8119	-1.3589	3.6348	C	-2.1218	-1.2657	3.9404
C	2.7513	-2.7848	3.6864	C	-4.4623	-1.6187	3.4949
C	3.0286	-3.9986	-1.2717	C	-4.85	1.476	-0.6376
C	4.7449	0.7357	-0.3432	C	-2.8836	-3.1183	-1.7532
O	5.9273	0.4403	-0.2375	O	-3.9349	-3.6327	-2.1089
C	-3.5338	-4.3229	1.4684	C	-0.4695	5.2418	1.7822
C	-3.0472	-2.9141	1.2134	C	0.1781	3.9099	1.4749
C	-3.0291	-2.3344	-0.0129	C	0.7034	3.5926	0.265
C	-3.5795	-3.0687	-1.252	C	0.7165	4.6101	-0.894
C	-4.4124	-4.3226	-0.8684	C	0.3785	6.0502	-0.4195
C	-2.461	-0.9542	-0.3212	C	1.3138	2.2455	-0.0973
C	-3.4465	-0.0542	-1.0932	C	2.7277	2.3632	-0.7047
C	-3.9252	-0.7628	-2.3696	C	2.7066	3.3104	-1.9134
C	-4.5254	-2.1309	-2.0487	C	2.1289	4.6729	-1.5344
C	-2.8258	1.3032	-1.3412	C	3.2718	0.9854	-1.0124

C	-2.4819	1.8544	-2.5038	C	3.6096	0.4752	-2.1953
O	-2.5987	2.0595	-0.1936	O	3.4243	0.1573	0.0975
C	-2.402	-3.5168	-2.1497	C	-0.3259	4.1864	-1.9559
C	-2.5754	-2.2314	2.4624	C	0.1576	2.9779	2.6497
O	-2.47	-2.822	3.5338	O	-0.2816	3.3154	3.7449
O	5.0513	-2.1049	-0.9513	O	-4.9833	-1.1002	-1.6764
C	-3.7347	-5.1541	0.2078	C	-0.791	6.0765	0.5497
O	0.0757	-0.5504	3.0814	O	-0.9731	-1.0139	3.5964
H	0.6597	-1.6499	4.6879	H	-2.3617	-1.5262	4.9852
H	-3.6808	5.6776	1.3532	H	6.2089	-2.1209	2.0197
H	-3.6597	3.9646	1.7039	H	5.0284	-0.8554	2.2735
H	-3.9992	4.2182	-0.6571	H	5.9333	-0.5792	0.0663
H	-2.6856	5.3754	-0.8108	H	5.7194	-2.2792	-0.327
H	-1.8733	5.0486	2.9627	H	4.1386	-2.9592	3.1373
H	-1.2865	5.8763	1.5343	H	4.5169	-3.799	1.6467
H	0.0917	1.4985	0.035	H	1.0398	-1.0851	-0.293
H	0.5666	2.4274	-1.3815	H	1.5242	-1.9498	-1.7447
H	2.1514	3.76	-0.1294	H	0.8785	-4.0904	-0.8568
H	1.4881	2.1083	2.354	H	-0.1066	-2.74	1.6934
H	2.6694	3.3975	2.2358	H	-0.1502	-4.4462	1.3107
H	0.9801	5.0772	1.8135	H	2.2617	-4.6362	1.3535
H	0.5826	4.2011	3.2754	H	1.7174	-3.8915	2.841
H	-0.7282	1.6015	2.0655	H	1.2507	-0.9313	1.8929
H	-1.1646	2.6267	3.4303	H	2.008	-1.5873	3.3417
H	-2.3324	2.3013	2.1721	H	2.8791	-0.4517	2.3398
H	-0.1421	4.7813	-1.466	H	3.5778	-3.3331	-1.5752
H	4.7281	2.7765	0.6309	H	-1.6118	-4.9563	-1.3972
H	2.858	-0.5744	-4.3606	H	-1.8538	0.749	-4.0715
H	1.7335	-0.2787	-3.0461	H	-1.071	0.5659	-2.5116
H	4.7957	-0.2475	-2.8886	H	-3.2035	-1.2726	-3.7251
H	3.7194	1.1421	-2.8266	H	-1.4893	-1.6214	-3.5402
H	3.7045	-2.5823	-3.3403	H	-4.017	1.1096	-3.0715
H	1.9578	-2.6915	-3.4476	H	-2.8699	2.2438	-2.3871
H	3.9432	-2.835	1.15	H	-5.0102	-0.9776	0.8075
H	4.2469	-1.1648	1.4781	H	-4.0899	-2.4194	0.5441
H	1.8763	-0.6082	1.3504	H	-2.0259	-1.3416	1.2985
H	0.1084	-2.2285	0.9212	H	-1.9095	0.9627	2.0989
H	1.2446	-3.5531	0.846	H	-3.6235	1.1987	1.8574
H	0.5724	-2.913	-1.3975	H	-2.3545	2.2241	0.0425
H	0.9304	-1.2328	-1.1031	H	-1.4741	0.7466	-0.2556
H	2.5586	-2.9616	4.7413	H	-4.5901	-1.899	4.537
H	3.616	-3.2968	3.2776	H	-5.3629	-1.6475	2.8906
H	3.0557	-4.3392	-0.2334	H	-5.2676	1.1911	0.3316
H	2.2734	-4.6006	-1.7911	H	-4.6687	2.5571	-0.6088
H	3.9978	-4.2477	-1.7182	H	-5.63	1.3033	-1.3876
H	-2.8288	-4.8626	2.1124	H	-1.4051	5.0944	2.3356
H	-4.485	-4.2633	2.0132	H	0.2049	5.8098	2.436

H	-5.4016	-4.022	-0.4962	H	1.2474	6.4983	0.0821
H	-4.5963	-4.9455	-1.7528	H	0.158	6.6951	-1.2795
H	-2.1363	-0.4293	0.5791	H	1.362	1.5744	0.7616
H	-1.5472	-1.0835	-0.9145	H	0.6497	1.7447	-0.8132
H	-4.3294	0.1103	-0.4584	H	3.3905	2.8065	0.0525
H	-4.6866	-0.1527	-2.8721	H	3.7258	3.4537	-2.2941
H	-3.101	-0.8821	-3.0828	H	2.1236	2.8799	-2.7364
H	-5.4483	-1.965	-1.4757	H	2.8296	5.1495	-0.8348
H	-4.8301	-2.6141	-2.986	H	2.1075	5.3108	-2.4275
H	-2.5459	1.491	-3.5112	H	3.5833	0.891	-3.184
H	-2.7634	-4.0808	-3.0173	H	-0.3615	4.9081	-2.7801
H	-1.8226	-2.6731	-2.5369	H	-0.1057	3.2092	-2.3965
H	-1.7004	-4.159	-1.6064	H	-1.3327	4.1217	-1.5299
H	-2.3385	-1.1629	2.3896	H	0.5549	1.9661	2.5003
H	5.729	-1.5174	-0.5541	H	-5.1045	-2.0689	-1.7712
H	-2.7706	-5.5336	-0.1492	H	-1.7001	5.6999	0.0671
H	-4.3462	-6.0331	0.4424	H	-1.0039	7.1086	0.8516
5c-5	X axis(Å)	Y axis(Å)	Z axis(Å)	5c-6	X axis(Å)	Y axis(Å)	Z axis(Å)
C	2.3119	4.3822	-1.8708	C	0.7583	5.6821	0.0382
C	2.6198	4.3028	-0.3758	C	0.9023	4.7657	1.2524
C	1.8558	3.1745	0.3338	C	0.3852	3.3406	0.9941
C	0.3269	3.2445	0.046	C	-1.062	3.348	0.4215
C	0.0404	3.2276	-1.5009	C	-1.1595	4.2301	-0.8747
C	0.8094	4.3998	-2.1687	C	-0.6541	5.6626	-0.5526
C	-0.4883	2.1405	0.7525	C	-1.6305	1.9385	0.1523
C	-2.0042	2.2541	0.4769	C	-3.0964	1.9709	-0.3413
C	-2.3269	2.3671	-1.0206	C	-3.2717	2.9281	-1.5376
C	-1.4833	3.4305	-1.7285	C	-2.648	4.3079	-1.3084
C	0.4499	1.909	-2.2117	C	-0.3441	3.6886	-2.0785
C	2.1477	3.2244	1.8175	C	0.4774	2.5431	2.2744
O	1.7804	4.0943	2.5948	O	-0.2237	2.6822	3.267
O	-0.1723	4.5109	0.5464	O	-1.9308	3.9673	1.4061
C	-2.7217	1.0893	1.1128	C	-3.6276	0.5727	-0.6039
O	-2.4167	-0.18	0.6207	O	-3.3031	-0.3965	0.3512
C	-3.6031	1.1663	2.1075	C	-4.3707	0.1712	-1.6347
C	-1.0388	-2.6361	1.479	C	-4.5797	-2.0688	2.4238
C	-1.9528	-1.7793	2.3473	C	-5.1585	-1.752	1.0496
C	-3.057	-1.135	1.4981	C	-4.0381	-1.5963	0.0143
C	-3.9197	-2.2173	0.7566	C	-3.1573	-2.8933	-0.0845
C	-3.0298	-3.2073	-0.0858	C	-2.6044	-3.3445	1.3201
C	-1.8238	-3.7215	0.7531	C	-3.7352	-3.3372	2.3894
C	-5.0426	-1.6182	-0.1274	C	-2.0001	-2.7812	-1.1094
C	-4.5652	-0.9802	-1.4442	C	-0.802	-1.9346	-0.6505
C	-3.6658	-1.9471	-2.2341	C	-0.302	-2.3626	0.7387
C	-2.5287	-2.5212	-1.383	C	-1.4348	-2.4301	1.7676
C	-5.7483	-0.4286	-2.2242	C	0.2674	-1.9215	-1.7294
C	-6.3348	0.8549	-1.7316	C	0.1305	-0.8947	-2.8045

C	-6.3076	-0.9504	-3.328	C	1.3246	-2.7441	-1.8214
C	-3.8235	-4.4846	-0.4912	C	-2.0811	-4.8112	1.2828
C	-3.9067	-0.232	2.3658	C	-4.6276	-1.2249	-1.3264
O	-4.7352	-0.5994	3.1877	O	-5.2382	-1.9744	-2.0767
C	7.0967	-3.1513	-0.5867	C	5.7218	-3.2377	-0.5173
C	6.5458	-1.7619	-0.3603	C	4.6764	-2.452	0.2379
C	5.2212	-1.4722	-0.3313	C	4.6603	-1.0991	0.3214
C	4.1567	-2.5774	-0.5098	C	5.7498	-0.2441	-0.3569
C	4.7609	-4.0041	-0.3904	C	6.5884	-1.0612	-1.3791
C	4.6339	-0.0785	-0.1401	C	3.6081	-0.289	1.0673
C	3.58	-0.0297	0.9809	C	2.9874	0.8333	0.2087
C	2.4762	-1.0664	0.7429	C	4.0935	1.7422	-0.3454
C	3.0666	-2.4652	0.5896	C	5.1139	0.9323	-1.1422
C	2.9744	1.3431	1.1161	C	1.9359	1.6534	0.924
C	2.897	2.0521	2.2396	C	1.5176	1.532	2.1826
O	2.4187	1.8948	-0.0337	O	1.3127	2.6284	0.144
C	3.5077	-2.4332	-1.9071	C	6.7001	0.3084	0.7318
C	7.6207	-0.7324	-0.1976	C	3.669	-3.3243	0.9158
O	8.8087	-1.0251	-0.1117	O	3.5126	-4.5034	0.6183
O	-4.5799	-3.0256	1.7625	O	-4.006	-3.9742	-0.5468
C	6.0765	-4.1385	-1.1382	C	6.9719	-2.4337	-0.8501
O	-5.9075	1.4443	-0.7459	O	-0.8027	-0.1021	-2.8502
H	-7.1866	1.2506	-2.3104	H	0.9239	-0.8895	-3.5711
H	2.77	5.2889	-2.2839	H	1.0106	6.7083	0.331
H	2.7898	3.5427	-2.3877	H	1.4919	5.3982	-0.7243
H	3.7018	4.1648	-0.2534	H	1.961	4.7407	1.5411
H	2.376	5.2686	0.0855	H	0.3614	5.2131	2.0963
H	0.6612	4.3779	-3.2559	H	-0.6706	6.2819	-1.4585
H	0.3996	5.3597	-1.8282	H	-1.3343	6.1504	0.1578
H	-0.1187	1.1495	0.4647	H	-1.0004	1.4031	-0.5645
H	-0.3486	2.2165	1.8391	H	-1.6042	1.3587	1.0838
H	-2.3602	3.1776	0.955	H	-3.7086	2.3691	0.4805
H	-2.1813	1.403	-1.521	H	-2.8414	2.483	-2.4432
H	-3.3876	2.6156	-1.1496	H	-4.3405	3.0675	-1.7454
H	-1.7949	4.4219	-1.3757	H	-3.2396	4.8389	-0.5515
H	-1.7125	3.4105	-2.8018	H	-2.7443	4.899	-2.2283
H	0.0236	1.0213	-1.7371	H	-0.5971	2.6565	-2.331
H	0.1037	1.9132	-3.2526	H	-0.5381	4.2924	-2.9735
H	1.5304	1.7588	-2.2531	H	0.7351	3.7209	-1.9173
H	0.1153	4.619	1.4772	H	-1.8151	3.5027	2.2616
H	-4.0003	2.0138	2.6317	H	-4.7408	0.6995	-2.4918
H	-0.2725	-3.1025	2.1091	H	-5.3995	-2.1999	3.1398
H	-0.5056	-2.0098	0.7554	H	-3.9822	-1.2259	2.789
H	-2.3861	-2.3884	3.1502	H	-5.859	-2.5406	0.748
H	-1.3406	-1.0092	2.8344	H	-5.7439	-0.8268	1.1275
H	-2.1834	-4.4314	1.5106	H	-4.4151	-4.1805	2.2056
H	-1.1361	-4.2879	0.1118	H	-3.3085	-3.5068	3.3864

H	-5.7763	-2.4045	-0.3549	H	-1.6513	-3.7927	-1.3619
H	-5.621	-0.8954	0.4611	H	-2.3863	-2.3993	-2.0632
H	-3.937	-0.1177	-1.2118	H	-1.1308	-0.9008	-0.5285
H	-3.2317	-1.4239	-3.0958	H	0.4519	-1.6482	1.0916
H	-4.2514	-2.7766	-2.6453	H	0.1993	-3.3352	0.6976
H	-1.9689	-3.2423	-1.9931	H	-1.0198	-2.7929	2.7172
H	-1.8175	-1.7206	-1.158	H	-1.7853	-1.4142	1.9741
H	-7.1483	-0.4826	-3.8331	H	2.0511	-2.6794	-2.6265
H	-5.9523	-1.8752	-3.7702	H	1.4894	-3.5465	-1.1083
H	-4.7361	-4.2584	-1.0486	H	-1.3129	-4.9683	0.5212
H	-3.2099	-5.1384	-1.1224	H	-1.6451	-5.0921	2.2489
H	-4.1198	-5.0728	0.3846	H	-2.8872	-5.5244	1.0771
H	7.941	-3.12	-1.2864	H	6.0321	-4.1169	0.0607
H	7.4848	-3.5281	0.3684	H	5.2707	-3.6076	-1.4471
H	4.9423	-4.2518	0.6646	H	6.0192	-1.2024	-2.3083
H	4.0496	-4.7532	-0.7604	H	7.4946	-0.5091	-1.6584
H	4.1937	0.2393	-1.0941	H	2.7896	-0.9184	1.4222
H	5.3938	0.6705	0.0919	H	4.0748	0.1352	1.9656
H	4.0833	-0.2832	1.9254	H	2.4823	0.3557	-0.6435
H	1.7775	-1.0665	1.5893	H	3.6655	2.5047	-1.0087
H	1.8832	-0.8113	-0.144	H	4.5887	2.2857	0.4684
H	3.4916	-2.7558	1.5604	H	4.6053	0.5454	-2.0363
H	2.2537	-3.1746	0.3873	H	5.8985	1.608	-1.5064
H	3.2269	1.8329	3.2369	H	1.8049	0.8646	2.9717
H	2.9812	-1.4814	-2.0297	H	7.5131	0.8914	0.2839
H	4.2537	-2.4876	-2.7074	H	6.1871	0.9659	1.4408
H	2.7745	-3.2289	-2.0828	H	7.155	-0.4967	1.3193
H	7.308	0.3181	-0.1575	H	3.0595	-2.8637	1.7045
H	-5.0767	-2.4277	2.3611	H	-4.4488	-3.6896	-1.3745
H	5.9287	-3.9675	-2.2106	H	7.6063	-2.3394	0.0387
H	6.4625	-5.1594	-1.0359	H	7.5641	-2.9712	-1.5998
5c-7	X axis(Å)	Y axis(Å)	Z axis(Å)	5c-8	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-2.2252	4.5119	1.6843	C	2.5945	4.6529	-0.0169
C	-2.4283	4.3673	0.1759	C	2.3013	3.8285	1.2376
C	-1.5948	3.2286	-0.4316	C	1.553	2.5228	0.9298
C	-0.0904	3.353	-0.0493	C	0.2739	2.7858	0.0825
C	0.0906	3.3966	1.5136	C	0.6203	3.5469	-1.2496
C	-0.7474	4.5733	2.0841	C	1.3567	4.8677	-0.8948
C	0.8001	2.2515	-0.6625	C	-0.5381	1.5111	-0.2227
C	2.2915	2.4168	-0.2877	C	-1.8175	1.8028	-1.0329
C	2.5023	2.5769	1.2243	C	-1.5485	2.6458	-2.2887
C	1.5896	3.6424	1.8368	C	-0.7032	3.8883	-1.9903
C	-0.3365	2.0945	2.2447	C	1.5108	2.7411	-2.2333
C	-1.7913	3.1998	-1.9312	C	1.2317	1.7995	2.2203
O	-1.3935	4.0403	-2.7257	O	0.4427	2.1685	3.0795
O	0.4059	4.6156	-0.5622	O	-0.5999	3.6594	0.8431
C	3.1245	1.2802	-0.8314	C	-2.5512	0.528	-1.3724

O	2.5441	0.0116	-0.8365	O	-3.8429	0.4183	-0.8612
C	4.3612	1.3882	-1.3138	C	-2.079	-0.506	-2.0671
C	1.5465	-1.9255	-2.8387	C	-6.6562	0.2067	-1.7648
C	2.8231	-1.1034	-2.9523	C	-5.454	-0.4696	-2.4116
C	3.4393	-0.8575	-1.5676	C	-4.394	-0.8216	-1.3603
C	3.7589	-2.2044	-0.8293	C	-4.9708	-1.7549	-0.2376
C	2.5019	-3.1534	-0.7613	C	-6.2757	-1.1574	0.4102
C	1.8073	-3.2588	-2.1497	C	-7.2705	-0.676	-0.6853
C	4.3604	-2.0079	0.5853	C	-3.9389	-2.1159	0.8635
C	3.3587	-1.5656	1.6686	C	-3.621	-0.9932	1.8709
C	2.1216	-2.4806	1.689	C	-4.9135	-0.3822	2.4446
C	1.4931	-2.6505	0.3033	C	-5.9219	0.0125	1.3631
C	4.0612	-1.4185	3.0099	C	-2.6435	-1.4919	2.9276
C	4.9196	-0.2084	3.1887	C	-1.2178	-1.6651	2.5176
C	3.9736	-2.2415	4.0677	C	-2.9122	-1.7689	4.2148
C	2.9076	-4.6109	-0.3919	C	-7.0514	-2.2324	1.2274
C	4.6595	0.0239	-1.7197	C	-3.1944	-1.4369	-2.0455
O	5.7537	-0.3306	-2.1366	O	-3.1343	-2.5632	-2.5196
C	-6.8526	-3.0832	0.4577	C	7.8726	-2.6788	-0.3108
C	-6.2921	-1.7054	0.1878	C	7.0063	-1.5816	0.2639
C	-4.9709	-1.4048	0.2468	C	5.7778	-1.2632	-0.2145
C	-3.919	-2.4856	0.5808	C	5.1546	-2.0366	-1.3975
C	-4.5043	-3.923	0.5046	C	5.9221	-3.3505	-1.7132
C	-4.3771	-0.0202	0.0139	C	4.8927	-0.1438	0.321
C	-3.2346	-0.0312	-1.0183	C	3.4687	-0.6249	0.6528
C	-2.1497	-1.0399	-0.624	C	2.8213	-1.3	-0.5621
C	-2.7445	-2.4319	-0.4323	C	3.6925	-2.4452	-1.0721
C	-2.6304	1.3384	-1.1896	C	2.6068	0.5084	1.1436
C	-2.4912	1.9922	-2.3404	C	1.9636	0.5467	2.3077
O	-2.1525	1.9544	-0.038	O	2.4515	1.5914	0.2851
C	-3.3855	-2.2468	2.0136	C	5.1794	-1.1376	-2.6567
C	-7.3554	-0.6993	-0.1264	C	7.66	-0.8641	1.4035
O	-8.5311	-1.0091	-0.2886	O	8.7148	-1.2405	1.904
O	4.7575	-2.9121	-1.6046	O	-5.3638	-3.0067	-0.8542
C	-5.8754	-4.0233	1.1512	C	7.4292	-3.1601	-1.6861
O	5.0699	0.6335	2.3114	O	-0.8083	-1.4306	1.3866
H	5.4191	-0.1102	4.1674	H	-0.532	-2.0234	3.3041
H	-2.7279	5.4237	2.0284	H	2.9963	5.6288	0.281
H	-2.7214	3.6828	2.2007	H	3.387	4.1664	-0.5962
H	-3.4963	4.1998	-0.0136	H	3.2538	3.6119	1.7382
H	-2.173	5.319	-0.3077	H	1.7166	4.4418	1.9351
H	-0.6748	4.5924	3.179	H	1.6563	5.3909	-1.8119
H	-0.3345	5.5299	1.7383	H	0.6739	5.5482	-0.3696
H	0.4326	1.264	-0.3616	H	0.0875	0.7723	-0.7354
H	0.7344	2.2862	-1.758	H	-0.8567	1.0532	0.721
H	2.646	3.3423	-0.7641	H	-2.4805	2.3966	-0.3873
H	2.3423	1.6221	1.7367	H	-1.0521	2.0438	-3.0593

H	3.5451	2.855	1.4233	H	-2.5028	2.9648	-2.7277
H	1.9032	4.6288	1.4717	H	-1.3037	4.5885	-1.3955
H	1.7456	3.6635	2.9231	H	-0.4876	4.4075	-2.933
H	0.1317	1.1999	1.8255	H	1.1102	1.747	-2.4486
H	-0.0511	2.1396	3.3029	H	1.5945	3.2678	-3.1918
H	-1.415	1.9254	2.2311	H	2.533	2.6025	-1.8758
H	0.1836	4.6771	-1.5148	H	-0.7474	3.2602	1.7259
H	5.0119	2.2369	-1.3963	H	-1.1233	-0.6699	-2.5256
H	1.1423	-2.1087	-3.8411	H	-7.41	0.4164	-2.5328
H	0.7822	-1.3603	-2.2958	H	-6.3667	1.176	-1.3437
H	3.5388	-1.6138	-3.6089	H	-5.7778	-1.3691	-2.9501
H	2.5754	-0.1519	-3.4404	H	-5.039	0.2131	-3.1644
H	2.4305	-3.8624	-2.8237	H	-7.7133	-1.549	-1.1842
H	0.857	-3.7998	-2.0528	H	-8.1071	-0.1381	-0.221
H	4.8402	-2.9448	0.9023	H	-4.3014	-2.9963	1.4132
H	5.1976	-1.3014	0.5267	H	-3.0167	-2.4755	0.3908
H	2.9823	-0.5706	1.4193	H	-3.1089	-0.1783	1.35
H	1.3676	-2.0642	2.3693	H	-4.6659	0.5075	3.0378
H	2.3746	-3.4704	2.0844	H	-5.4018	-1.0798	3.1338
H	0.6566	-3.3567	0.3865	H	-6.8325	0.3785	1.8557
H	1.0403	-1.7009	0.0024	H	-5.5293	0.8709	0.8104
H	4.5035	-2.0548	4.9978	H	-2.1516	-2.1085	4.9124
H	3.3729	-3.1446	4.0458	H	-3.9097	-1.6707	4.6301
H	3.4593	-4.6724	0.5497	H	-6.4403	-2.6976	2.0051
H	2.02	-5.247	-0.2918	H	-7.9246	-1.789	1.7208
H	3.5394	-5.0639	-1.1642	H	-7.4228	-3.0393	0.5857
H	-7.7507	-3.0162	1.0839	H	8.9129	-2.3413	-0.3959
H	-7.1605	-3.5236	-0.4994	H	7.8657	-3.5252	0.388
H	-4.5984	-4.2388	-0.5436	H	5.6639	-4.126	-0.9789
H	-3.8215	-4.64	0.9778	H	5.6192	-3.7452	-2.6913
H	-4.0184	0.363	0.978	H	5.3003	0.3199	1.2216
H	-5.1195	0.7041	-0.3274	H	4.8611	0.6565	-0.4297
H	-3.6569	-0.3491	-1.9828	H	3.5461	-1.3752	1.4533
H	-1.385	-1.0868	-1.4082	H	1.8352	-1.6969	-0.2887
H	-1.6325	-0.724	0.2902	H	2.6474	-0.5754	-1.3669
H	-3.0886	-2.7857	-1.4141	H	3.6926	-3.2312	-0.3041
H	-1.948	-3.1203	-0.1218	H	3.2189	-2.8851	-1.9593
H	-2.7584	1.7208	-3.3435	H	1.9138	-0.1664	3.107
H	-2.8771	-1.283	2.1176	H	4.7828	-1.6718	-3.5278
H	-4.1931	-2.26	2.7536	H	4.578	-0.2308	-2.5372
H	-2.6633	-3.0212	2.2972	H	6.1964	-0.8129	-2.9023
H	-7.0459	0.3497	-0.2082	H	7.157	0.0316	1.7878
H	5.5214	-2.3123	-1.7441	H	-4.6005	-3.3567	-1.3606
H	-5.8158	-3.7834	2.2189	H	7.7403	-2.4429	-2.4543
H	-6.2467	-5.0524	1.0835	H	7.9302	-4.1061	-1.9221
5c-9	X axis(Å)	Y axis(Å)	Z axis(Å)	5c-10	X axis(Å)	Y axis(Å)	Z axis(Å)
C	2.7907	5.0649	0.1263	C	-2.9095	4.5799	1.8507

C	2.3632	4.3349	1.4001	C	-3.2616	4.3223	0.3853
C	1.6905	2.9839	1.1145	C	-2.3998	3.2214	-0.2505
C	0.5204	3.1313	0.0978	C	-0.8797	3.4943	-0.0486
C	1.0122	3.7966	-1.2404	C	-0.5354	3.6516	1.4794
C	1.6665	5.1661	-0.9099	C	-1.4085	4.7888	2.0765
C	-0.218	1.8086	-0.1984	C	0.0355	2.4339	-0.6985
C	-1.3934	1.996	-1.179	C	1.5369	2.7482	-0.5046
C	-0.9863	2.7442	-2.459	C	1.8944	3.0171	0.9637
C	-0.2159	4.0344	-2.163	C	0.9619	4.04	1.6179
C	2.0376	2.9458	-2.0371	C	-0.7628	2.3676	2.3234
C	1.2274	2.3606	2.4111	C	-2.753	3.0787	-1.7128
O	0.3317	2.7748	3.1343	O	-2.5327	3.9015	-2.5906
O	-0.4631	4.0323	0.6693	O	-0.5568	4.7585	-0.6817
C	-2.0522	0.6723	-1.4844	C	2.4106	1.6601	-1.0828
O	-3.3174	0.4824	-0.9299	O	1.9504	0.3462	-0.9815
C	-1.5469	-0.3259	-2.2077	C	3.5806	1.8535	-1.6889
C	-6.1302	0.1858	-1.8228	C	0.9698	-1.7871	-2.7982
C	-4.907	-0.4274	-2.4925	C	2.1374	-0.8467	-3.0655
C	-3.8273	-0.7645	-1.4557	C	2.8536	-0.4752	-1.7586
C	-4.3618	-1.7467	-0.3548	C	3.3731	-1.7471	-0.9993
C	-5.6864	-1.2185	0.3135	C	2.2323	-2.8113	-0.7774
C	-6.7047	-0.7481	-0.7649	C	1.4348	-3.0531	-2.0907
C	-3.3106	-2.0935	0.7316	C	4.0736	-1.4234	0.3449
C	-3.0372	-0.9878	1.7697	C	3.1306	-1.0297	1.4982
C	-4.3496	-0.4455	2.3648	C	2.0011	-2.0611	1.6678
C	-5.3751	-0.0608	1.2958	C	1.2745	-2.3583	0.3537
C	-2.0375	-1.4833	2.8063	C	3.9264	-0.7489	2.7638
C	-0.605	-1.5572	2.3936	C	4.6866	0.5367	2.8086
C	-2.2953	-1.8434	4.0748	C	3.9959	-1.5131	3.8661
C	-6.415	-2.3448	1.1047	C	2.8162	-4.2018	-0.3887
C	-2.6099	-1.3157	-2.1639	C	3.965	0.5039	-2.068
O	-2.5004	-2.4365	-2.642	O	5.0424	0.23	-2.5786
C	5.7186	-3.1867	-2.0373	C	-3.2372	-4.3276	2.0089
C	4.8116	-2.042	-1.6468	C	-2.6545	-3.0031	1.5789
C	4.2303	-1.9257	-0.427	C	-2.8774	-2.4637	0.3556
C	4.4905	-2.9612	0.6861	C	-3.6617	-3.2212	-0.7371
C	5.6841	-3.8988	0.3531	C	-4.1144	-4.6422	-0.2974
C	3.277	-0.8108	-0.0142	C	-2.4798	-1.0578	-0.0642
C	3.7045	-0.109	1.2919	C	-3.7262	-0.2184	-0.4229
C	3.8664	-1.1425	2.4166	C	-4.5795	-0.9277	-1.4898
C	4.8474	-2.2425	2.0146	C	-4.9111	-2.3718	-1.0909
C	2.7453	1.0137	1.6202	C	-3.3043	1.1857	-0.7887
C	1.9628	1.1385	2.6904	C	-3.3568	1.7819	-1.9782
O	2.6836	2.0325	0.6703	O	-2.7924	1.9323	0.2707
C	3.2235	-3.8281	0.8799	C	-2.7899	-3.4299	-2.0001
C	4.6074	-1.0601	-2.7592	C	-1.852	-2.3306	2.6483
O	5.2057	-1.1375	-3.8274	O	-1.6316	-2.8497	3.7376

O	-4.7078	-2.9976	-1.0004	O	4.3654	-2.3913	-1.8358
C	5.6567	-4.3769	-1.0889	C	-4.4532	-4.7239	1.1805
O	-0.2026	-1.2	1.2927	O	4.6872	1.3393	1.8827
H	0.0934	-1.9535	3.1502	H	5.2557	0.7301	3.7336
H	3.1292	6.0746	0.3878	H	-3.4514	5.4673	2.1994
H	3.6603	4.5605	-0.3094	H	-3.2706	3.7477	2.4648
H	3.2504	4.1922	2.0302	H	-4.3243	4.054	0.3279
H	1.6815	4.9824	1.9664	H	-3.1475	5.2592	-0.175
H	2.0645	5.6246	-1.8242	H	-1.2198	4.8838	3.1535
H	0.9074	5.8623	-0.53	H	-1.1226	5.7523	1.6347
H	0.481	1.0537	-0.5756	H	-0.2045	1.44	-0.3045
H	-0.6363	1.41	0.7342	H	-0.1514	2.393	-1.7797
H	-2.1448	2.6223	-0.6768	H	1.75	3.671	-1.0635
H	-0.3806	2.1024	-3.1096	H	1.8756	2.0853	1.5392
H	-1.8846	2.9938	-3.0384	H	2.9237	3.3922	1.0298
H	-0.9026	4.7585	-1.7062	H	1.1452	5.024	1.1677
H	0.1035	4.4845	-3.1117	H	1.2318	4.142	2.6769
H	1.6901	1.9253	-2.2186	H	-0.2646	1.49	1.9029
H	2.2298	3.3984	-3.0176	H	-0.3698	2.5033	3.3385
H	3.0091	2.8688	-1.5452	H	-1.8169	2.1094	2.4412
H	-0.7066	3.7045	1.5602	H	-0.8913	4.7444	-1.6028
H	-0.6033	-0.4289	-2.707	H	4.1397	2.7515	-1.8673
H	-6.8955	0.3869	-2.5817	H	0.4961	-2.0571	-3.7493
H	-5.8751	1.1538	-1.3773	H	0.2031	-1.2783	-2.2052
H	-5.1992	-1.3253	-3.0514	H	2.8375	-1.3133	-3.7699
H	-4.524	0.2891	-3.2306	H	1.7474	0.0513	-3.5618
H	-7.1155	-1.6244	-1.2849	H	2.0588	-3.6171	-2.7976
H	-7.5593	-0.2557	-0.2833	H	0.5636	-3.6878	-1.887
H	-3.6323	-3.0045	1.2563	H	4.6733	-2.2915	0.6532
H	-2.3744	-2.3978	0.247	H	4.8252	-0.6416	0.1801
H	-2.5616	-0.138	1.2703	H	2.6337	-0.0897	1.2456
H	-4.1346	0.4364	2.982	H	1.2718	-1.6887	2.3983
H	-4.8083	-1.1799	3.0355	H	2.3884	-3.0008	2.0764
H	-6.2975	0.2576	1.7991	H	0.5247	-3.1381	0.5397
H	-5.016	0.8255	0.7644	H	0.7049	-1.4721	0.0586
H	-1.5201	-2.1773	4.759	H	4.58	-1.2302	4.7376
H	-3.2989	-1.8243	4.4866	H	3.4721	-2.4603	3.9442
H	-5.7813	-2.8075	1.8656	H	3.4528	-4.162	0.4989
H	-7.3013	-1.9492	1.6149	H	2.0107	-4.9161	-0.1803
H	-6.7593	-3.1474	0.4428	H	3.4198	-4.6285	-1.1977
H	5.4684	-3.5488	-3.0421	H	-2.4607	-5.0988	1.9321
H	6.7492	-2.8112	-2.0786	H	-3.5543	-4.2902	3.058
H	6.6357	-3.3755	0.5202	H	-4.9764	-4.9709	-0.8914
H	5.6909	-4.7644	1.0273	H	-3.3166	-5.3713	-0.4973
H	3.1732	-0.0514	-0.7905	H	-1.9177	-0.5333	0.7103
H	2.2731	-1.2379	0.1018	H	-1.7942	-1.1086	-0.9172
H	4.6878	0.3544	1.1249	H	-4.3502	-0.1356	0.4795

H	4.2407	-0.6527	3.3244	H	-5.5176	-0.3781	-1.639
H	2.8995	-1.5886	2.6783	H	-4.0668	-0.9294	-2.4587
H	5.8433	-1.7857	1.93	H	-5.5962	-2.3427	-0.2332
H	4.9152	-2.974	2.8302	H	-5.4667	-2.8422	-1.9122
H	1.8206	0.5058	3.5442	H	-3.6925	1.4336	-2.9358
H	3.3909	-4.6032	1.6367	H	-3.34	-3.9945	-2.7623
H	2.3592	-3.2428	1.2088	H	-2.4689	-2.4956	-2.4682
H	2.9307	-4.3299	-0.0489	H	-1.8829	-3.9961	-1.7586
H	3.8915	-0.2472	-2.5886	H	-1.4372	-1.3417	2.4187
H	-3.9342	-3.3034	-1.5201	H	5.0512	-1.7289	-2.0675
H	4.7526	-4.9654	-1.282	H	-4.7566	-5.745	1.4384
H	6.5075	-5.0414	-1.2791	H	-5.3024	-4.0707	1.4147
5d-1	X axis(Å)	Y axis(Å)	Z axis(Å)	5d-2	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-2.3265	5.0331	-1.1273	C	-2.3812	5.0591	-0.9536
C	-2.39	4.596	0.3344	C	-2.3943	4.5612	0.4899
C	-1.5446	3.3386	0.6168	C	-1.5398	3.2938	0.6884
C	-0.0759	3.5244	0.1375	C	-0.087	3.5046	0.1718
C	-0.0252	3.9074	-1.3904	C	-0.0883	3.9503	-1.3403
C	-0.8899	5.175	-1.6325	C	-0.9628	5.2243	-1.5016
C	0.857	2.3214	0.4225	C	0.863	2.2972	0.3796
C	2.3104	2.6197	-0.0104	C	2.3005	2.6293	-0.0864
C	2.4029	3.0895	-1.4723	C	2.3376	3.1472	-1.5342
C	1.4412	4.2362	-1.7815	C	1.3626	4.3	-1.7676
C	-0.5262	2.7858	-2.339	C	-0.6182	2.8669	-2.3171
C	-1.6338	3.0173	2.0915	C	-1.5812	2.9047	2.1484
O	-1.0753	3.6253	2.9947	O	-0.9798	3.4602	3.058
O	0.4854	4.6533	0.8619	O	0.492	4.6066	0.9239
C	3.241	1.4527	0.2013	C	3.2626	1.4764	0.0464
O	2.9811	0.2896	-0.5233	O	2.9238	0.2823	-0.5882
C	4.3283	1.4643	0.97	C	4.4449	1.5306	0.6571
C	4.1654	-0.9945	-2.9138	C	3.7596	-1.0905	-3.0624
C	4.9394	-0.3598	-1.7643	C	4.6895	-0.4006	-2.0705
C	4.1772	-0.5218	-0.4407	C	4.134	-0.5115	-0.6433
C	3.9159	-2.0313	-0.1122	C	3.9557	-2.0085	-0.2165
C	3.1936	-2.7772	-1.296	C	3.0748	-2.8138	-1.242
C	3.8952	-2.4715	-2.651	C	3.5517	-2.557	-2.7013
C	3.149	-2.2591	1.2128	C	3.4071	-2.192	1.2192
C	1.6423	-1.9495	1.1595	C	1.9103	-1.878	1.3961
C	0.9526	-2.6025	-0.0472	C	1.0577	-2.6014	0.3417
C	1.699	-2.3742	-1.3633	C	1.5815	-2.4339	-1.0873
C	0.9438	-2.3307	2.4546	C	1.385	-2.1684	2.796
C	0.1026	-1.3058	3.1305	C	0.2052	-1.3832	3.2594
C	1.0118	-3.5318	3.0532	C	1.8853	-3.0424	3.6855
C	3.2683	-4.3233	-1.1292	C	3.2032	-4.3509	-1.0296
C	4.9315	0.176	0.6701	C	5.0267	0.2423	0.3179
O	5.9203	-0.2511	1.2501	O	6.0992	-0.1443	0.7614
C	-4.4349	-4.4237	-0.4283	C	-4.4945	-4.423	-0.4793

C	-3.5867	-3.2753	0.0667	C	-3.6348	-3.2834	0.0151
C	-3.7531	-1.9897	-0.331	C	-3.8016	-1.9946	-0.3706
C	-4.9028	-1.5877	-1.2796	C	-4.9718	-1.5727	-1.2833
C	-5.9416	-2.7289	-1.4654	C	-6.0194	-2.7076	-1.4582
C	-2.8691	-0.8172	0.0805	C	-2.8983	-0.8347	0.0279
C	-3.6815	0.3352	0.6914	C	-3.6881	0.2982	0.6986
C	-4.7848	0.7945	-0.2724	C	-4.8122	0.7891	-0.2257
C	-5.6747	-0.3754	-0.6899	C	-5.7203	-0.3652	-0.6523
C	-2.7877	1.4864	1.0719	C	-2.7791	1.4301	1.0989
C	-2.515	1.8827	2.3137	C	-2.468	1.771	2.3481
O	-2.1933	2.1905	0.027	O	-2.2076	2.173	0.0684
C	-4.3229	-1.2229	-2.6664	C	-4.4288	-1.188	-2.6793
C	-2.5377	-3.7037	1.0427	C	-2.58	-3.7205	0.9824
O	-2.3834	-4.8701	1.3891	O	-2.3885	-4.8972	1.2713
O	5.2025	-2.6801	0.0494	O	5.2647	-2.6327	-0.2291
C	-5.2802	-4.0845	-1.6493	C	-5.3668	-4.0632	-1.6758
O	-0.1751	-0.2297	2.6157	O	-0.3796	-0.578	2.545
H	-0.2875	-1.5808	4.1252	H	-0.1271	-1.5735	4.2941
H	-2.8787	4.3198	-1.7491	H	-2.9541	4.3715	-1.5854
H	-2.8432	5.9938	-1.2384	H	-2.9017	6.0228	-1.0067
H	-2.0542	5.4263	0.9692	H	-2.0367	5.364	1.1476
H	-3.4419	4.4169	0.5921	H	-3.4368	4.3702	0.7757
H	-0.433	6.0405	-1.1348	H	-0.4903	6.0704	-0.9855
H	-0.9105	5.4195	-2.7023	H	-1.0204	5.5115	-2.5594
H	0.8737	2.1143	1.5	H	0.9139	2.0424	1.4459
H	0.4828	1.4132	-0.0631	H	0.4804	1.4078	-0.1335
H	2.675	3.4475	0.6147	H	2.6734	3.4406	0.5551
H	3.4266	3.422	-1.6889	H	3.351	3.4924	-1.778
H	2.209	2.2555	-2.1581	H	2.1218	2.3339	-2.2383
H	1.505	4.4771	-2.8504	H	1.3898	4.5816	-2.8282
H	1.7849	5.1349	-1.2532	H	1.721	5.1796	-1.2172
H	-0.0192	1.832	-2.1711	H	-0.1075	1.9073	-2.2014
H	-1.5981	2.5972	-2.254	H	-1.6875	2.6753	-2.2084
H	-0.3484	3.0626	-3.3855	H	-0.4712	3.1844	-3.3567
H	0.3567	4.4927	1.8215	H	0.3922	4.4076	1.8795
H	4.7382	2.2303	1.5996	H	4.9273	2.3278	1.189
H	3.223	-0.46	-3.0781	H	2.7955	-0.5709	-3.1039
H	4.7439	-0.8921	-3.8395	H	4.1899	-1.0235	-4.0685
H	5.938	-0.8086	-1.6931	H	5.6937	-0.8381	-2.1312
H	5.0914	0.7017	-1.9983	H	4.7897	0.651	-2.3685
H	4.86	-2.9958	-2.6875	H	4.5059	-3.0757	-2.8678
H	3.301	-2.8766	-3.4803	H	2.8408	-2.9997	-3.4109
H	3.311	-3.2997	1.5227	H	3.6118	-3.227	1.5208
H	3.6112	-1.6777	2.0213	H	3.9936	-1.5925	1.9274
H	1.5462	-0.867	1.036	H	1.7935	-0.8006	1.2412
H	0.8283	-3.6798	0.1165	H	0.9846	-3.6689	0.5836
H	-0.0615	-2.1988	-0.1512	H	0.0321	-2.2185	0.37

H	1.1935	-2.9473	-2.1518	H	0.9682	-3.0532	-1.7552
H	1.5851	-1.3256	-1.6541	H	1.4014	-1.4034	-1.4081
H	0.4873	-3.7624	3.9762	H	1.4547	-3.185	4.673
H	1.5847	-4.3474	2.6202	H	2.7419	-3.6693	3.4603
H	2.8379	-4.6693	-0.1857	H	2.9214	-4.6655	-0.0214
H	2.7251	-4.827	-1.9378	H	2.5576	-4.8939	-1.7302
H	4.3018	-4.6856	-1.1645	H	4.2273	-4.7001	-1.2026
H	-3.8035	-5.2823	-0.6877	H	-3.8697	-5.2777	-0.7661
H	-5.0936	-4.7441	0.3891	H	-5.1357	-4.7559	0.347
H	-6.6018	-2.7884	-0.5891	H	-6.6581	-2.7767	-0.5669
H	-6.5937	-2.5181	-2.3223	H	-6.6915	-2.4836	-2.2961
H	-2.0963	-1.1026	0.7945	H	-2.0943	-1.1402	0.6953
H	-2.3194	-0.4693	-0.8038	H	-2.3868	-0.4641	-0.87
H	-4.1685	-0.0421	1.6025	H	-4.1555	-0.1077	1.6078
H	-5.4051	1.5611	0.2093	H	-5.4155	1.5467	0.2905
H	-4.3547	1.2648	-1.165	H	-4.3999	1.2793	-1.1161
H	-6.2389	-0.6957	0.1971	H	-6.2694	-0.6997	0.239
H	-6.4189	-0.0167	-1.4126	H	-6.4759	0.0151	-1.3517
H	-2.8231	1.4931	3.2638	H	-2.7503	1.3387	3.2878
H	-5.1238	-0.9809	-3.3747	H	-5.2482	-0.939	-3.3635
H	-3.6583	-0.3542	-2.6302	H	-3.7666	-0.3172	-2.6486
H	-3.7429	-2.0493	-3.0916	H	-3.8578	-2.0071	-3.13
H	-1.9031	-2.9195	1.4675	H	-1.9823	-2.935	1.459
H	5.715	-2.1872	0.7251	H	5.8649	-2.1046	0.3391
H	-4.658	-4.0897	-2.5516	H	-4.7654	-4.0574	-2.5921
H	-6.044	-4.8577	-1.7923	H	-6.1364	-4.8318	-1.8123
5d-3	X axis(Å)	Y axis(Å)	Z axis(Å)	5d-4	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-2.2901	4.9798	-1.0735	C	-2.2669	5.0311	-1.0781
C	-1.9008	4.6191	0.3633	C	-2.3507	4.571	0.3756
C	-1.1358	3.2913	0.4475	C	-1.514	3.3059	0.6476
C	0.0896	3.2903	-0.5124	C	-0.0386	3.4937	0.19
C	-0.3536	3.5453	-1.9992	C	0.0336	3.9005	-1.3306
C	-1.1181	4.897	-2.0612	C	-0.8234	5.1751	-1.5635
C	0.955	2.0191	-0.4145	C	0.8861	2.2831	0.4684
C	2.1914	2.079	-1.3345	C	2.3462	2.5841	0.0616
C	1.7998	2.3807	-2.7878	C	2.4605	3.0749	-1.3918
C	0.9148	3.6297	-2.8954	C	1.5066	4.2295	-1.6971
C	-1.2646	2.4406	-2.5983	C	-0.4589	2.7961	-2.3035
C	-0.7268	2.9934	1.875	C	-1.62	2.9594	2.1155
O	0.0682	3.6288	2.553	O	-1.074	3.5536	3.0353
O	0.9484	4.3987	-0.1392	O	0.5169	4.6092	0.9393
C	3.0348	0.8299	-1.2435	C	3.2699	1.4119	0.2741
O	2.3784	-0.3917	-1.0799	O	3.0383	0.2695	-0.4921
C	4.3663	0.8167	-1.2482	C	4.3274	1.4016	1.0833
C	1.9864	-3.0427	-2.3539	C	4.32	-0.9423	-2.8726
C	3.2721	-2.2248	-2.3524	C	5.0455	-0.3416	-1.6745
C	3.4018	-1.4183	-1.0551	C	4.2315	-0.5436	-0.3876

C	3.3685	-2.3461	0.2173	C	3.959	-2.0622	-0.115
C	2.1207	-3.3086	0.2239	C	3.2867	-2.7725	-1.3493
C	1.9384	-3.9909	-1.1622	C	4.0428	-2.4267	-2.6647
C	3.4543	-1.5669	1.5574	C	3.1387	-2.3294	1.1701
C	2.1593	-0.8465	1.9726	C	1.6345	-2.0212	1.0643
C	0.9589	-1.8051	1.9535	C	0.996	-2.6364	-0.19
C	0.8353	-2.5368	0.6149	C	1.7959	-2.3672	-1.4661
C	2.3504	-0.0897	3.2761	C	0.8881	-2.4474	2.3182
C	3.0699	1.2185	3.1922	C	0.0491	-1.4376	3.0192
C	1.9117	-0.4512	4.4927	C	0.9117	-3.678	2.8574
C	2.306	-4.4774	1.237	C	3.3564	-4.3228	-1.2256
C	4.6704	-0.5941	-1.0969	C	4.9412	0.1211	0.7718
O	5.8115	-1.0252	-1.0003	O	5.9057	-0.3241	1.3784
C	-4.5016	-4.0587	-0.8681	C	-4.7863	-4.2367	-0.3387
C	-3.5575	-2.8838	-0.7676	C	-3.7271	-3.211	-0.0162
C	-3.9027	-1.6745	-0.2611	C	-3.7571	-1.9406	-0.4878
C	-5.3409	-1.3965	0.2228	C	-4.8418	-1.4689	-1.4794
C	-6.154	-2.7046	0.4269	C	-5.7981	-2.6094	-1.9275
C	-2.96	-0.4824	-0.143	C	-2.8339	-0.8142	-0.042
C	-2.9983	0.1928	1.2451	C	-3.6469	0.2996	0.6459
C	-4.4322	0.5699	1.6276	C	-4.8036	0.7955	-0.2404
C	-5.3376	-0.6579	1.5865	C	-5.6623	-0.3579	-0.7727
C	-2.109	1.4096	1.3121	C	-2.7603	1.4453	1.0566
C	-1.3752	1.7826	2.3577	C	-2.4981	1.8172	2.308
O	-2.0478	2.2027	0.1738	O	-2.1602	2.171	0.0301
C	-6.059	-0.5265	-0.8371	C	-4.2082	-0.9147	-2.7794
C	-2.2046	-3.1742	-1.3344	C	-2.6723	-3.7133	0.9158
O	-1.8286	-4.3112	-1.5972	O	-2.69	-4.8372	1.4059
O	4.5331	-3.2089	0.1738	O	5.2385	-2.7158	0.0796
C	-5.971	-3.6871	-0.7183	C	-6.0876	-3.6067	-0.8194
O	3.5159	1.6602	2.1396	O	-0.1793	-0.327	2.5562
H	3.18	1.7724	4.1399	H	-0.3853	-1.7554	3.9824
H	-3.1033	4.3241	-1.4043	H	-2.814	4.3301	-1.7181
H	-2.6999	5.9969	-1.0891	H	-2.7784	5.9956	-1.1803
H	-1.2957	5.4321	0.7841	H	-2.0198	5.3894	1.028
H	-2.8161	4.5695	0.967	H	-3.4064	4.3916	0.6171
H	-0.4303	5.7262	-1.8499	H	-0.3695	6.0309	-1.0468
H	-1.4947	5.0711	-3.0772	H	-0.8299	5.4363	-2.6295
H	1.3209	1.9185	0.612	H	0.8867	2.0582	1.5424
H	0.3542	1.1278	-0.6268	H	0.5166	1.3842	-0.0376
H	2.8165	2.9152	-0.9886	H	2.7032	3.4025	0.7033
H	2.7033	2.5397	-3.3905	H	3.4883	3.407	-1.5893
H	1.2885	1.518	-3.232	H	2.273	2.252	-2.0925
H	0.6299	3.7762	-3.9451	H	1.5856	4.4859	-2.7614
H	1.5134	4.5087	-2.6237	H	1.8462	5.1191	-1.151
H	-0.8554	1.4361	-2.4613	H	0.0424	1.8378	-2.1443
H	-2.2724	2.4381	-2.1787	H	-1.5325	2.6103	-2.2356

H	-1.3912	2.592	-3.6773	H	-0.2664	3.0889	-3.343
H	1.2202	4.2814	0.7951	H	0.3749	4.4347	1.8945
H	5.075	1.619	-1.3191	H	4.7121	2.1491	1.7498
H	1.1129	-2.3811	-2.3499	H	3.3839	-0.404	-3.0589
H	1.9293	-3.6248	-3.2811	H	4.9352	-0.8119	-3.7706
H	4.1358	-2.8884	-2.484	H	6.0414	-0.7915	-1.5766
H	3.2559	-1.5551	-3.222	H	5.2047	0.7265	-1.8706
H	2.7279	-4.7415	-1.3054	H	5.0094	-2.9487	-2.6768
H	0.9912	-4.5442	-1.1854	H	3.484	-2.8077	-3.5292
H	3.7501	-2.2609	2.3568	H	3.2903	-3.3782	1.457
H	4.2896	-0.8571	1.5139	H	3.5656	-1.7705	2.0132
H	1.9276	-0.0901	1.2238	H	1.5387	-0.9357	0.9706
H	1.0312	-2.5416	2.7609	H	0.8662	-3.7183	-0.0662
H	0.0338	-1.2433	2.1344	H	-0.0138	-2.2297	-0.3231
H	-0.0113	-3.2318	0.6795	H	1.3242	-2.9155	-2.2924
H	0.5643	-1.8107	-0.1578	H	1.6928	-1.31	-1.7286
H	2.0812	0.1568	5.3773	H	0.3538	-3.9418	3.7516
H	1.3777	-1.3814	4.6571	H	1.4829	-4.483	2.4029
H	2.5094	-4.1297	2.2532	H	2.8891	-4.6966	-0.3107
H	1.4047	-5.1007	1.2793	H	2.8466	-4.8023	-2.0698
H	3.1348	-5.1349	0.9512	H	4.3909	-4.684	-1.2301
H	-4.3825	-4.5664	-1.8333	H	-4.3953	-4.9187	-1.104
H	-4.2313	-4.7838	-0.0896	H	-5.0229	-4.8432	0.5437
H	-5.8418	-3.202	1.3556	H	-6.7413	-2.1924	-2.3025
H	-7.2207	-2.4765	0.5467	H	-5.3567	-3.1618	-2.769
H	-1.9196	-0.7562	-0.3358	H	-2.0649	-1.1478	0.6556
H	-3.2343	0.2356	-0.9263	H	-2.2801	-0.4275	-0.9056
H	-2.6315	-0.5391	1.9797	H	-4.0953	-0.1323	1.5531
H	-4.4532	0.9894	2.6417	H	-5.4428	1.4776	0.335
H	-4.8198	1.3521	0.9638	H	-4.4213	1.3824	-1.0844
H	-5.0064	-1.3454	2.3772	H	-6.2199	-0.7853	0.071
H	-6.3588	-0.356	1.8526	H	-6.4131	0.0526	-1.4601
H	-1.2548	1.3407	3.3278	H	-2.8128	1.4079	3.2477
H	-7.0989	-0.335	-0.5481	H	-4.9852	-0.6297	-3.4987
H	-5.5783	0.4473	-0.9746	H	-3.5878	-0.0289	-2.6178
H	-6.0727	-1.0114	-1.8193	H	-3.5727	-1.6695	-3.2579
H	-1.549	-2.3142	-1.5233	H	-1.8504	-3.029	1.1488
H	5.3314	-2.6537	0.0454	H	5.723	-2.2426	0.7892
H	-6.3475	-3.26	-1.6547	H	-6.7604	-4.3896	-1.1878
H	-6.5603	-4.5924	-0.5317	H	-6.6012	-3.1141	0.0146
5d-5	X axis(Å)	Y axis(Å)	Z axis(Å)	5d-6	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-2.3421	5.0588	-0.8795	C	1.8438	4.7569	1.4174
C	-2.3713	4.5287	0.5524	C	1.9031	4.4581	-0.0797
C	-1.521	3.2559	0.7307	C	1.0517	3.243	-0.4837
C	-0.0625	3.4761	0.2346	C	-0.4089	3.3635	0.0392
C	-0.0467	3.9545	-1.2673	C	-0.4412	3.5873	1.5961
C	-0.9179	5.2333	-1.4096	C	0.4095	4.838	1.9466

C	0.884	2.2632	0.4268	C	-1.3041	2.1673	-0.3445
C	2.3268	2.6049	-0.0145	C	-2.7557	2.3372	0.145
C	2.3806	3.1519	-1.4511	C	-2.8474	2.6995	1.6376
C	1.4094	4.3108	-1.6712	C	-1.9103	3.8432	2.0322
C	-0.5676	2.8937	-2.2733	C	0.0944	2.3874	2.423
C	-1.5759	2.8322	2.1806	C	1.1017	3.0839	-1.9854
O	-0.9868	3.3687	3.1093	O	0.5969	3.8359	-2.8074
O	0.5093	4.5608	1.0167	O	-1.0081	4.5418	-0.5592
C	3.2882	1.4504	0.1088	C	-3.5676	1.1003	-0.1474
O	2.965	0.2714	-0.5615	O	-3.2477	-0.0494	0.5767
C	4.458	1.4921	0.744	C	-4.5646	1.0136	-1.0253
C	3.8568	-1.0286	-3.0564	C	-4.5168	-1.6129	2.7543
C	4.763	-0.3627	-2.0271	C	-5.2273	-1.0231	1.5428
C	4.1795	-0.5161	-0.615	C	-4.2998	-1.0073	0.3188
C	3.9998	-2.0251	-0.2337	C	-3.7823	-2.445	-0.0347
C	3.1452	-2.8059	-1.2997	C	-3.1254	-3.1606	1.2063
C	3.6503	-2.5057	-2.7411	C	-4.0258	-3.0262	2.468
C	3.4221	-2.2512	1.1845	C	-2.8183	-2.4772	-1.2476
C	1.9197	-1.9516	1.3386	C	-1.3847	-1.9909	-0.9695
C	1.0947	-2.6509	0.2467	C	-0.7847	-2.6555	0.2809
C	1.6469	-2.4385	-1.1655	C	-1.7177	-2.5769	1.4914
C	1.3668	-2.2856	2.7182	C	-0.5417	-2.1512	-2.2254
C	0.168	-1.5262	3.1761	C	-0.605	-1.0495	-3.2293
C	1.8569	-3.178	3.595	C	0.2611	-3.1843	-2.53
C	3.2785	-4.3477	-1.1279	C	-2.9765	-4.6924	0.9674
C	5.05	0.2141	0.3842	C	-5.0191	-0.3553	-0.8424
O	6.1138	-0.1819	0.84	O	-5.8757	-0.8775	-1.5427
C	-4.8076	-4.2527	-0.4086	C	5.7954	-2.718	1.9778
C	-3.7541	-3.2257	-0.0716	C	5.0393	-1.4476	1.6598
C	-3.7898	-1.9525	-0.535	C	4.7793	-1.023	0.3981
C	-4.8921	-1.4656	-1.4988	C	5.21	-1.8523	-0.8294
C	-5.8559	-2.5993	-1.9474	C	5.6529	-3.2913	-0.4451
C	-2.8553	-0.8337	-0.1007	C	4.0605	0.2729	0.0403
C	-3.6525	0.2503	0.6466	C	2.8594	0.0444	-0.9007
C	-4.8271	0.7714	-0.2022	C	3.3262	-0.689	-2.1678
C	-5.6973	-0.3674	-0.7524	C	4.0223	-2.0027	-1.817
C	-2.7567	1.3785	1.0839	C	2.133	1.3434	-1.1739
C	-2.456	1.6877	2.3438	C	1.8378	1.8857	-2.3543
O	-2.1838	2.1516	0.0771	O	1.6951	2.0268	-0.0388
C	-4.2888	-0.8855	-2.8017	C	6.3931	-1.1454	-1.5319
C	-2.7119	-3.7288	0.8764	C	4.6221	-0.7017	2.8903
O	-2.6653	-4.8941	1.2573	O	4.8059	-1.14	4.0213
O	5.3119	-2.643	-0.236	O	-4.9279	-3.2527	-0.4046
C	-6.1201	-3.6199	-0.8541	C	6.5396	-3.3106	0.7884
O	-0.4061	-0.7036	2.4729	O	-1.241	-0.0192	-3.046
H	-0.1882	-1.752	4.1957	H	-0.0309	-1.2085	-4.1578
H	-2.9097	4.3865	-1.5323	H	2.408	3.9949	1.9662

H	-2.8603	6.0244	-0.9165	H	2.3531	5.708	1.6142
H	-2.0196	5.3159	1.2318	H	1.5704	5.3483	-0.6292
H	-3.417	4.3328	0.8229	H	2.9528	4.2967	-0.3571
H	-0.4493	6.0671	-0.8705	H	-0.0618	5.74	1.5349
H	-0.9642	5.5434	-2.4614	H	0.4382	4.9827	3.0341
H	0.9222	1.9847	1.4877	H	-1.3398	2.0745	-1.4368
H	0.5074	1.3857	-0.1105	H	-0.8756	1.2332	0.0341
H	2.6911	3.4038	0.6473	H	-3.1971	3.1738	-0.4153
H	3.3971	3.5005	-1.6766	H	-3.8785	2.9869	1.8813
H	2.1713	2.3534	-2.1737	H	-2.6291	1.8252	2.2629
H	1.4487	4.6144	-2.7253	H	-1.9638	3.9888	3.1188
H	1.7627	5.1782	-1.0987	H	-2.2847	4.7748	1.5888
H	-0.0602	1.9308	-2.1725	H	-0.4056	1.4466	2.1782
H	-1.6385	2.7024	-2.1813	H	1.1656	2.2202	2.2952
H	-0.4078	3.2333	-3.304	H	-0.0616	2.5627	3.4945
H	0.398	4.3421	1.9668	H	-0.899	4.4864	-1.5323
H	4.9279	2.2769	1.3048	H	-4.977	1.7411	-1.697
H	2.8909	-0.513	-3.1026	H	-3.68	-0.9724	3.0545
H	4.3067	-0.9309	-4.0514	H	-5.2092	-1.6359	3.6041
H	5.7704	-0.794	-2.0795	H	-6.1384	-1.596	1.329
H	4.8641	0.6972	-2.2936	H	-5.5514	-0.0058	1.7975
H	4.6107	-3.0145	-2.9024	H	-4.9107	-3.6675	2.3544
H	2.9567	-2.932	-3.4773	H	-3.4927	-3.4025	3.3506
H	3.6274	-3.2927	1.4619	H	-2.7799	-3.5041	-1.6387
H	3.9896	-1.6677	1.921	H	-3.2516	-1.904	-2.0775
H	1.7985	-0.8709	1.2116	H	-1.4161	-0.9214	-0.744
H	1.0253	-3.7255	0.4565	H	-0.5427	-3.7068	0.0945
H	0.0654	-2.2775	0.2641	H	0.1659	-2.1681	0.5332
H	1.0513	-3.0409	-1.8641	H	-1.2513	-3.1194	2.3243
H	1.4677	-1.3998	-1.4594	H	-1.7795	-1.5359	1.8228
H	1.406	-3.3517	4.5685	H	0.8337	-3.2282	-3.4523
H	2.7258	-3.789	3.3732	H	0.3654	-4.0421	-1.8736
H	2.9794	-4.692	-0.1345	H	-2.409	-4.9277	0.0633
H	2.6496	-4.8743	-1.8558	H	-2.4604	-5.168	1.8099
H	4.3077	-4.6865	-1.2909	H	-3.951	-5.1843	0.8712
H	-4.4206	-4.9104	-1.1968	H	6.5291	-2.5387	2.7732
H	-5.0279	-4.8848	0.4601	H	5.0804	-3.4578	2.3607
H	-6.8076	-2.177	-2.2936	H	4.7733	-3.9178	-0.2419
H	-5.4316	-3.134	-2.8088	H	6.1777	-3.7673	-1.2829
H	-2.0513	-1.1822	0.5453	H	3.7087	0.8033	0.9262
H	-2.3418	-0.4175	-0.9753	H	4.7796	0.9547	-0.4323
H	-4.0828	-0.2152	1.5459	H	2.1423	-0.609	-0.3826
H	-5.4547	1.4365	0.4047	H	2.4694	-0.9106	-2.8147
H	-4.4601	1.3818	-1.0364	H	4.0019	-0.0552	-2.7548
H	-6.2438	-0.8139	0.0889	H	3.2675	-2.6734	-1.3835
H	-6.457	0.0619	-1.418	H	4.3625	-2.4837	-2.7431
H	-2.7415	1.228	3.2695	H	2.0305	1.5614	-3.3584

H	-5.0822	-0.6008	-3.5032	H	6.7513	-1.7341	-2.3843
H	-3.6786	0.0072	-2.6393	H	6.1236	-0.1574	-1.9178
H	-3.6523	-1.6253	-3.3018	H	7.2391	-0.9996	-0.8512
H	-1.9697	-3.0069	1.2341	H	4.1321	0.2691	2.7499
H	5.8976	-2.128	0.3587	H	-5.4213	-2.7844	-1.1117
H	-6.7955	-4.3988	-1.2261	H	7.4645	-2.7515	0.6064
H	-6.6214	-3.1463	-0.0016	H	6.8381	-4.3399	1.0189
5d-7	X axis(Å)	Y axis(Å)	Z axis(Å)	5d-8	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-1.9473	4.8271	-0.8039	C	-1.1979	5.4909	-1.1373
C	-1.826	4.3018	0.6267	C	-1.5334	4.8711	0.2185
C	-0.9569	3.0376	0.7264	C	-0.917	3.473	0.3982
C	0.4313	3.2461	0.0552	C	0.6183	3.4901	0.1405
C	0.2742	3.6926	-1.4456	C	0.938	4.0559	-1.2952
C	-0.5908	4.9814	-1.4992	C	0.302	5.4662	-1.4421
C	1.361	2.0194	0.1545	C	1.3312	2.1303	0.3608
C	2.7453	2.2785	-0.4773	C	2.8585	2.2603	0.1598
C	2.6415	2.8176	-1.9127	C	3.2115	2.8755	-1.2046
C	1.6816	4.0054	-2.0254	C	2.4761	4.192	-1.4562
C	-0.3822	2.6271	-2.3644	C	0.4242	3.1642	-2.4569
C	-0.8306	2.6257	2.1755	C	-1.2487	2.9562	1.777
O	-0.2098	3.2178	3.0468	O	-0.7853	3.3717	2.8307
O	1.1041	4.332	0.7426	O	1.2167	4.4158	1.0893
C	3.6093	1.0423	-0.4488	C	3.6114	0.9646	0.3266
O	3.0568	-0.1285	-0.9679	O	3.1525	-0.1513	-0.3743
C	4.8459	0.9747	0.0397	C	4.7272	0.8241	1.0401
C	3.4079	-2.0086	-3.2127	C	4.0005	-1.5883	-2.8116
C	4.5296	-1.3459	-2.4215	C	4.9253	-1.0584	-1.7221
C	4.1058	-1.125	-0.9643	C	4.2326	-1.1175	-0.3533
C	3.7112	-2.4752	-0.2646	C	3.8058	-2.5822	0.0094
C	2.6252	-3.2717	-1.0819	C	2.9367	-3.2496	-1.1212
C	3.0043	-3.3398	-2.5899	C	3.5743	-3.0225	-2.5227
C	3.2572	-2.3017	1.2076	C	3.0941	-2.7042	1.3806
C	1.8474	-1.7121	1.3914	C	1.6343	-2.2114	1.4142
C	0.8111	-2.4867	0.5604	C	0.8212	-2.8491	0.2773
C	1.2266	-2.6254	-0.9075	C	1.4915	-2.695	-1.0901
C	1.5176	-1.5846	2.8705	C	0.9388	-2.4258	2.7526
C	2.1471	-0.4408	3.5986	C	-0.2656	-1.5913	3.0363
C	0.705	-2.3738	3.5917	C	1.3067	-3.2647	3.7357
C	2.5319	-4.7544	-0.6134	C	2.8615	-4.7963	-0.9503
C	5.2085	-0.4092	-0.2148	C	5.1382	-0.5283	0.7064
O	6.2689	-0.9027	0.1447	O	6.0964	-1.0823	1.2276
C	-6.3659	-2.2594	-1.9022	C	-7.0415	-2.4328	-0.8128
C	-5.5277	-1.0772	-1.4701	C	-6.27	-1.3536	-0.0873
C	-4.9782	-0.9553	-0.236	C	-4.9233	-1.2121	-0.1627
C	-5.1407	-2.0647	0.8245	C	-4.0691	-2.1448	-1.047
C	-5.6899	-3.3857	0.2181	C	-4.9334	-2.9895	-2.024
C	-4.1664	0.2411	0.2473	C	-4.1043	-0.1702	0.5912

C	-2.7942	-0.1679	0.819	C	-3.1832	0.6532	-0.3319
C	-2.9822	-1.1902	1.9497	C	-2.2804	-0.2773	-1.1535
C	-3.7667	-2.4064	1.4613	C	-3.0974	-1.3116	-1.9231
C	-1.9967	1.0536	1.2174	C	-2.3406	1.6842	0.3866
C	-1.5451	1.3836	2.4257	C	-2.2043	1.8652	1.6995
O	-1.6741	1.9125	0.1678	O	-1.6174	2.5366	-0.4469
C	-6.1217	-1.5811	1.9187	C	-3.2675	-3.11	-0.1421
C	-5.3834	-0.0478	-2.5491	C	-7.1509	-0.4699	0.7404
O	-5.8385	-0.2057	-3.6773	O	-8.3727	-0.5793	0.7542
O	4.8876	-3.3215	-0.2294	O	5.0113	-3.3837	0.1096
C	-6.833	-3.1423	-0.7525	C	-6.1713	-3.5599	-1.3531
O	2.8852	0.3665	3.047	O	-0.7192	-0.7813	2.2372
H	1.9069	-0.3588	4.6722	H	-0.7389	-1.7449	4.021
H	-2.595	4.1607	-1.3842	H	-1.752	4.9702	-1.9261
H	-2.4544	5.7993	-0.7875	H	-1.5512	6.5288	-1.1556
H	-1.409	5.0951	1.2604	H	-1.185	5.5431	1.0133
H	-2.8361	4.1008	1.0063	H	-2.6259	4.8214	0.3125
H	-0.0528	5.8142	-1.0278	H	0.8021	6.1742	-0.7683
H	-0.7565	5.282	-2.5417	H	0.4659	5.8502	-2.4571
H	1.5258	1.7708	1.2095	H	1.1639	1.7832	1.3885
H	0.8836	1.1447	-0.301	H	0.9142	1.3611	-0.2988
H	3.2435	3.052	0.1245	H	3.231	2.9514	0.9298
H	3.6339	3.1339	-2.2595	H	4.2917	3.0648	-1.2583
H	2.3257	2.0224	-2.5993	H	2.9914	2.1664	-2.0123
H	1.6013	4.3003	-3.0795	H	2.7234	4.5527	-2.463
H	2.1244	4.8664	-1.5083	H	2.8663	4.95	-0.7647
H	0.1137	1.6547	-2.3062	H	0.7486	2.1243	-2.3664
H	-1.4385	2.4602	-2.1453	H	-0.664	3.154	-2.5432
H	-0.3375	2.9473	-3.4127	H	0.7998	3.5346	-3.4186
H	1.1501	4.1143	1.6976	H	0.9144	4.1701	1.9896
H	5.4609	1.7222	0.5021	H	5.2739	1.5273	1.6385
H	2.5408	-1.3415	-3.2762	H	3.1199	-0.9436	-2.9112
H	3.7434	-2.1784	-4.2425	H	4.5205	-1.5531	-3.7761
H	5.4372	-1.9602	-2.4728	H	5.8593	-1.6337	-1.7099
H	4.7715	-0.3894	-2.9025	H	5.1987	-0.0261	-1.9758
H	3.8458	-4.0338	-2.7223	H	4.4658	-3.6567	-2.6233
H	2.1716	-3.7634	-3.1663	H	2.8809	-3.3519	-3.3073
H	3.3064	-3.2765	1.7133	H	3.1355	-3.7591	1.6819
H	3.9973	-1.6987	1.7482	H	3.6751	-2.1858	2.1542
H	1.8342	-0.6946	0.9964	H	1.6553	-1.1286	1.251
H	0.6407	-3.4849	0.9777	H	0.6437	-3.9107	0.489
H	-0.1546	-1.9697	0.6041	H	-0.1716	-2.3934	0.2228
H	0.4698	-3.2282	-1.4266	H	0.8764	-3.2121	-1.8383
H	1.1855	-1.6394	-1.3807	H	1.4692	-1.6385	-1.3761
H	0.5199	-2.2088	4.6496	H	0.7595	-3.3465	4.671
H	0.2029	-3.2311	3.1556	H	2.1716	-3.9142	3.6481
H	2.3247	-4.8495	0.4556	H	2.4748	-5.0979	0.0265

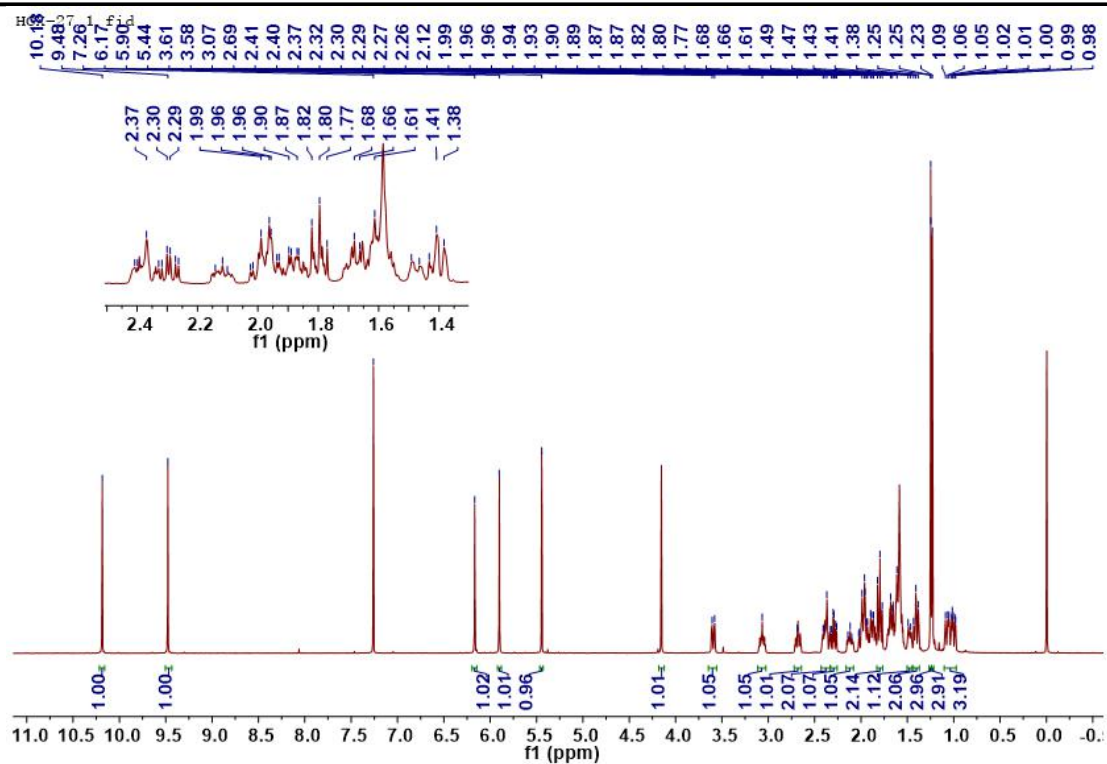
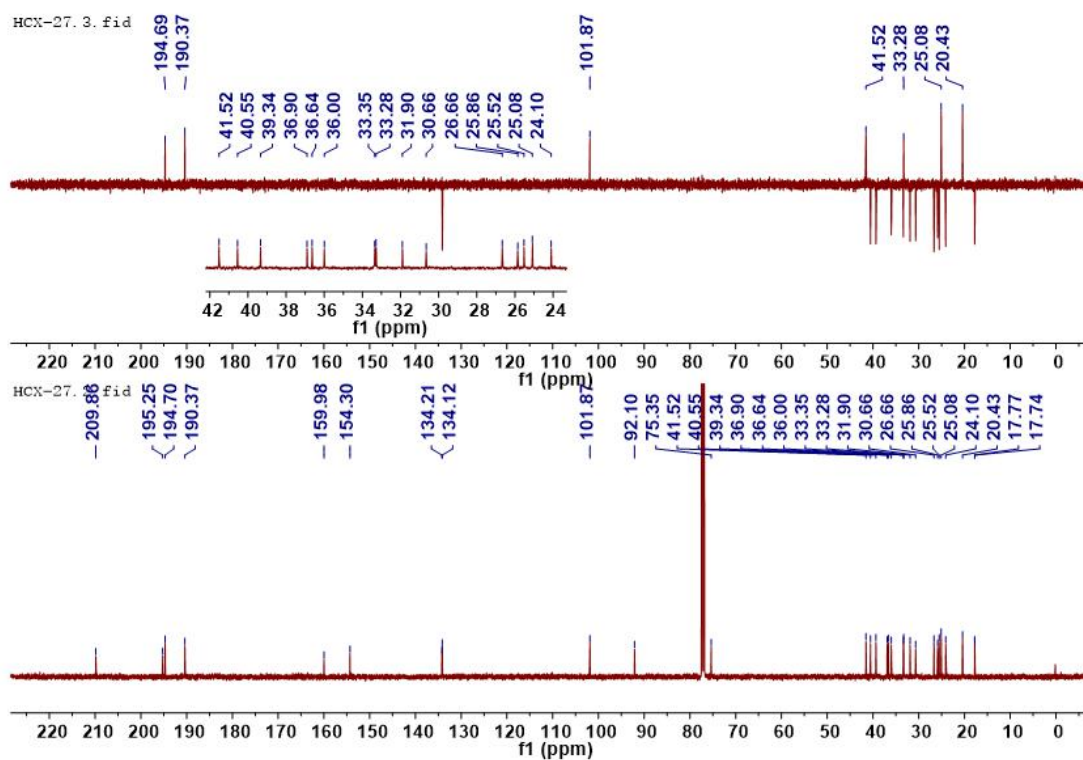
H	1.7326	-5.2807	-1.1487	H	2.2066	-5.2388	-1.7104
H	3.4611	-5.3011	-0.8099	H	3.8452	-5.2655	-1.0646
H	-7.2573	-1.9199	-2.4439	H	-7.7909	-2.8812	-0.149
H	-5.7745	-2.863	-2.6028	H	-7.5864	-1.967	-1.6441
H	-4.8926	-3.9161	-0.3208	H	-5.2602	-2.3724	-2.8723
H	-6.0216	-4.0639	1.0143	H	-4.3387	-3.8056	-2.4534
H	-4.0038	0.9752	-0.5433	H	-4.7328	0.5306	1.1436
H	-4.7464	0.7717	1.0138	H	-3.5107	-0.6914	1.3529
H	-2.227	-0.6629	0.0171	H	-3.8294	1.205	-1.0303
H	-2.0064	-1.5282	2.3177	H	-1.6892	0.3025	-1.8739
H	-3.4971	-0.7353	2.8044	H	-1.5585	-0.7772	-0.5005
H	-3.1407	-2.9326	0.727	H	-3.6672	-0.775	-2.6946
H	-3.9039	-3.1017	2.2994	H	-2.4103	-1.9786	-2.4599
H	-1.6341	0.8966	3.3773	H	-2.618	1.3371	2.5363
H	-6.2936	-2.365	2.6654	H	-2.6656	-3.8023	-0.7421
H	-5.7512	-0.7034	2.4573	H	-2.5791	-2.5841	0.5257
H	-7.0948	-1.3063	1.4972	H	-3.9269	-3.71	0.4944
H	-4.8434	0.873	-2.2984	H	-6.6618	0.2997	1.3493
H	5.6221	-2.8153	0.1791	H	5.6228	-2.9486	0.7414
H	-7.6808	-2.6746	-0.2391	H	-5.8903	-4.2406	-0.5414
H	-7.1975	-4.0972	-1.1487	H	-6.7466	-4.1542	-2.0725
5d-9	X axis(Å)	Y axis(Å)	Z axis(Å)	5d-10	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-2.4348	4.527	-1.8018	C	-1.2271	5.3217	-1.4705
C	-2.4747	4.4097	-0.2774	C	-1.6189	4.8239	-0.0799
C	-1.5871	3.2692	0.2477	C	-0.9919	3.4603	0.2593
C	-0.1317	3.3961	-0.2892	C	0.5527	3.4819	0.0679
C	-0.1004	3.4327	-1.8608	C	0.9359	3.9224	-1.3948
C	-1.008	4.5925	-2.3566	C	0.2864	5.3006	-1.6994
C	0.8366	2.3178	0.2425	C	1.2671	2.159	0.4377
C	2.2796	2.5566	-0.2459	C	2.7992	2.2889	0.3019
C	2.3586	2.6815	-1.7767	C	3.2221	2.7986	-1.086
C	1.3583	3.7023	-2.33	C	2.4794	4.0734	-1.4901
C	-0.5751	2.1183	-2.535	C	0.4939	2.9199	-2.4937
C	-1.6131	3.2524	1.7595	C	-1.3777	3.072	1.6666
O	-1.1179	4.0933	2.4971	O	-0.9811	3.6054	2.694
O	0.3945	4.6751	0.1597	O	1.0943	4.498	0.9562
C	3.2163	1.5051	0.2935	C	3.5231	1.0079	0.6293
O	3.354	0.3243	-0.4361	O	3.3505	-0.0702	-0.2407
C	3.9336	1.6239	1.4095	C	4.3616	0.8425	1.6505
C	5.4962	-0.9612	-2.0703	C	5.0286	-1.3288	-2.3442
C	5.6829	-0.2292	-0.7485	C	5.5065	-0.8581	-0.9764
C	4.4554	-0.4037	0.1582	C	4.3976	-1.0197	0.0745
C	4.1437	-1.9156	0.4365	C	3.9163	-2.5077	0.1795
C	4.0415	-2.7535	-0.8936	C	3.5018	-3.0994	-1.2205
C	5.235	-2.4441	-1.8417	C	4.5785	-2.7836	-2.2983
C	2.8826	-2.1353	1.3124	C	2.7838	-2.723	1.2139
C	1.5332	-1.9425	0.5943	C	1.3834	-2.2694	0.7641

C	1.4828	-2.7203	-0.7317	C	1.0218	-2.7947	-0.634
C	2.703	-2.4642	-1.6164	C	2.1255	-2.542	-1.6622
C	0.3907	-2.2573	1.5496	C	0.3404	-2.6592	1.7989
C	8.00E-04	-1.1938	2.52	C	-0.369	-1.5778	2.5365
C	-0.3254	-3.3921	1.6091	C	0.0028	-3.9204	2.1184
C	4.1228	-4.2828	-0.6119	C	3.4031	-4.653	-1.177
C	4.6779	0.3771	1.4351	C	4.8863	-0.4898	1.4052
O	5.3858	0.0383	2.3737	O	5.6286	-1.0712	2.1847
C	-4.5617	-4.274	-0.8881	C	-7.1271	-2.4539	-0.712
C	-3.7106	-3.0293	-0.8163	C	-6.3659	-1.331	-0.0435
C	-4.1623	-1.8211	-0.4002	C	-5.0133	-1.2287	-0.0525
C	-5.6371	-1.6219	0.0028	C	-4.1394	-2.2603	-0.7978
C	-6.3717	-2.9717	0.2357	C	-4.9721	-3.1645	-1.7481
C	-3.3066	-0.5612	-0.3044	C	-4.2098	-0.1376	0.6471
C	-3.4474	0.1682	1.0493	C	-3.2152	0.569	-0.2959
C	-4.923	0.4614	1.3488	C	-2.2881	-0.4609	-0.9533
C	-5.7454	-0.8235	1.3265	C	-3.0878	-1.5386	-1.6809
C	-2.6416	1.4438	1.1249	C	-2.3944	1.6561	0.3602
C	-2.3148	2.0783	2.2497	C	-2.3084	1.9557	1.6555
O	-2.2095	2.0042	-0.0739	O	-1.6434	2.4349	-0.5204
C	-6.3602	-0.8543	-1.1298	C	-3.4252	-3.1618	0.2364
C	-2.3155	-3.2461	-1.3026	C	-7.2674	-0.353	0.645
O	-1.8195	-4.3623	-1.4105	O	-8.4903	-0.4374	0.6023
O	5.2588	-2.4738	1.1756	O	5.0373	-3.3073	0.6348
C	-6.0587	-3.9979	-0.8411	C	-6.2616	-3.6442	-1.1039
O	0.4947	-0.073	2.5165	O	-0.2152	-0.3878	2.2928
H	-0.7815	-1.4684	3.2478	H	-1.0678	-1.9108	3.3227
H	-2.9735	3.6836	-2.2479	H	-1.7328	4.7184	-2.2324
H	-2.9799	5.4282	-2.1069	H	-1.596	6.3458	-1.6028
H	-2.1627	5.3659	0.1618	H	-1.3189	5.5735	0.6636
H	-3.5172	4.2539	0.029	H	-2.7139	4.7627	-0.0328
H	-0.5712	5.5582	-2.0704	H	0.7412	6.0762	-1.0694
H	-1.0512	4.5955	-3.4532	H	0.4944	5.5951	-2.736
H	0.8545	2.3514	1.3391	H	1.0542	1.906	1.4838
H	0.4936	1.3154	-0.035	H	0.8908	1.3271	-0.1681
H	2.6142	3.5207	0.1639	H	3.1296	3.0438	1.0301
H	3.3724	2.9827	-2.0702	H	4.3007	3.0033	-1.091
H	2.1828	1.7096	-2.2533	H	3.0608	2.025	-1.8466
H	1.4116	3.6959	-3.4263	H	2.7723	4.3487	-2.5114
H	1.6771	4.7066	-2.0225	H	2.822	4.8969	-0.8503
H	-0.0398	1.2379	-2.1697	H	0.8394	1.901	-2.3002
H	-1.6407	1.9252	-2.3975	H	-0.5891	2.8717	-2.6215
H	-0.4123	2.1646	-3.6188	H	0.9015	3.2164	-3.468
H	0.2868	4.7288	1.1333	H	0.7646	4.3196	1.8628
H	3.9846	2.4149	2.1323	H	4.6589	1.5126	2.4339
H	4.6764	-0.512	-2.6419	H	4.2145	-0.6895	-2.7039
H	6.3995	-0.843	-2.6803	H	5.8456	-1.2259	-3.068

H	6.5871	-0.5957	-0.246	H	6.4027	-1.4179	-0.681
H	5.8561	0.8325	-0.9666	H	5.8107	0.193	-1.0629
H	6.1531	-2.8842	-1.4288	H	5.4692	-3.4002	-2.1153
H	5.0781	-2.9307	-2.8131	H	4.211	-3.0732	-3.2913
H	2.9209	-3.1485	1.7374	H	2.7612	-3.7888	1.48
H	2.9327	-1.4854	2.1956	H	3.04	-2.2291	2.1604
H	1.426	-0.8889	0.32	H	1.3979	-1.1782	0.6895
H	1.3976	-3.7977	-0.5566	H	0.7951	-3.8667	-0.6046
H	0.5851	-2.4302	-1.289	H	0.1026	-2.3103	-0.9826
H	2.6198	-3.0926	-2.5129	H	1.825	-3.0005	-2.6135
H	2.6632	-1.4333	-1.9812	H	2.1802	-1.4677	-1.8634
H	-1.1347	-3.5418	2.3179	H	-0.7464	-4.1582	2.868
H	-0.1293	-4.2324	0.9488	H	0.4785	-4.7687	1.6336
H	3.3657	-4.6241	0.0989	H	2.7124	-5.0127	-0.4099
H	3.9841	-4.8556	-1.5366	H	3.0554	-5.0467	-2.1395
H	5.0986	-4.5681	-0.2029	H	4.3758	-5.1157	-0.9755
H	-4.3519	-4.8303	-1.81	H	-7.9219	-2.8242	-0.0529
H	-4.2873	-4.9277	-0.0501	H	-7.6152	-2.0521	-1.6093
H	-6.0805	-3.3975	1.2059	H	-5.2326	-2.6149	-2.6632
H	-7.4563	-2.8126	0.286	H	-4.3788	-4.0292	-2.0713
H	-2.2433	-0.7744	-0.4435	H	-4.8481	0.6277	1.092
H	-3.5949	0.1044	-1.1282	H	-3.6736	-0.5962	1.488
H	-3.0685	-0.5092	1.8286	H	-3.8048	1.0542	-1.0877
H	-5.0257	0.9215	2.3399	H	-1.6236	0.0277	-1.6773
H	-5.3264	1.1859	0.6309	H	-1.6382	-0.9179	-0.1997
H	-5.4089	-1.4503	2.164	H	-3.5896	-1.0603	-2.5336
H	-6.7953	-0.5777	1.5321	H	-2.391	-2.2709	-2.1088
H	-2.5172	1.8453	3.2771	H	-2.7553	1.5117	2.5231
H	-7.4228	-0.7199	-0.8964	H	-2.8159	-3.9249	-0.2616
H	-5.9387	0.1423	-1.2953	H	-2.757	-2.5962	0.8913
H	-6.2963	-1.3858	-2.0855	H	-4.1397	-3.6794	0.8857
H	-1.7432	-2.3494	-1.5748	H	-6.7924	0.4631	1.2023
H	5.4197	-1.914	1.965	H	5.3852	-2.9111	1.4623
H	-6.4069	-3.6468	-1.8191	H	-6.0463	-4.2591	-0.2226
H	-6.5969	-4.9307	-0.6363	H	-6.8134	-4.2841	-1.8022

Table S12 DP4+ results obtained for compounds **1– 5**

Exp NMR from	Cal NMR from	sDP4+	sDP4+	sDP4+	uDP4+	uDP4+	uDP4+	DP4+	DP4+	DP4+
		(H data)	(C data)	(all data)	(H data)	(C data)	(all data)	(H data)	(C data)	(all data)
1	1a&1b& 1c&1d	100.00%	91.39%	100.00%	100.00%	53.02%	100.00%	100.00%	92.50%	100.00%
2	2c&2d& 2c&2d	100.00%	90.64%	100.00%	100.00%	67.02%	100.00%	100.00%	95.16%	100.00%
3	3c&3d& 3c&3d	100.00%	87.82%	100.00%	100.00%	61.03%	100.00%	100.00%	97.44%	100.00%
4	4c&4d& 4c&4d	100.00%	72.22%	100.00%	100.00%	93.48%	100.00%	100.00%	98.84%	100.00%
5	5c&5d&	100.00%	68.40%	100.00%	100.00%	25.41%	100.00%	100.00%	63.89%	100.00%

Figure S31. ¹H NMR (600 MHz) spectrum of **1** in CDCl₃Figure S32. ¹³C NMR and DEPT (150 MHz) spectra of **1** in CDCl₃

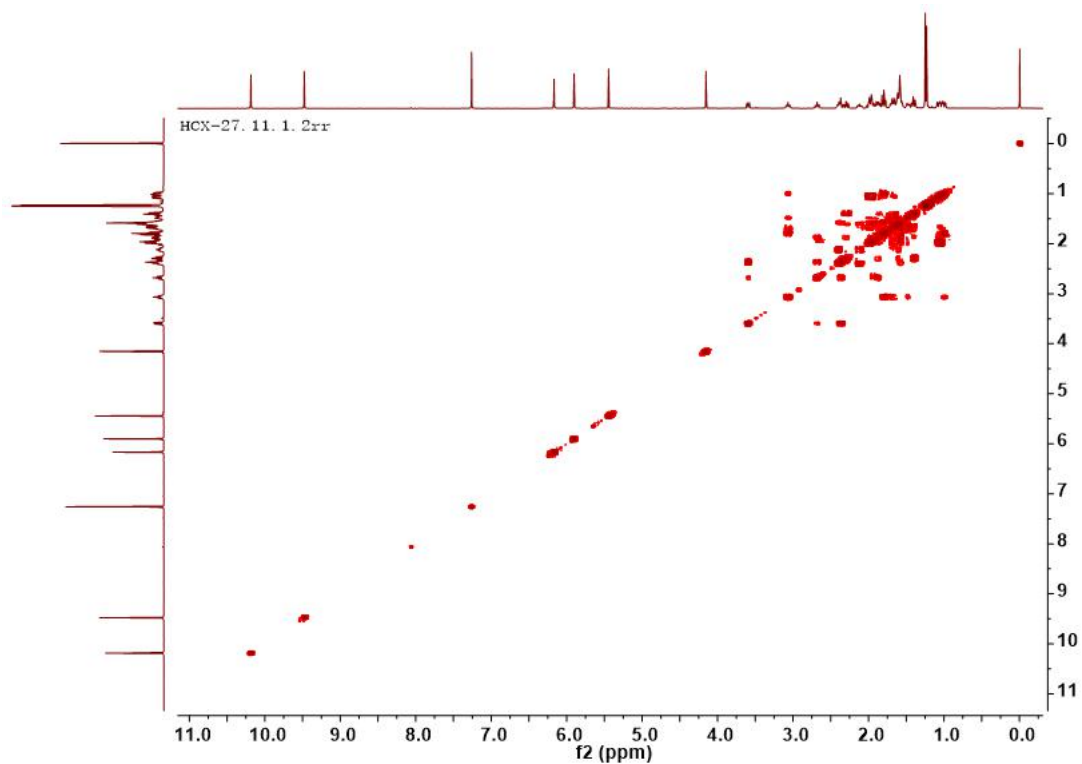


Figure S33. HSQC (600 MHz) spectrum of **1** in CDCl₃

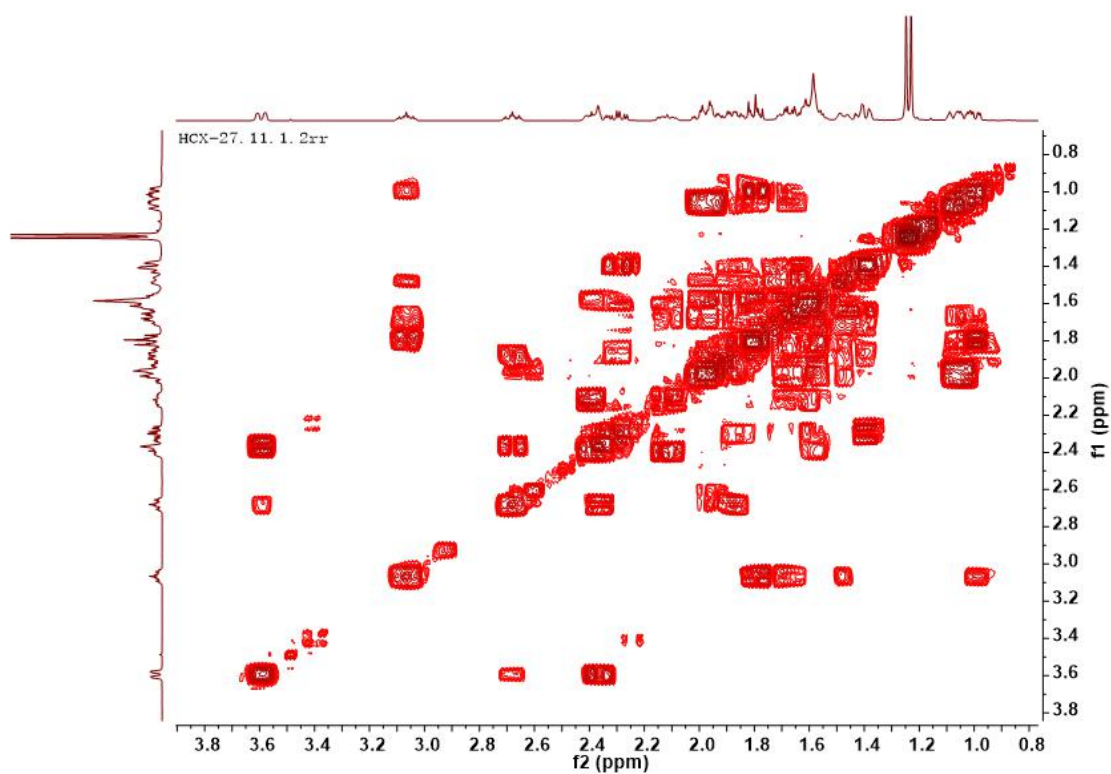


Figure S34. Enlarged ¹H-¹H COSY (600 MHz) spectrum of **1** in CDCl₃

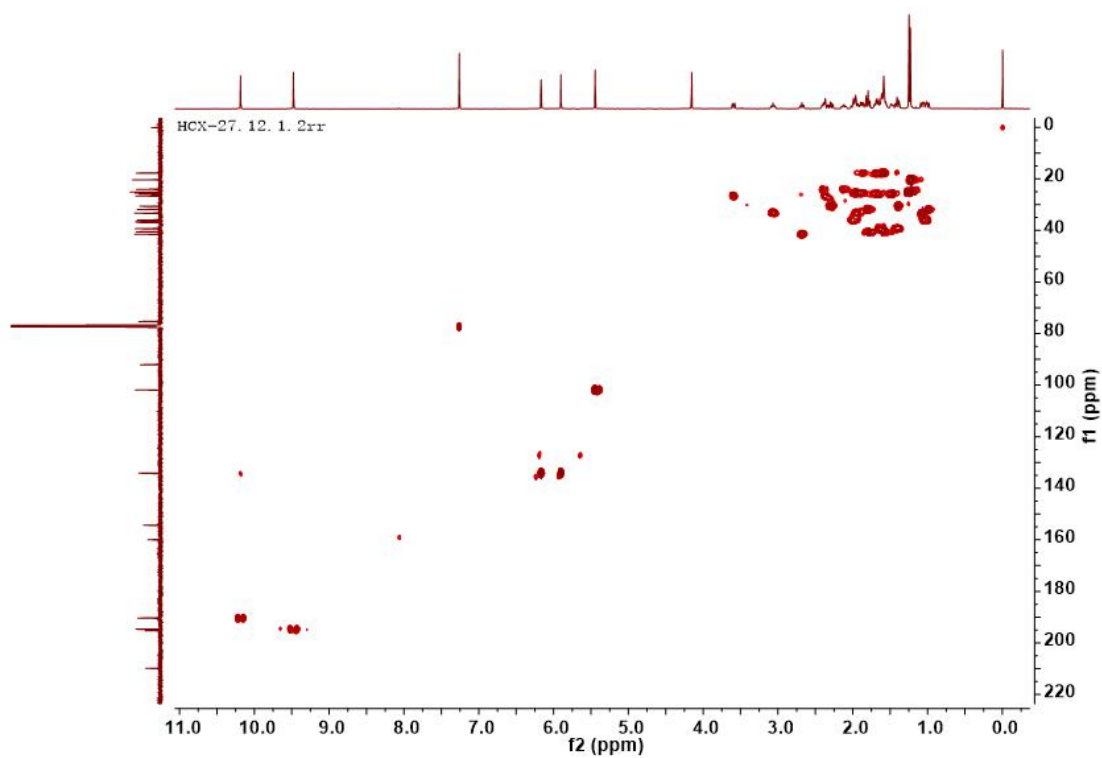


Figure S35. HSQC (600 MHz) spectrum of **1** in CDCl₃

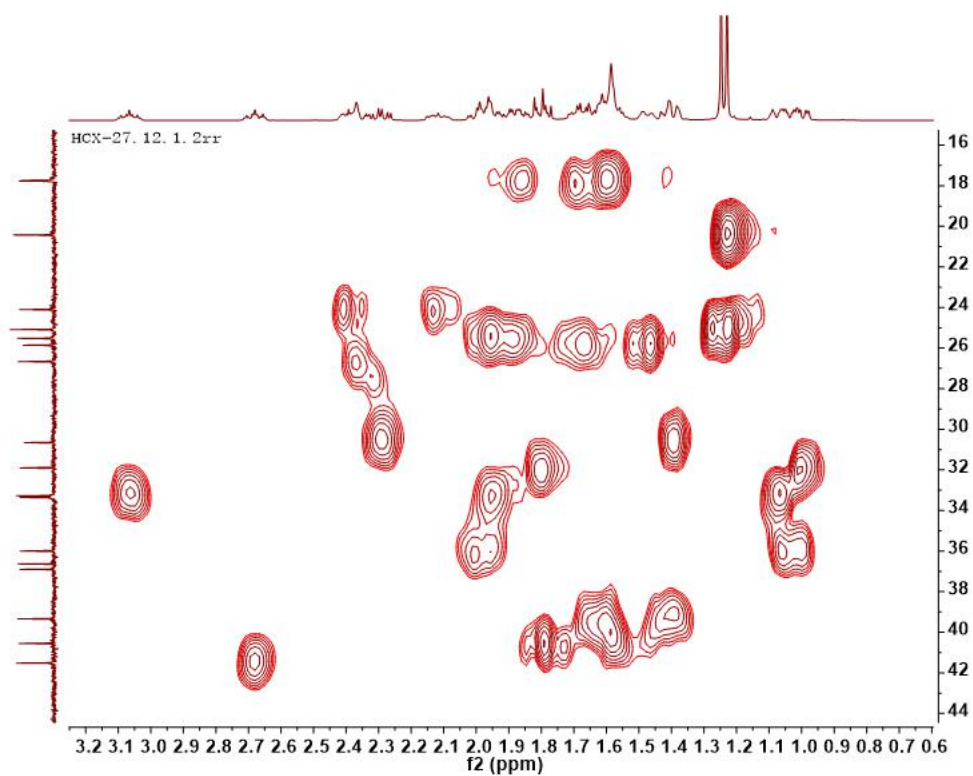


Figure S36. Enlarged HSQC (600 MHz) spectrum of **1** in CDCl₃

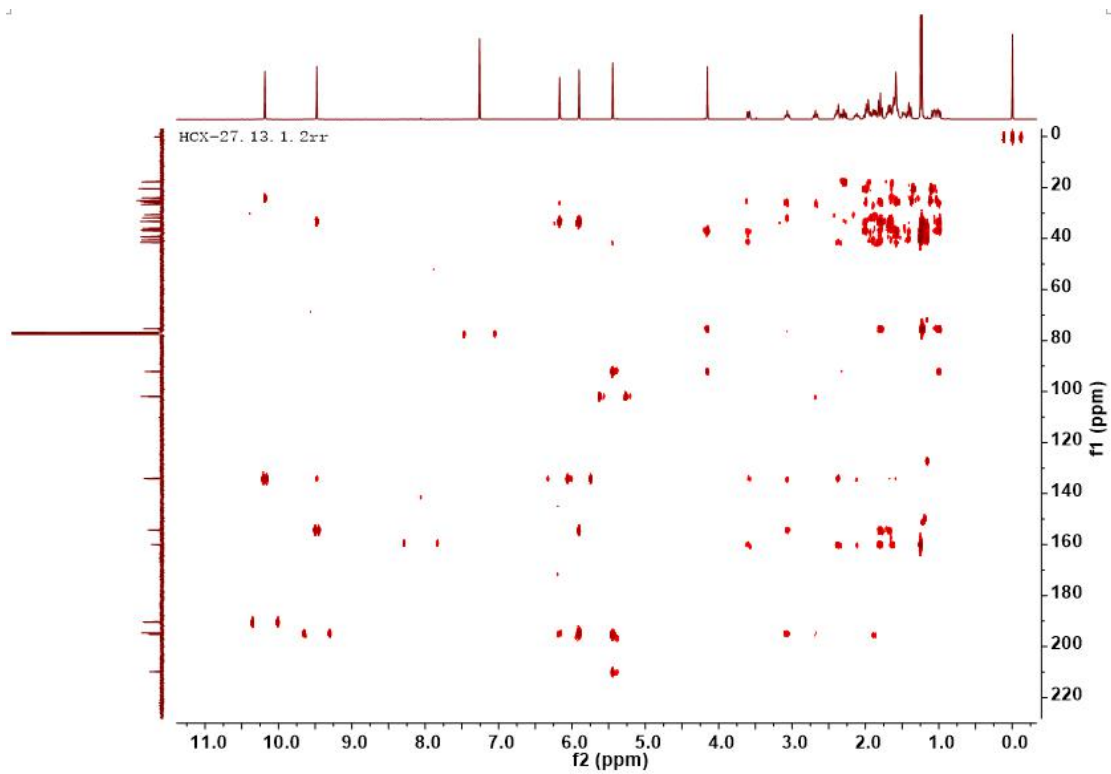


Figure S37. HMBC (600 MHz) spectrum of **1** in CDCl₃

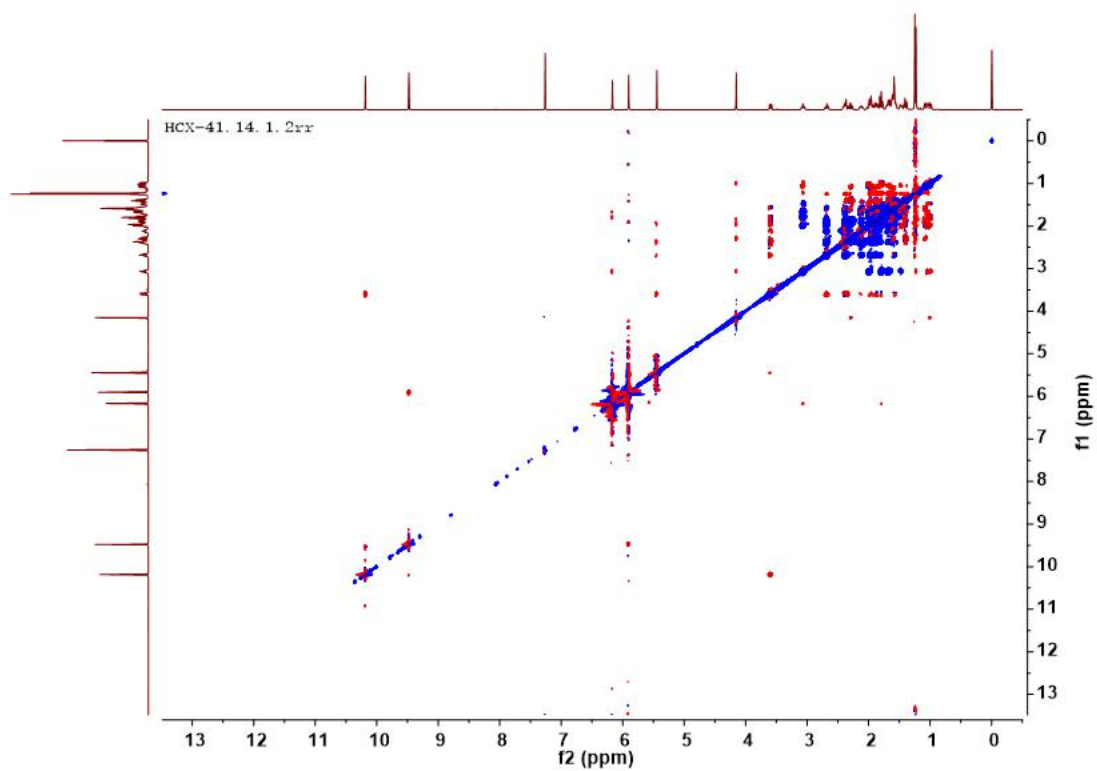


Figure S38. ROESY (600 MHz) spectrum of **1** in CDCl₃

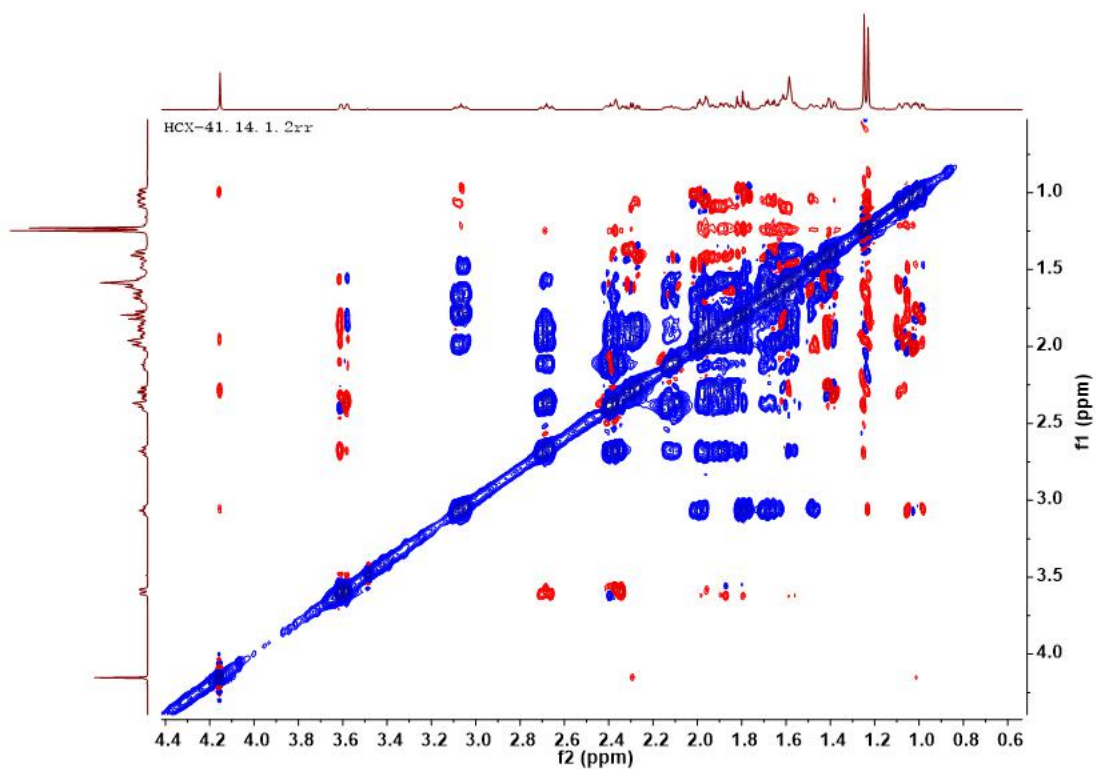


Figure S39. Enlarged ROESY (600 MHz) spectrum of **1** in CDCl₃

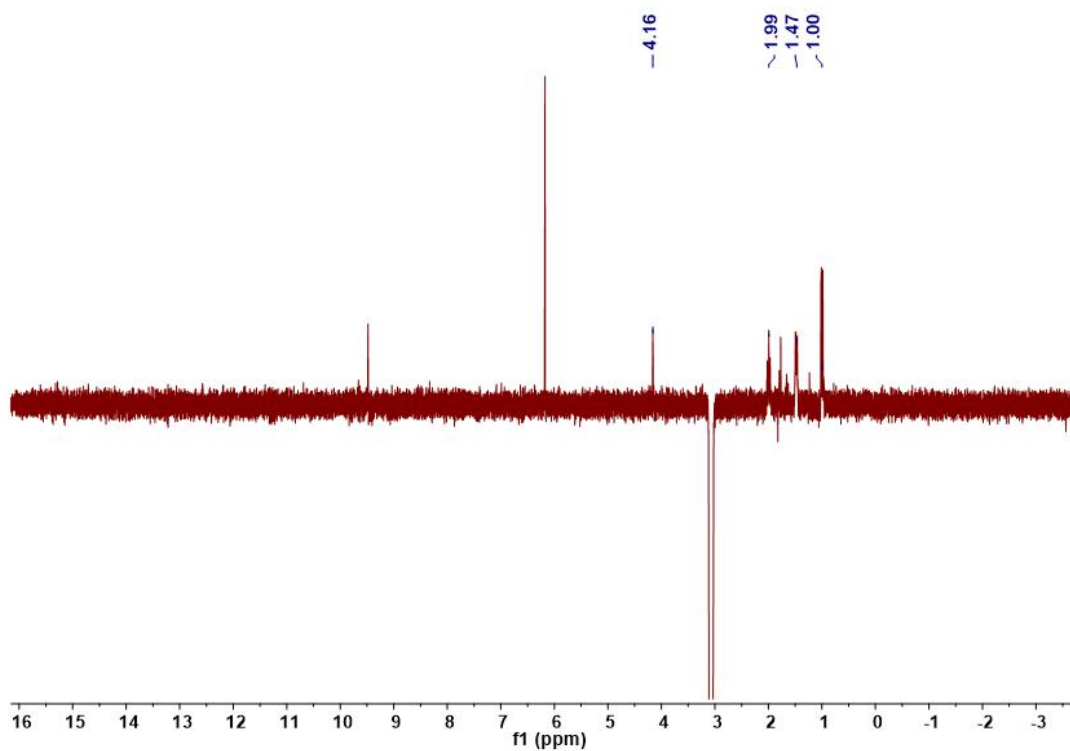


Figure S40. NOE irradiation spectrum (freq: 3.06 ppm) of compound **1** in CDCl₃

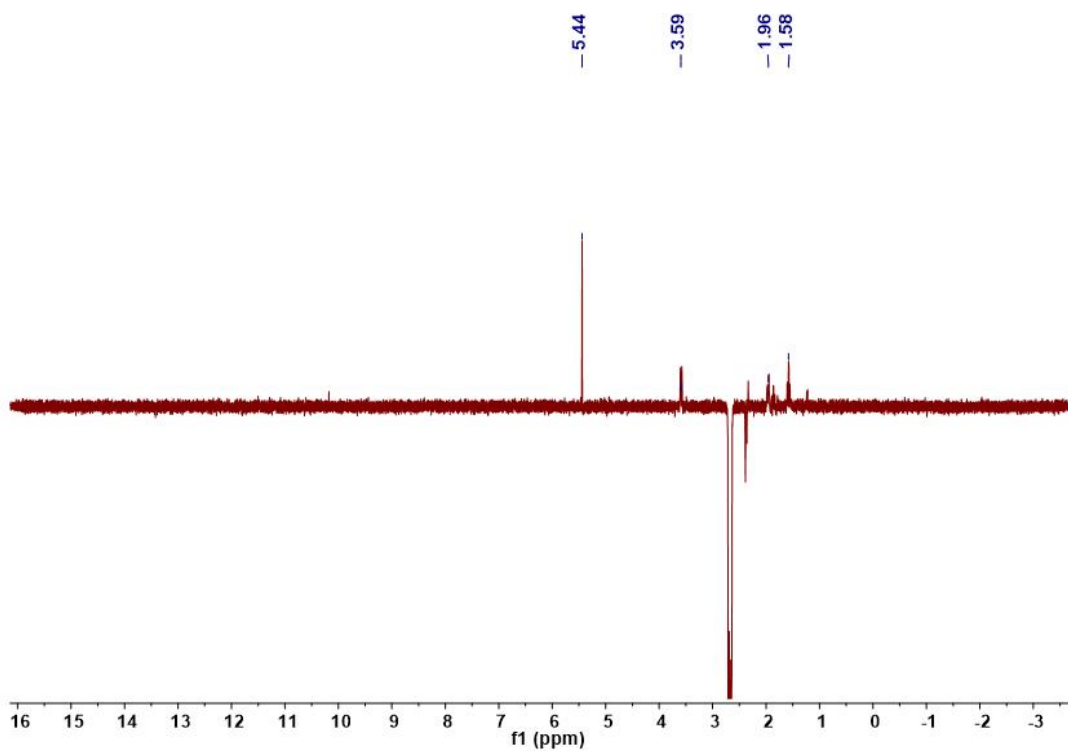


Figure S41. NOE irradiation spectrum (freq: 2.68 ppm) of compound **1** in CDCl₃

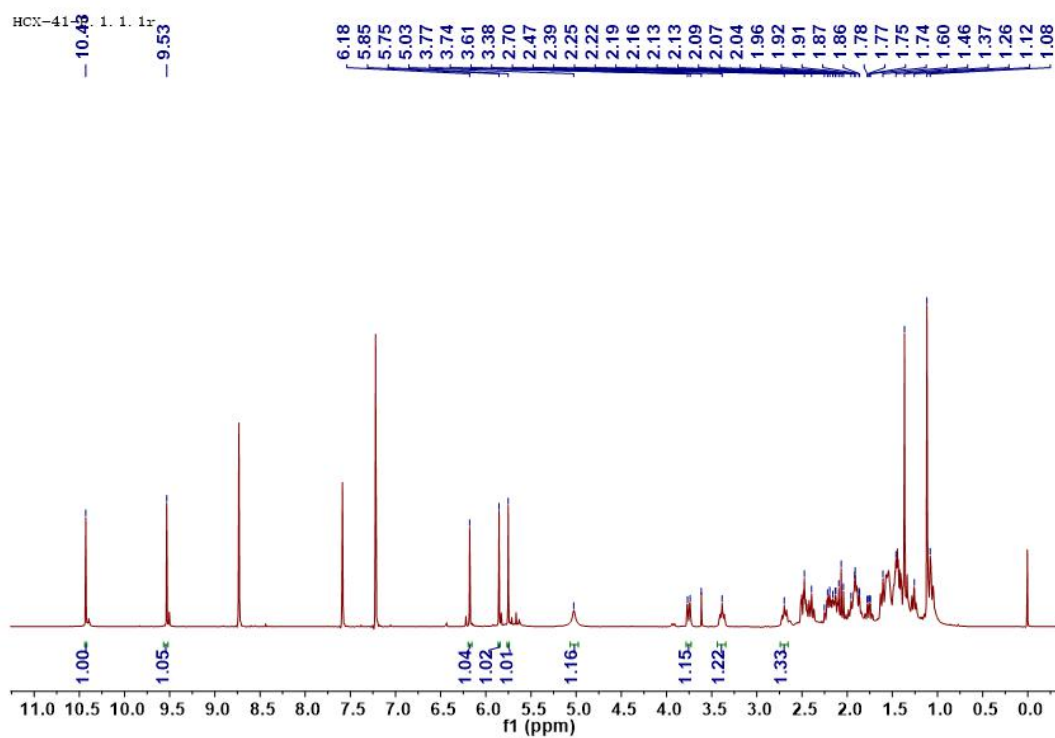


Figure S42. ¹H NMR (600 MHz) spectrum of **1** in Pyridine-*d*₃

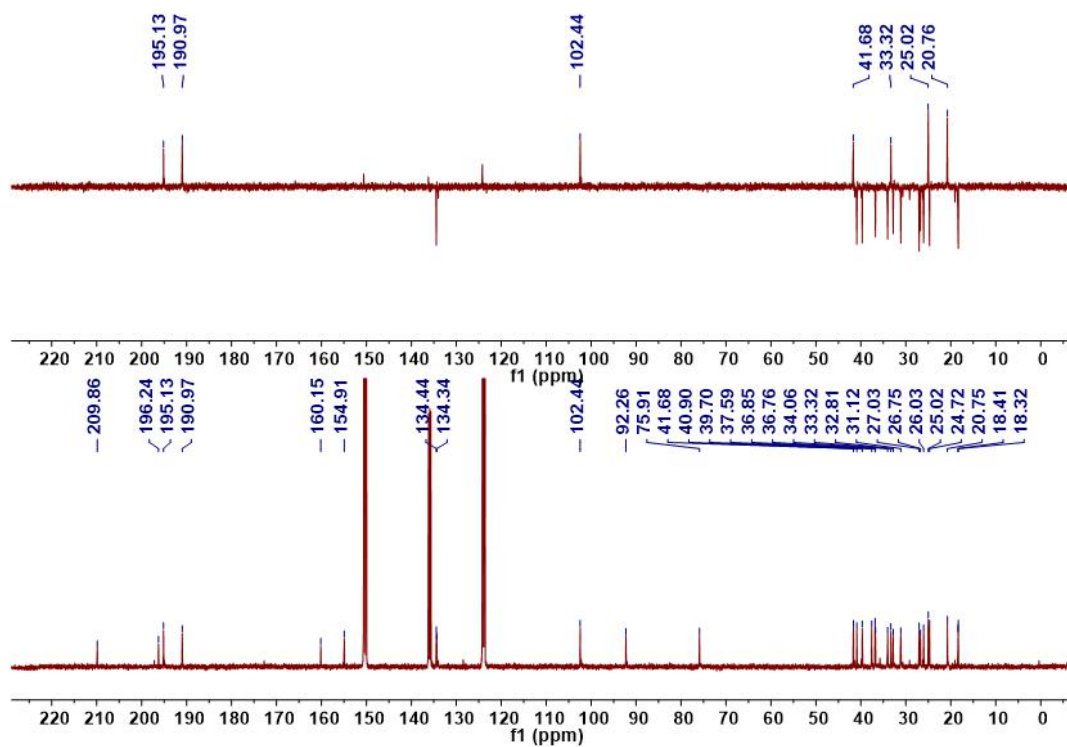


Figure S43. ^{13}C NMR and DEPT (150 MHz) spectra of **1** in pyridine- d_5

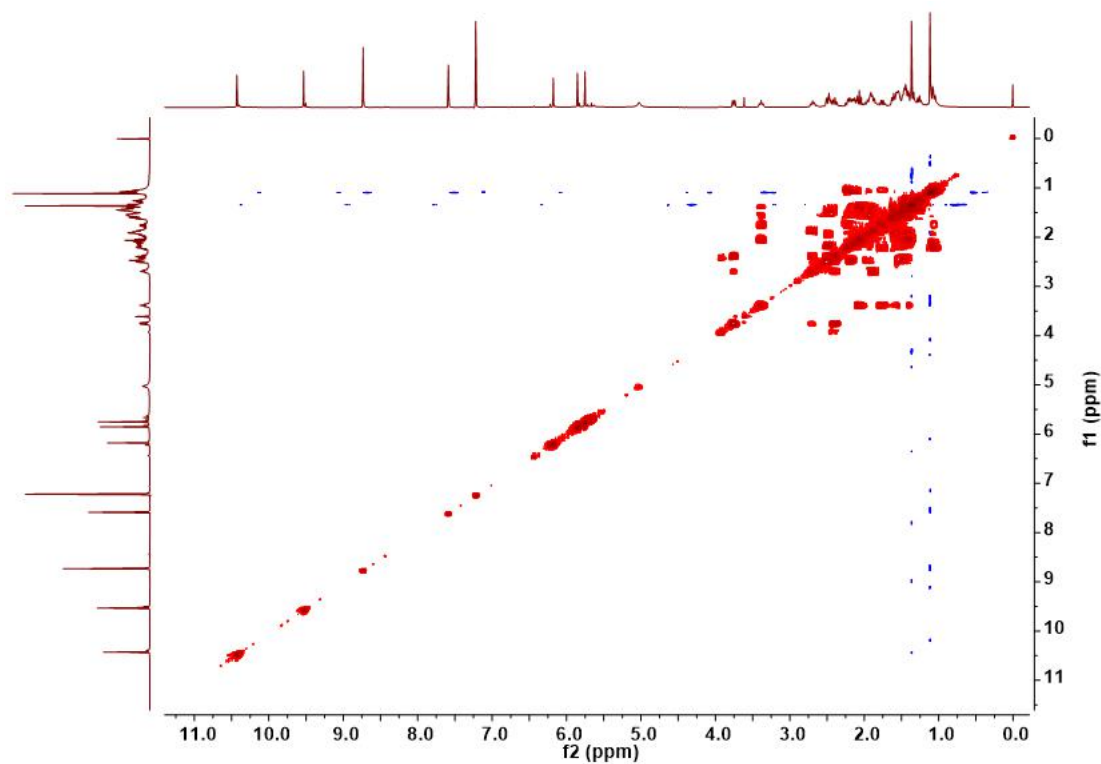


Figure S44. ^1H - ^1H COSY (600 MHz) spectrum of **1** in pyridine- d_5

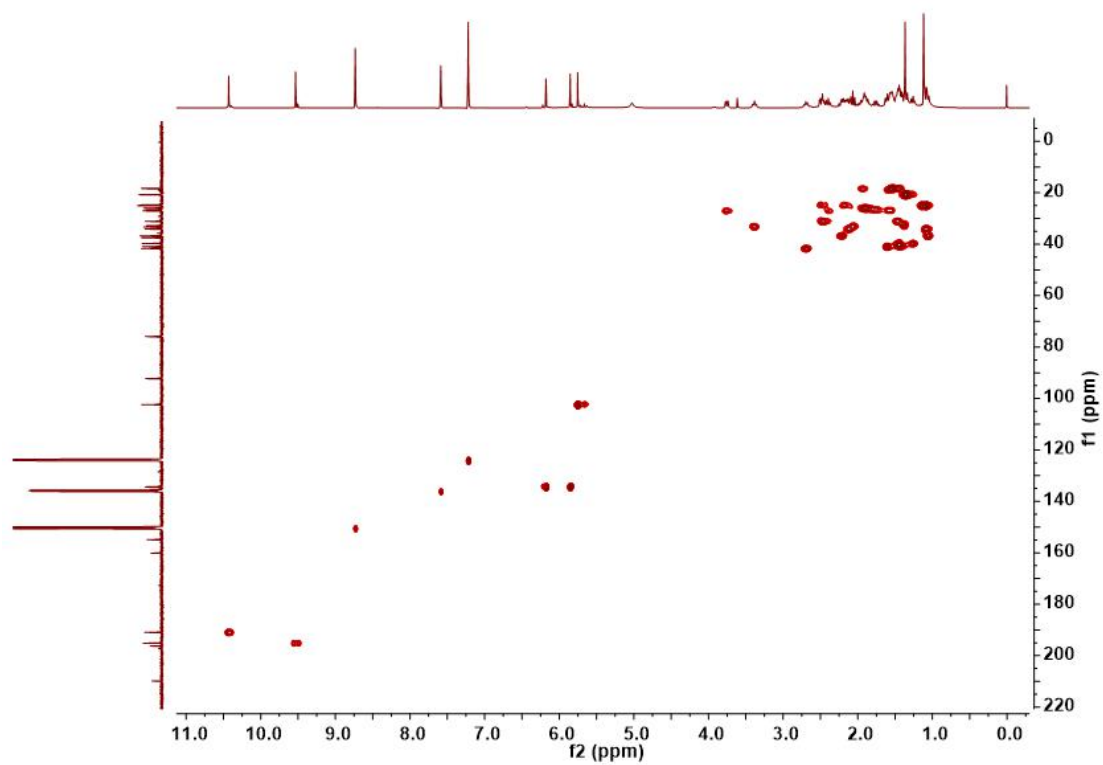


Figure S45. HSQC (600 MHz) spectrum of **1** in pyridine-*d*₅

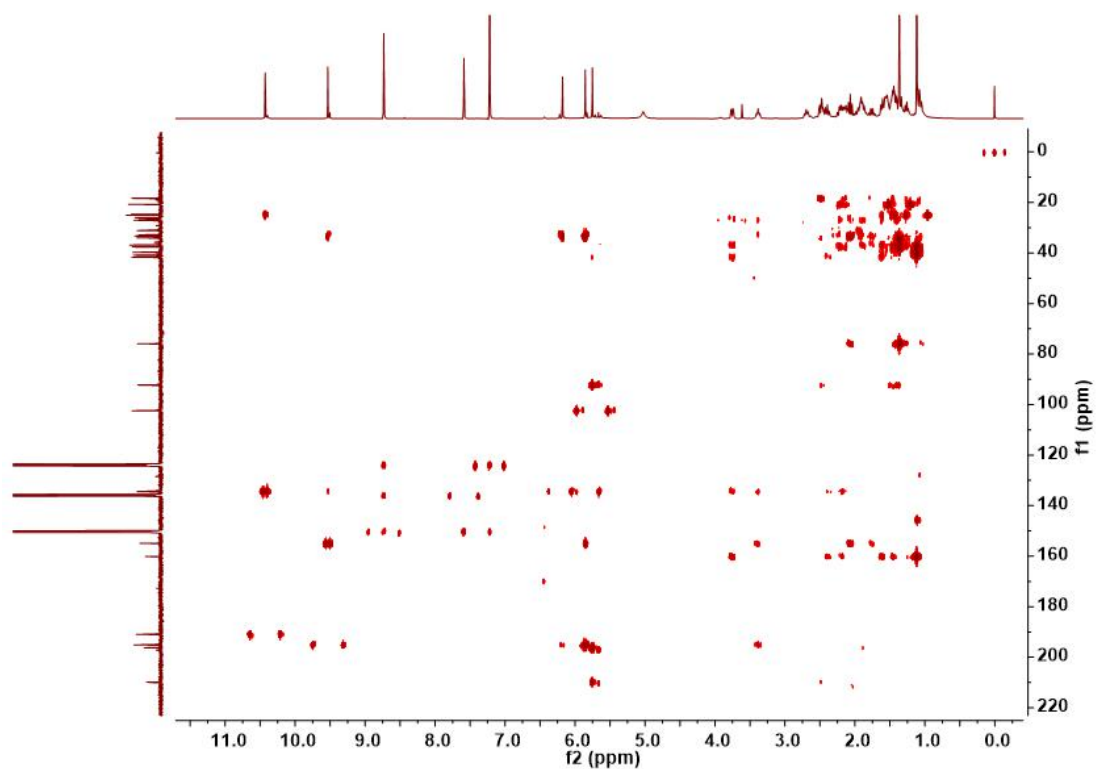


Figure S46. HMBC (600 MHz) spectrum of **1** in pyridine-*d*₅

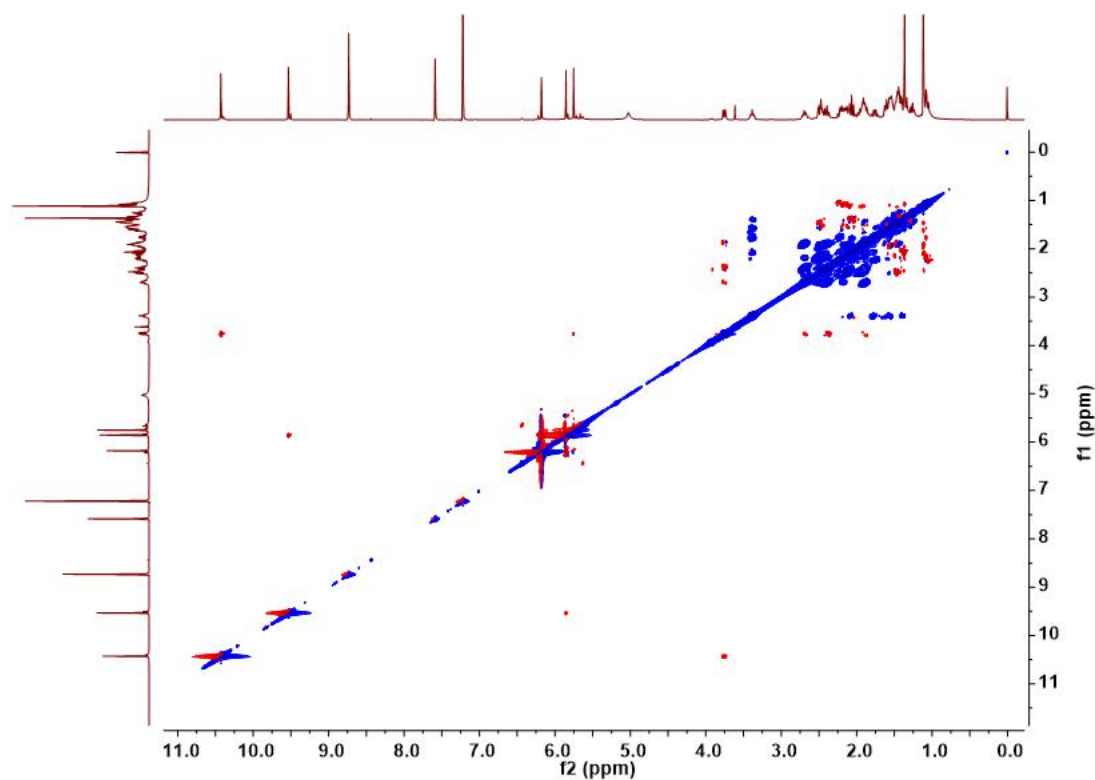


Figure S47. ROESY (600 MHz) spectrum of **1** in pyridine-*d*₅

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

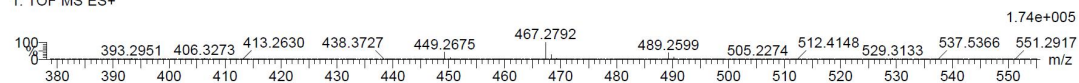
129 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 29-29 H: 0-80 N: 0-5 O: 0-10 Na: 0-1

HCX-41 241 (1.353)

1: TOF MS ES+



Minimum:

Maximum: 20.0 5.0 -1.5

50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
467.2792	467.2797	-0.5	-1.1	10.5	498.0	n/a	n/a	C ₂₉ H ₃₉ O ₅

Figure S48. HRESIMS of **1**

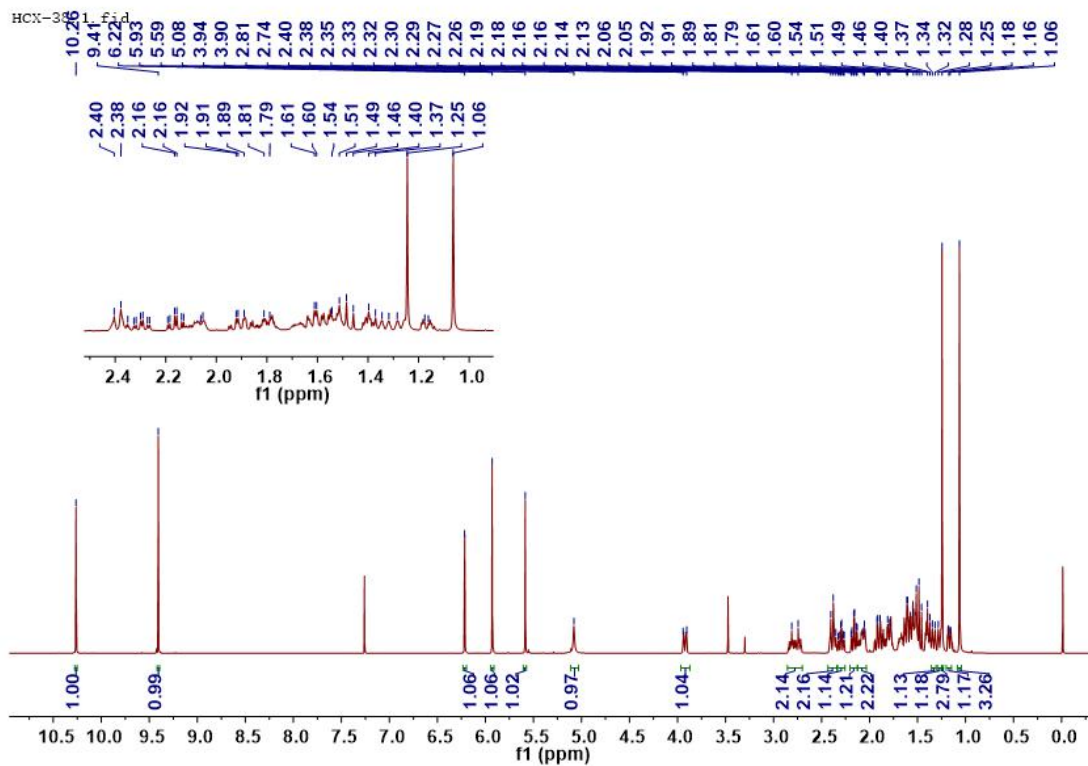


Figure S49. ^1H NMR (600 MHz) spectrum of **2** in CDCl_3

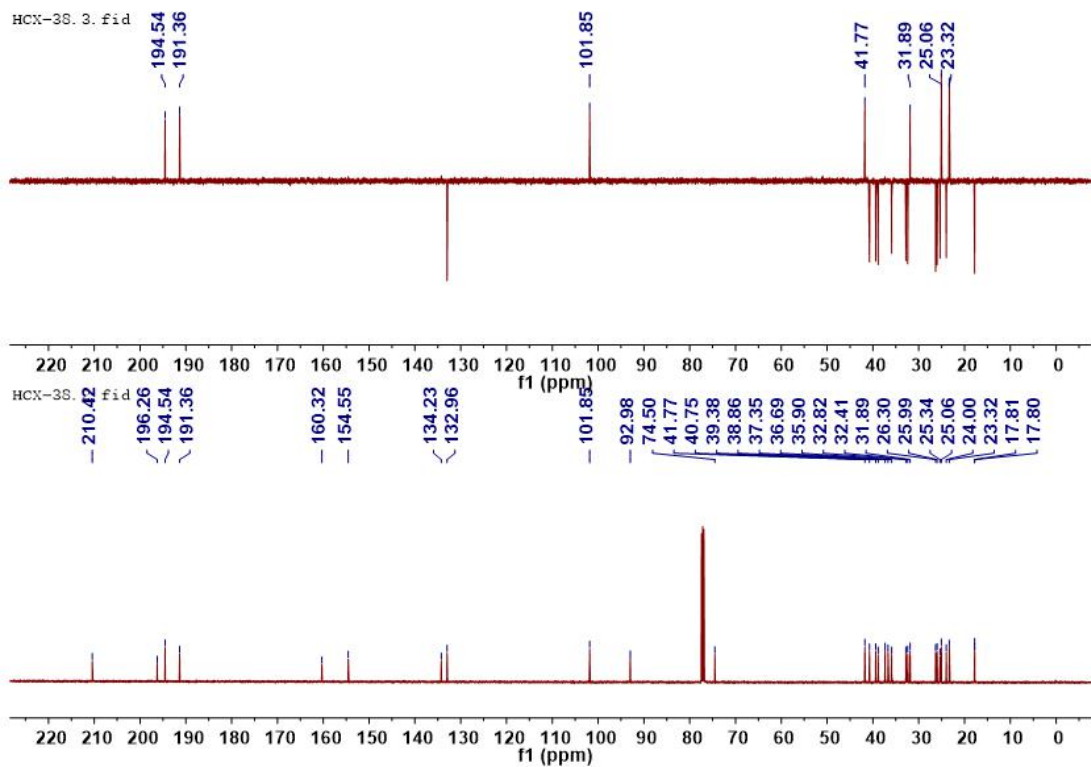


Figure S50. ^{13}C NMR and DEPT (150 MHz) spectra of **2** in CDCl_3

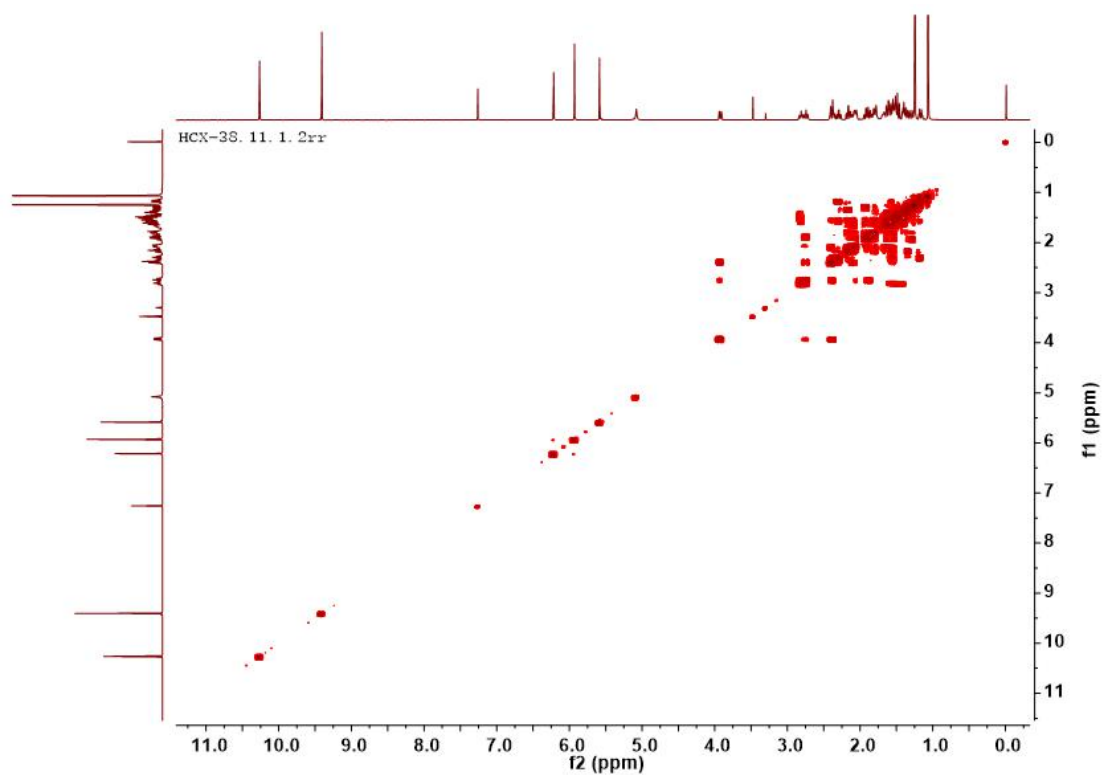


Figure S51. ^1H - ^1H COSY (600 MHz) spectrum of **2** in CDCl_3

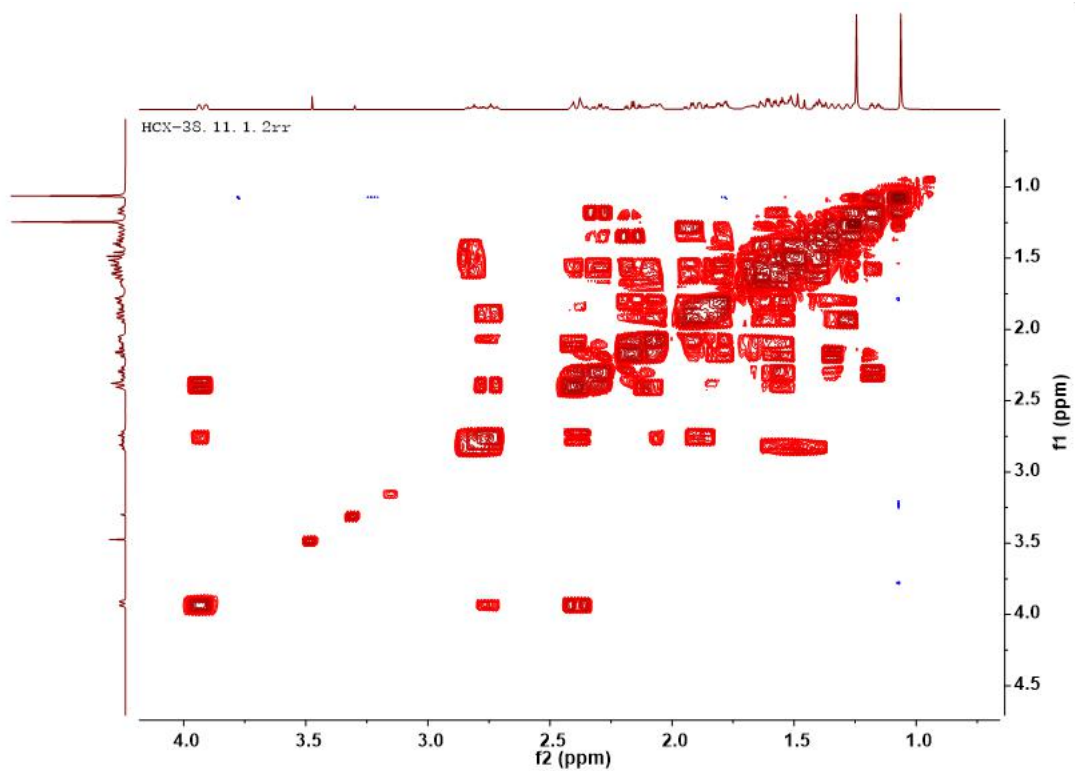


Figure S52. Enlarged ^1H - ^1H COSY (600 MHz) spectrum of **2** in CDCl_3

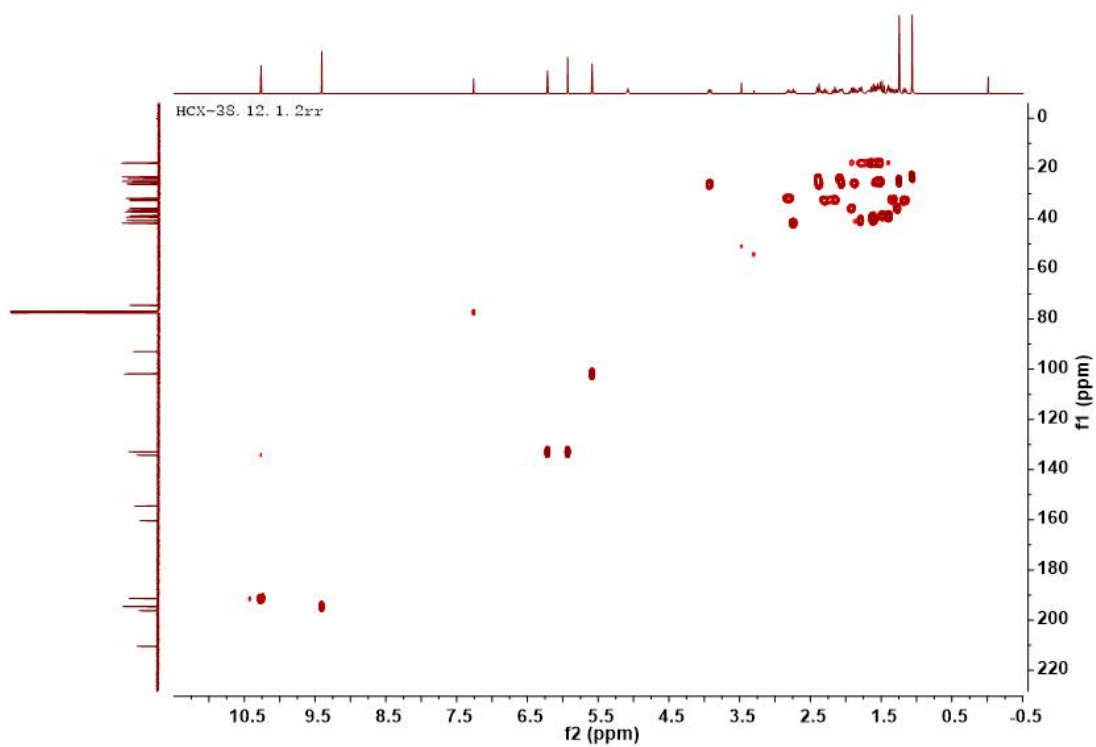


Figure S53. HSQC (600 MHz) spectrum of **2** in CDCl₃

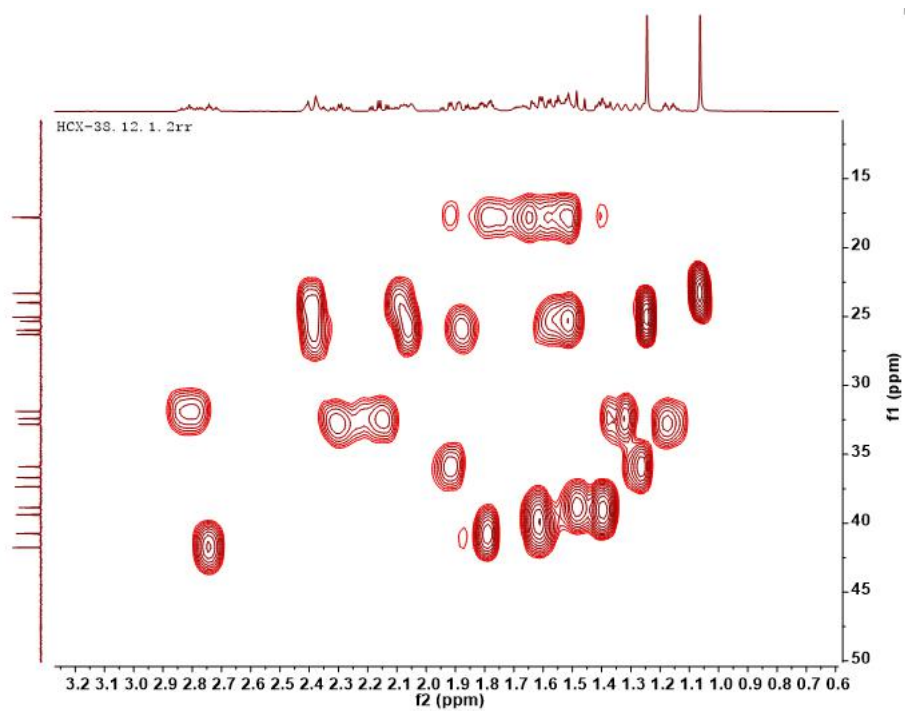


Figure S54. Enlarged HSQC (600 MHz) spectrum of **2** in CDCl₃

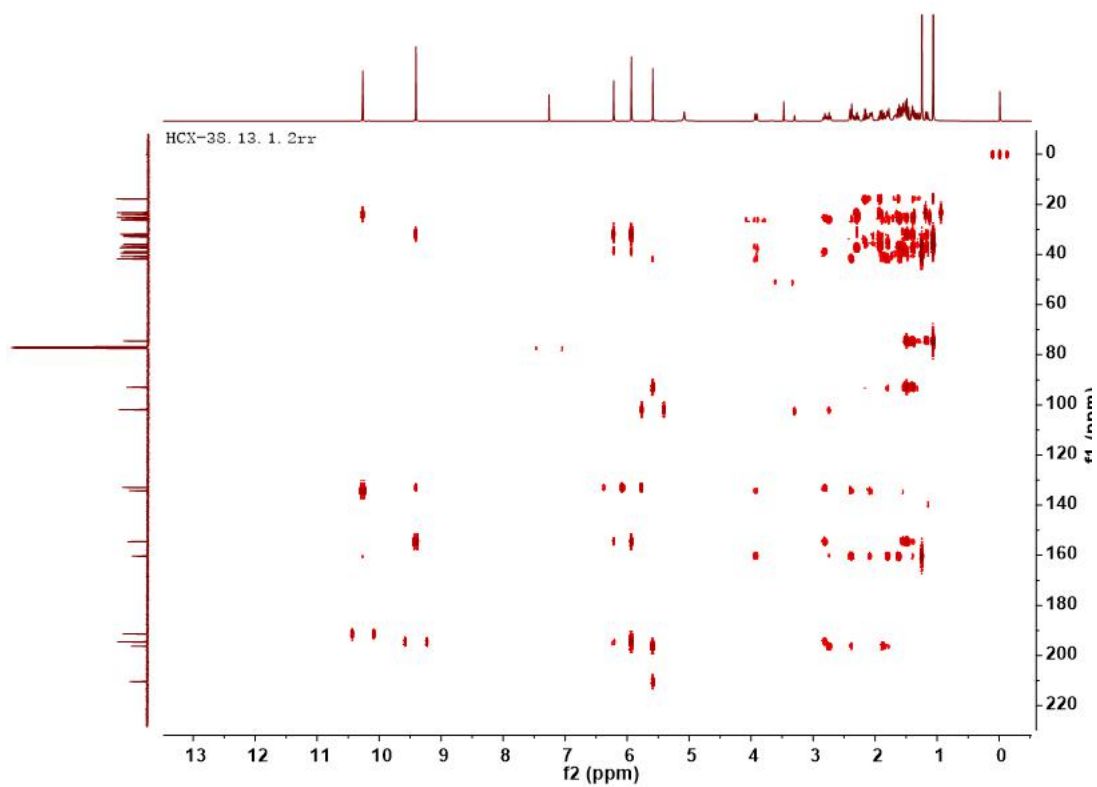


Figure S55. HMBC (600 MHz) spectrum of **2** in CDCl₃

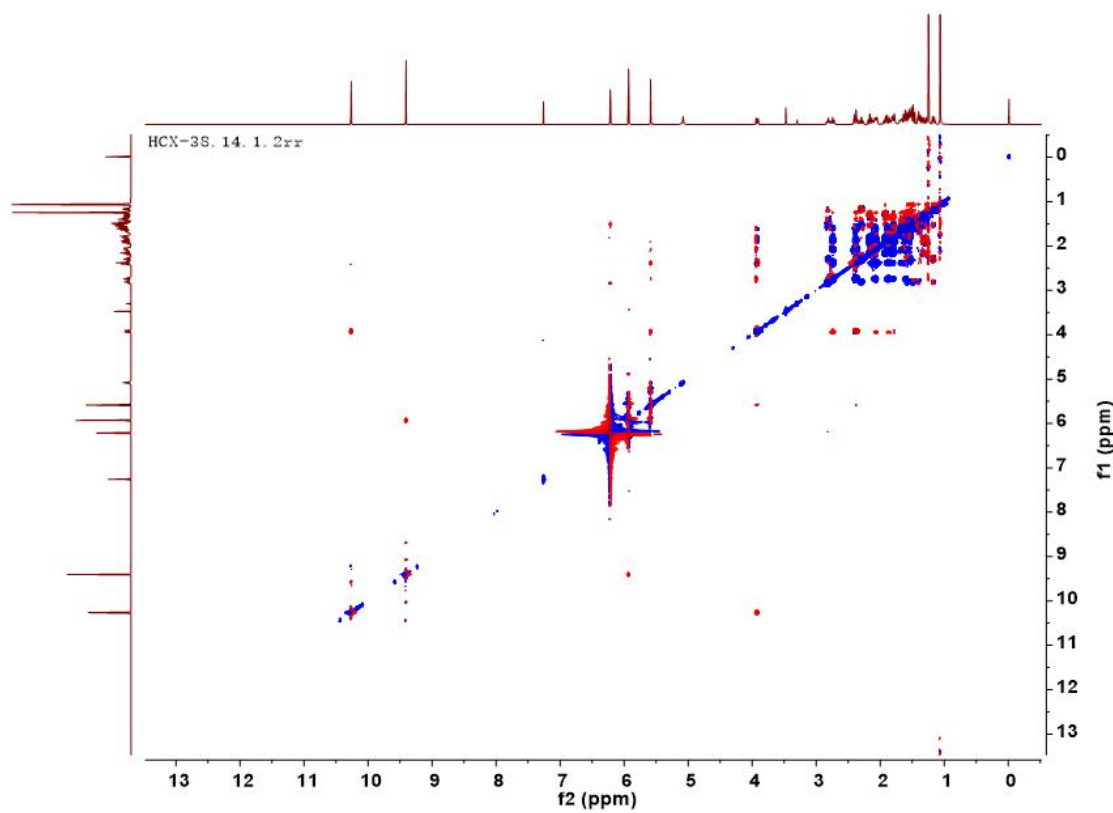


Figure S56. ROESY (600 MHz) spectrum of **2** in CDCl₃

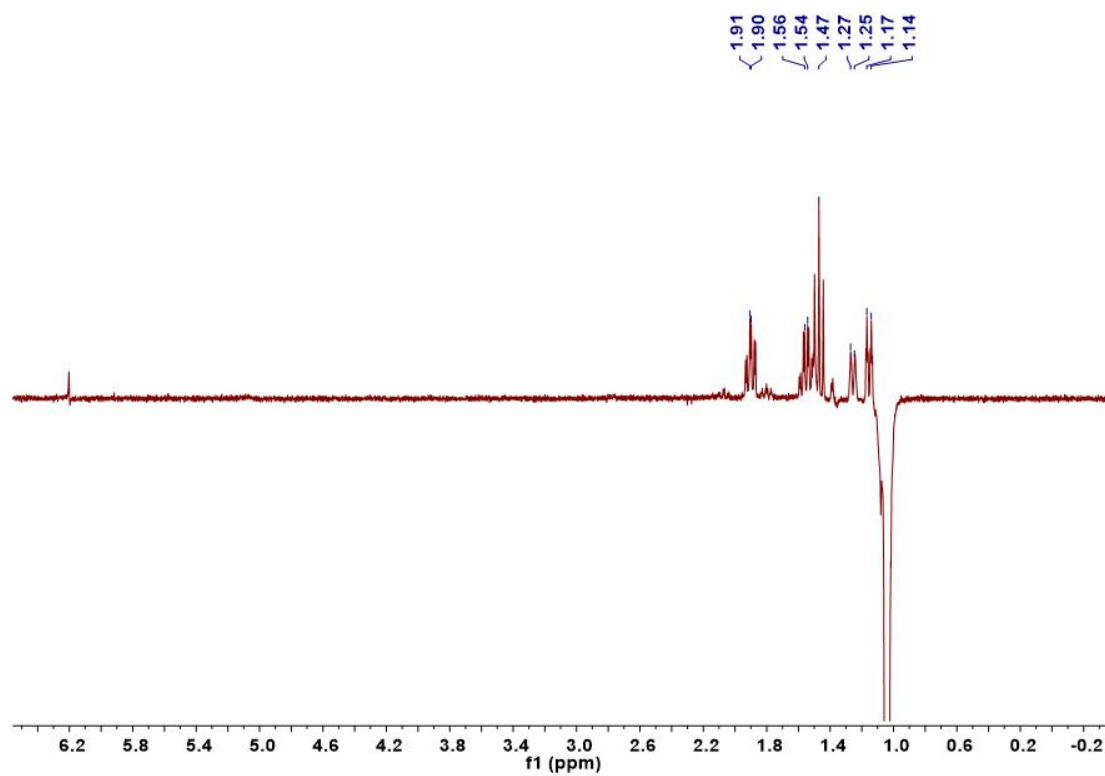


Figure S57. NOE irradiation spectrum (freq: 1.06 ppm) of compound **2** in CDCl₃

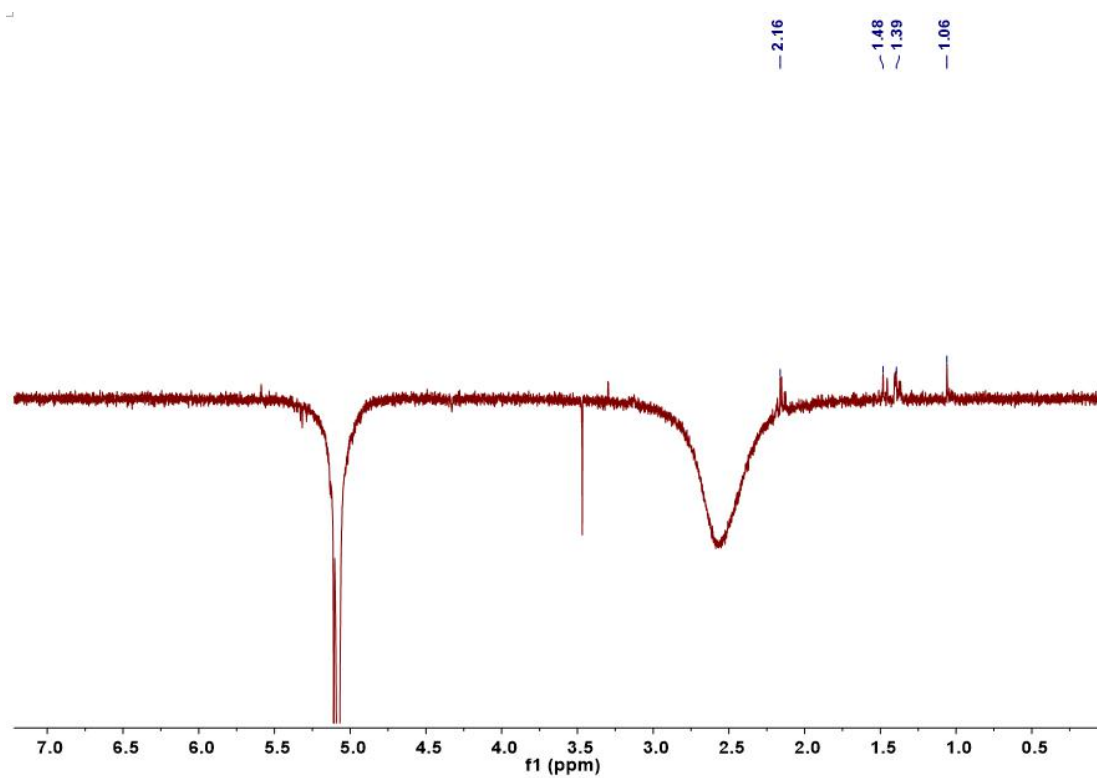


Figure S58. NOE irradiation spectrum (freq: 5.09 ppm) of compound **2** in CDCl₃

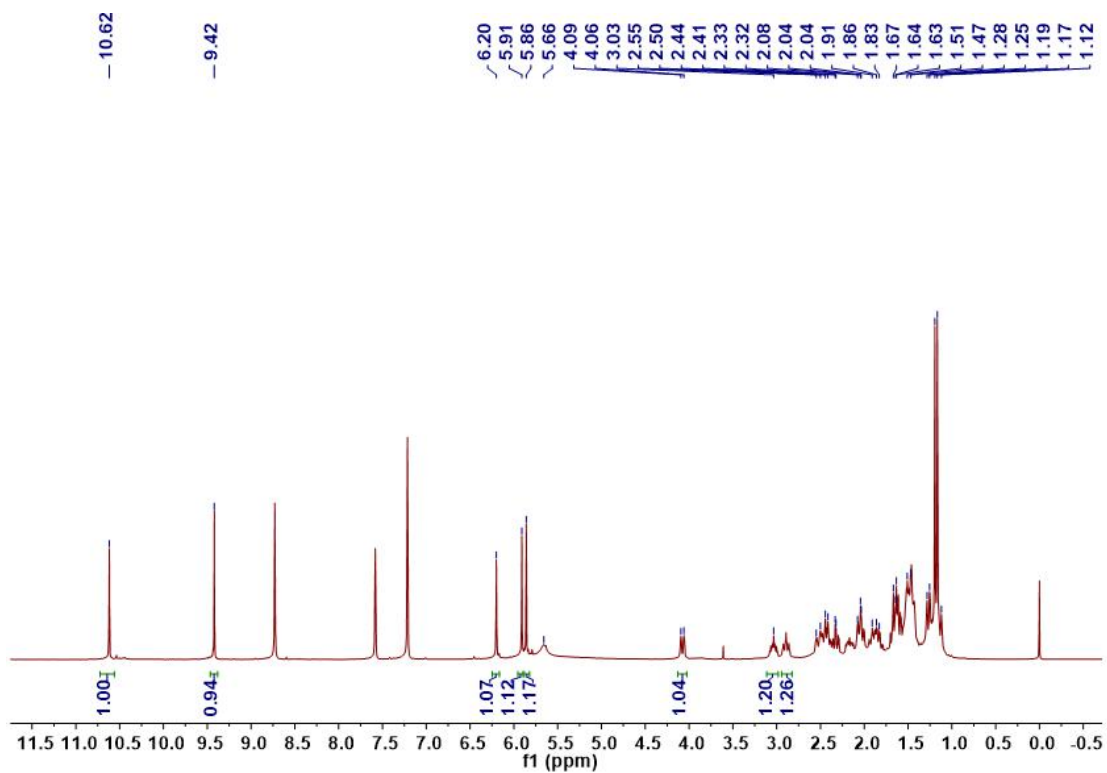


Figure S59. ^1H NMR (600 MHz) spectrum of **2** in pyridine- d_5

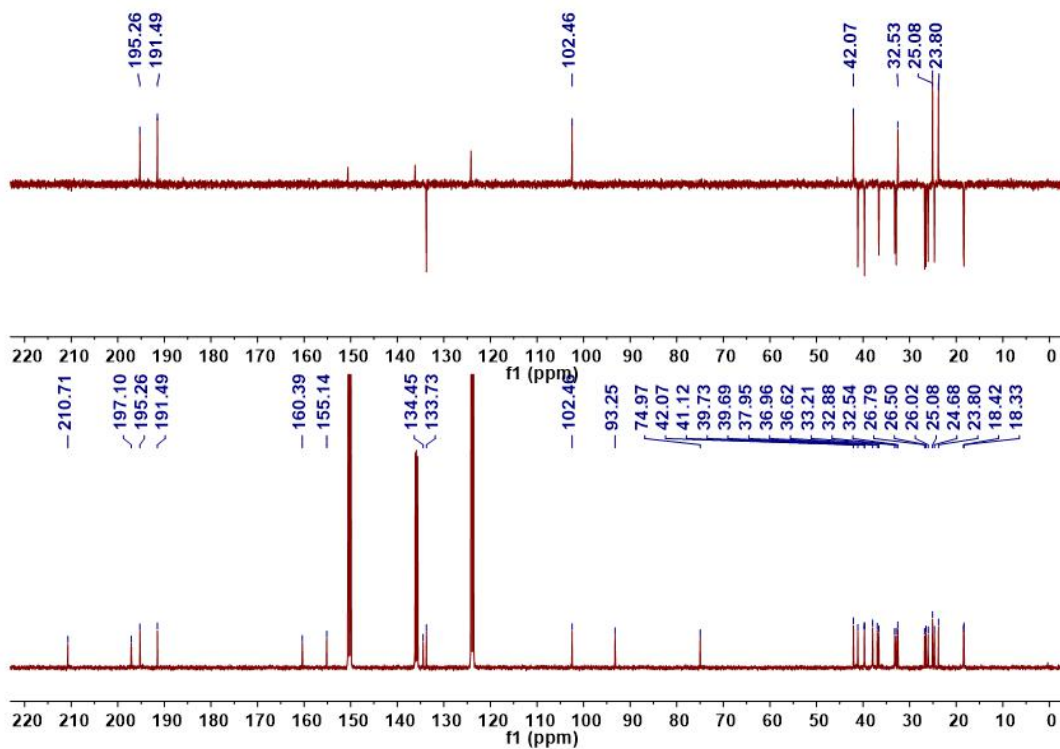


Figure S60. ^{13}C NMR and DEPT (150 MHz) spectra of **2** in pyridine- d_5

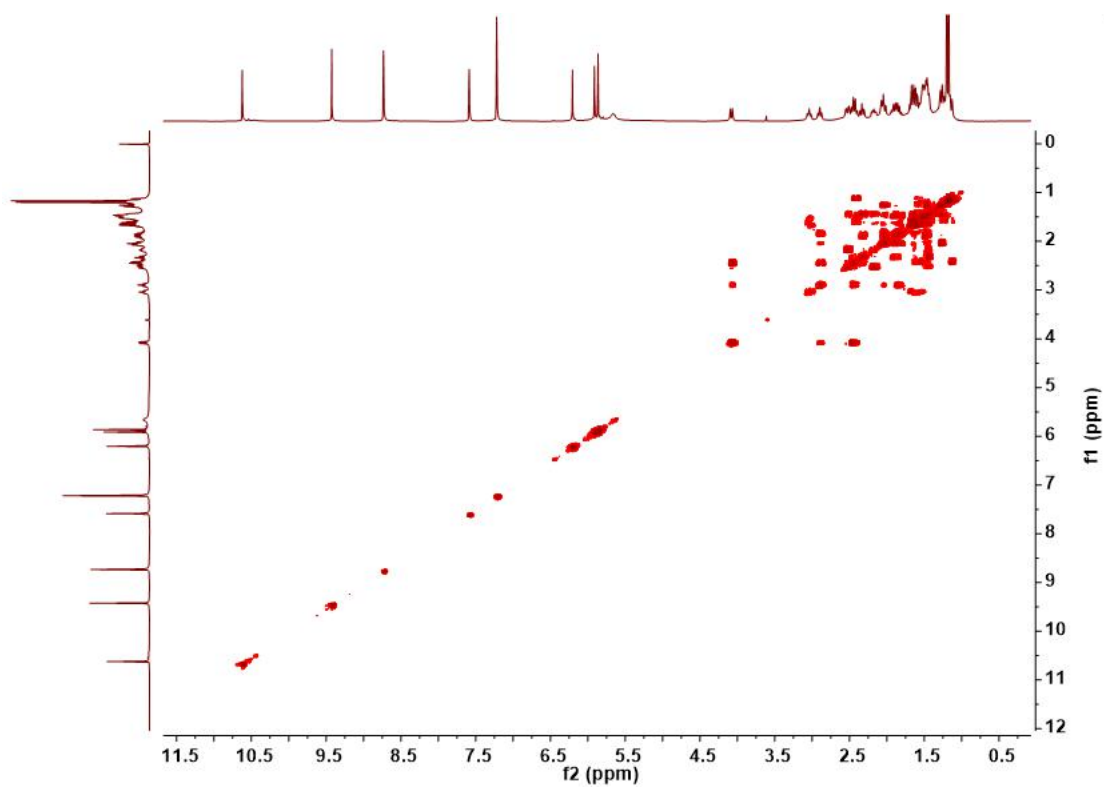


Figure S61. ^1H - ^1H COSY (600 MHz) spectrum of **2** in pyridine- d_5

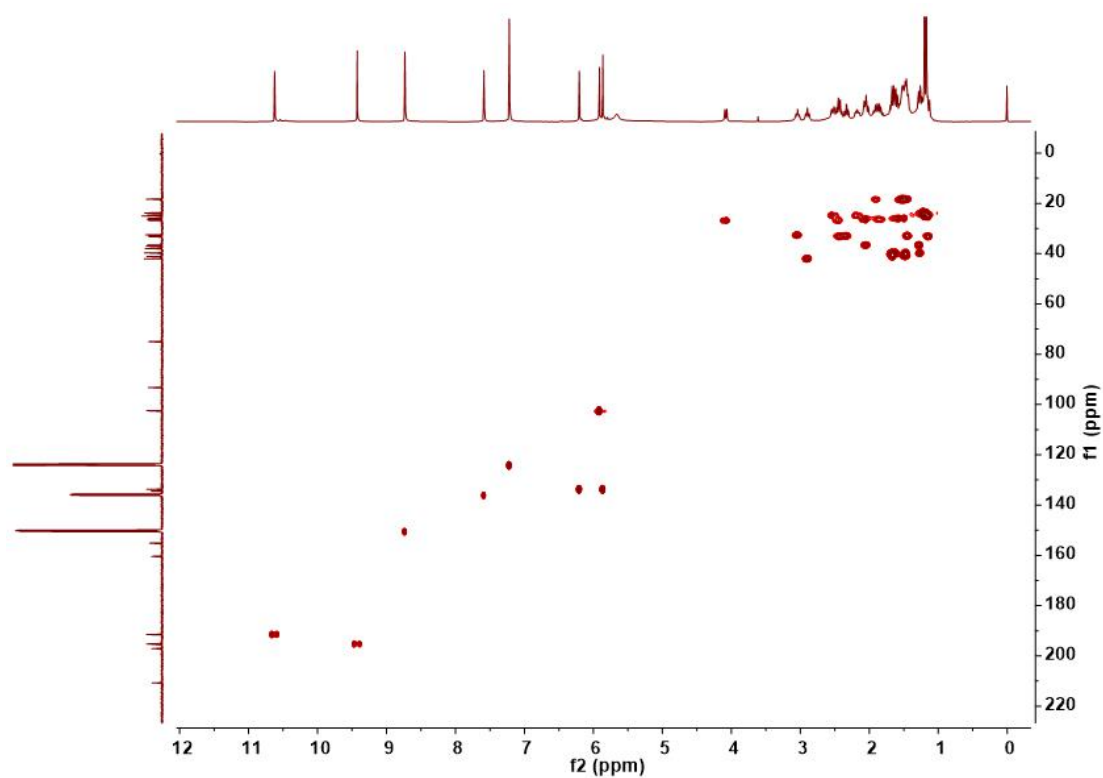


Figure S62. HSQC (600 MHz) spectrum of **2** in pyridine- d_5

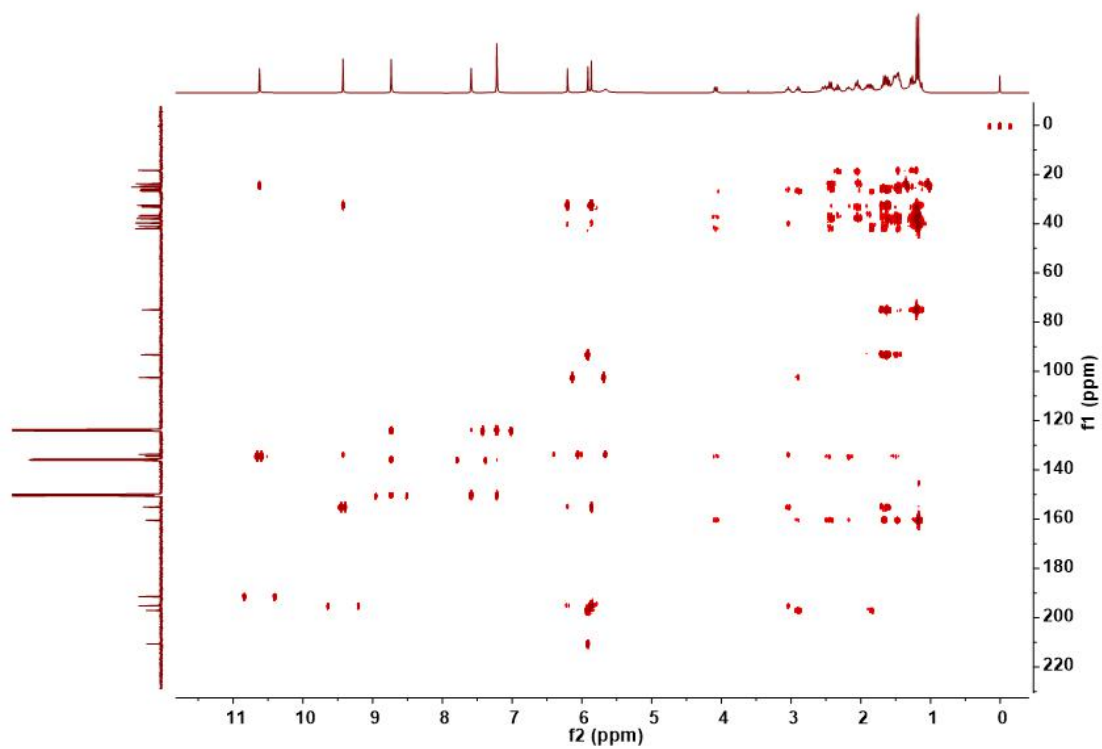


Figure S63. HMBC (600 MHz) spectrum of **2** in pyridine-*d*₅

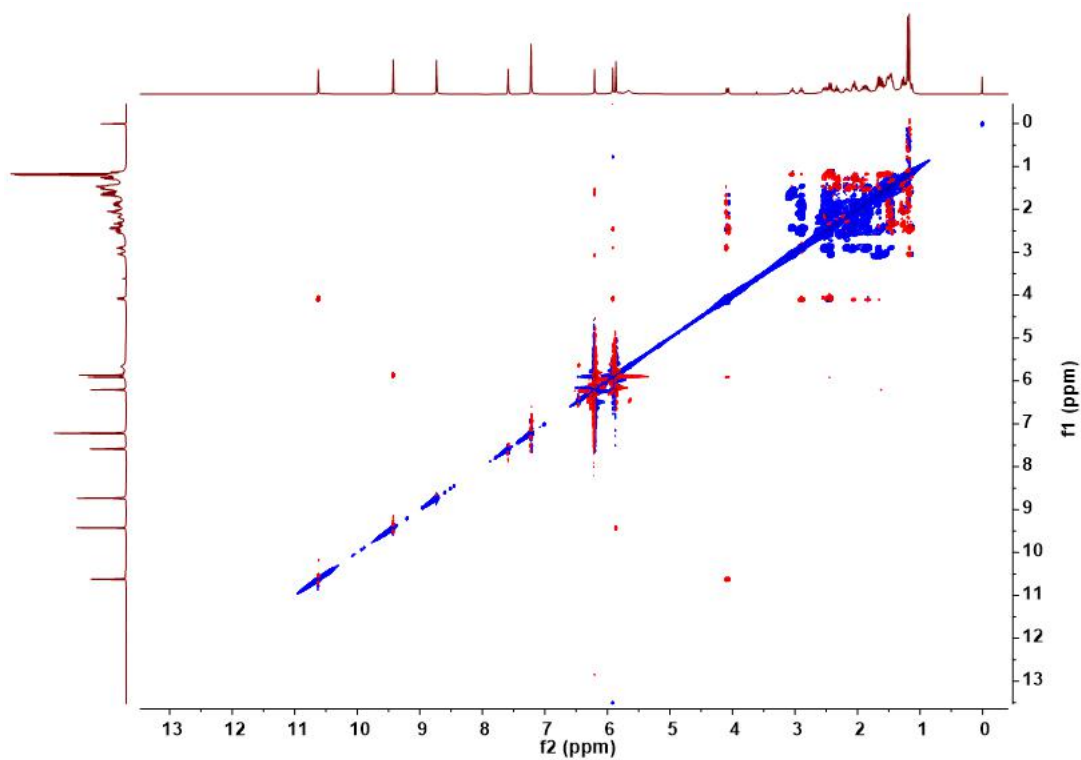


Figure S64. ROESY (600 MHz) spectrum of **2** in pyridine-*d*₅

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

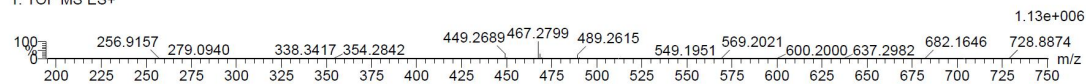
129 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 29-29 H: 0-80 N: 0-5 O: 0-10 Na: 0-1

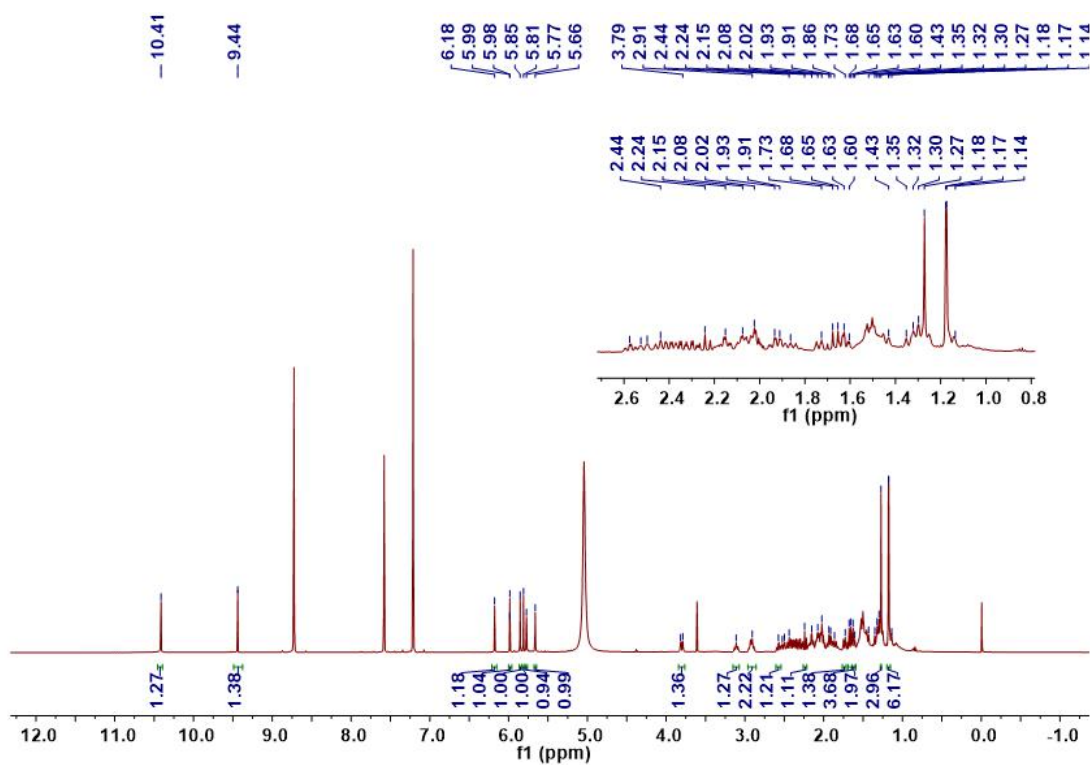
HCX-38 266 (1.484)

1: TOF MS ES+

Minimum: -1.5
Maximum: 20.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
467.2799	467.2797	0.2	0.4	10.5	636.5	n/a	n/a	C29 H39 O5

Figure S65. HRESIMS of 2

Figure S66. ¹H NMR (600 MHz) spectrum of 3 in pyridine-*d*₅

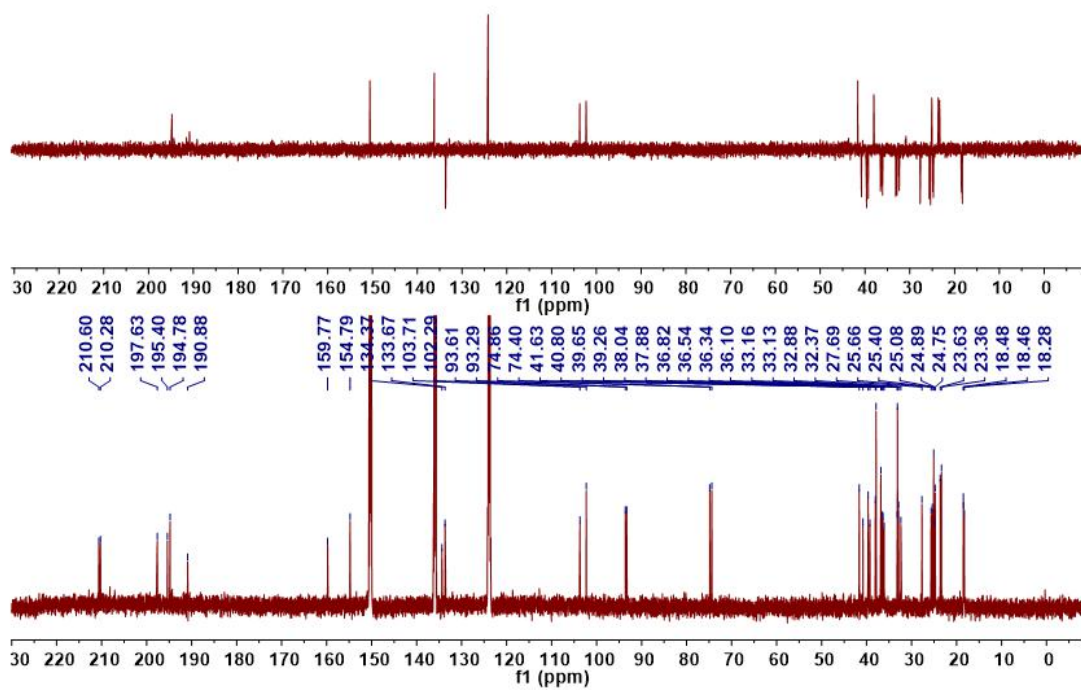


Figure S67. ^{13}C NMR and DEPT (150 MHz) spectra of **3** in pyridine- d_5

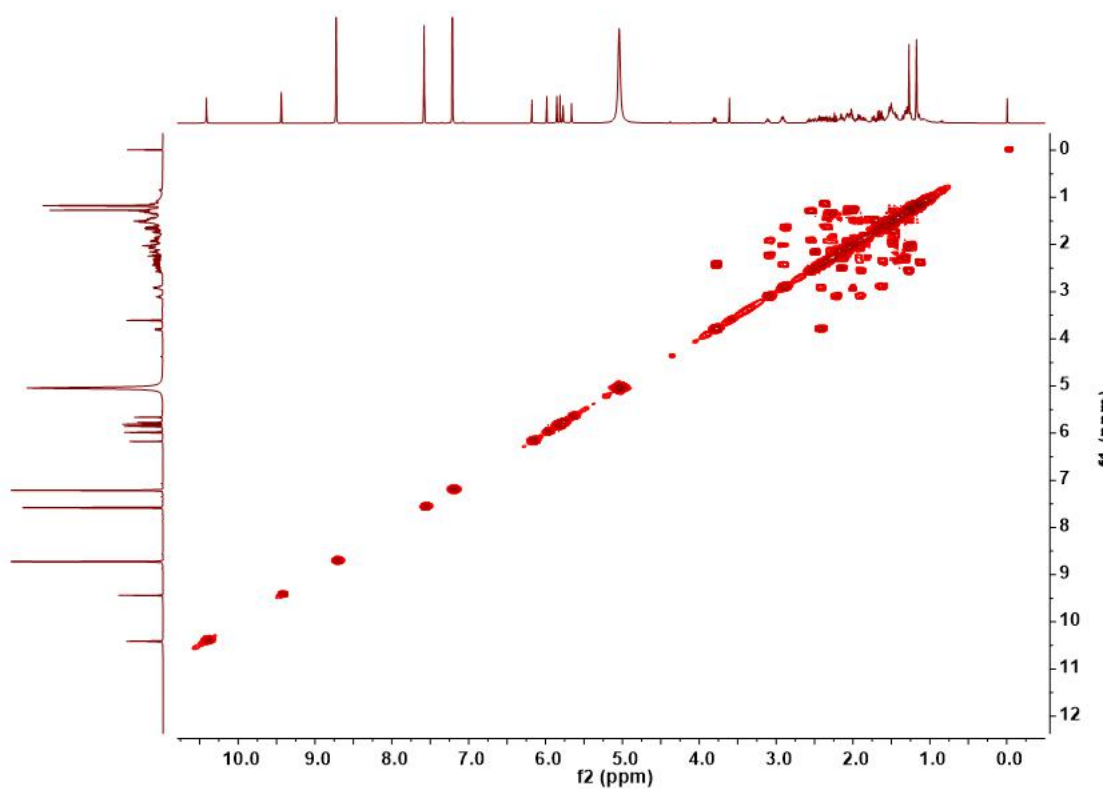


Figure S68. ^1H - ^1H COSY (600 MHz) spectrum of **3** in pyridine- d_5

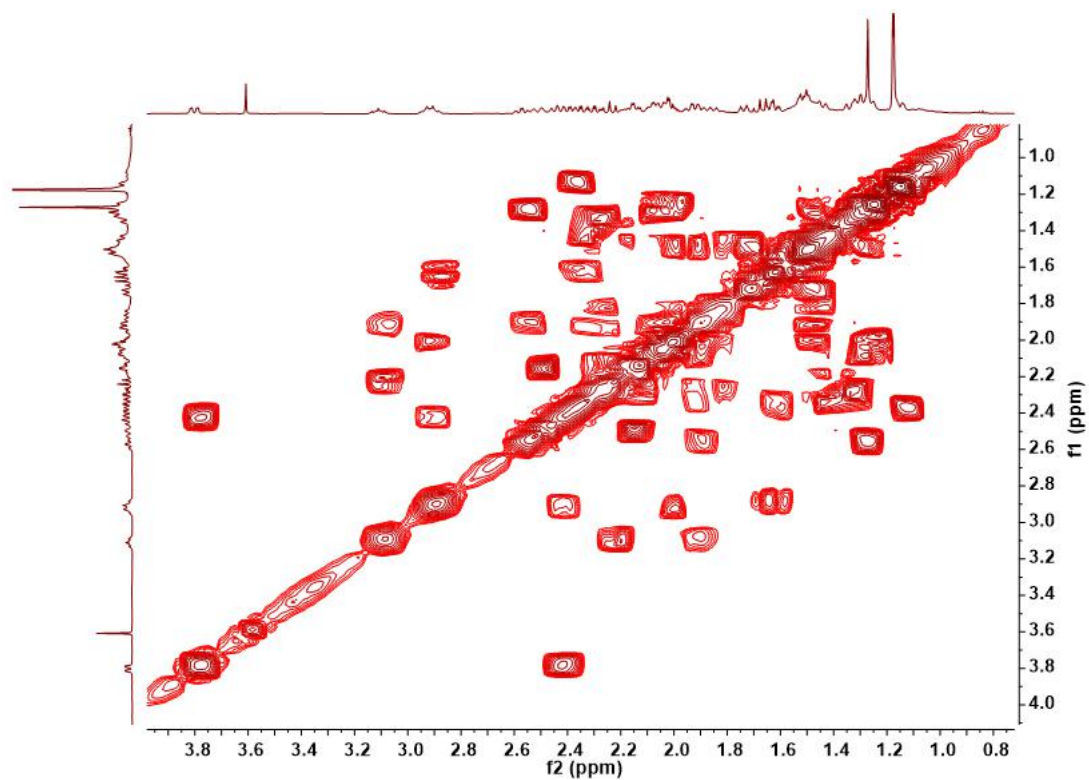


Figure S69. Enlarged ^1H - ^1H COSY (600 MHz) spectrum of **3** in pyridine- d_5

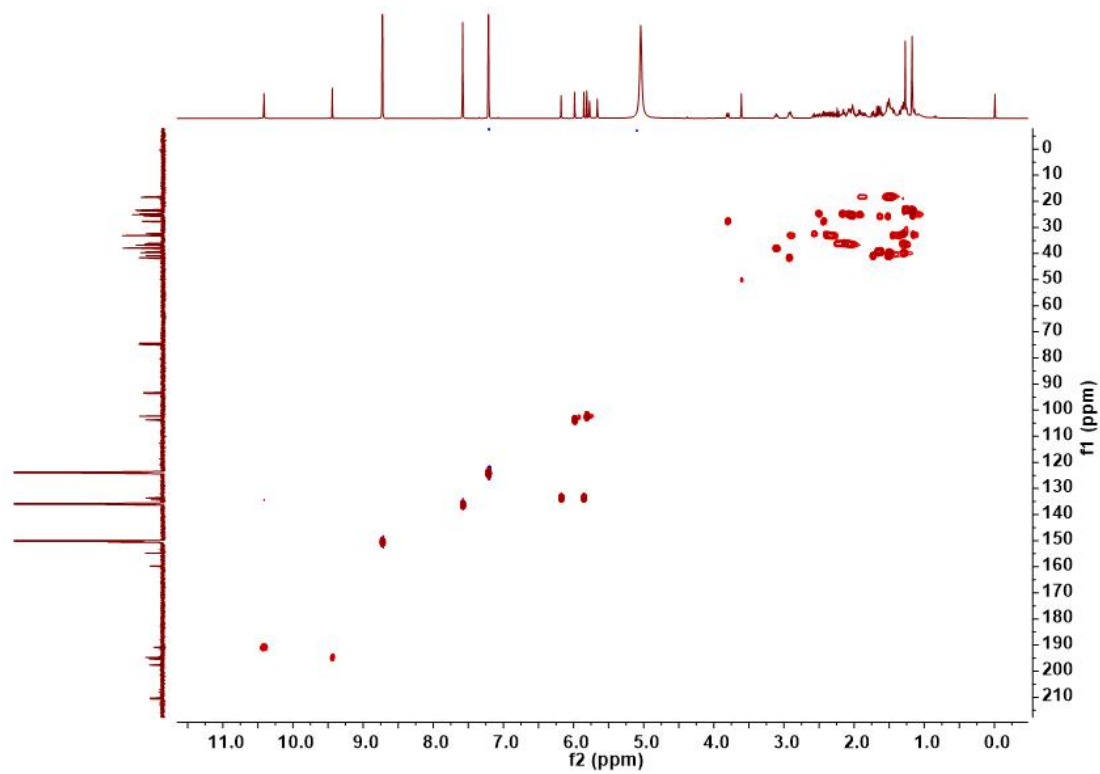


Figure S70. HSQC (600 MHz) spectrum of **3** in pyridine- d_5

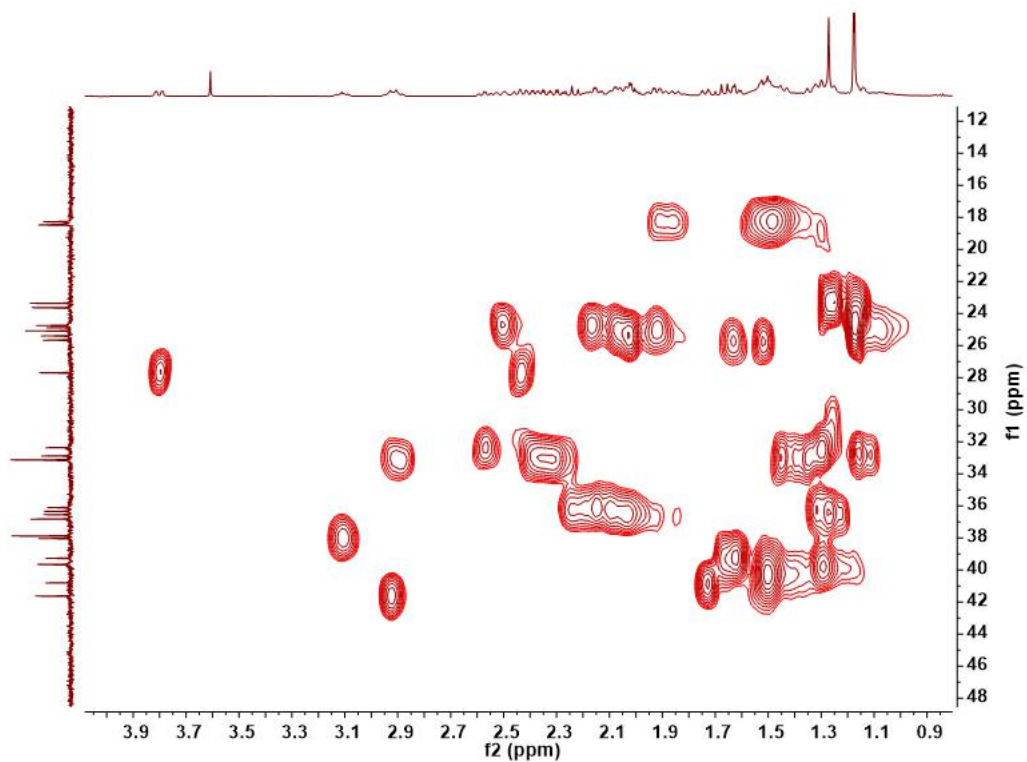


Figure S71. Enlarged HSQC (600 MHz) spectrum of **3** in pyridine-*d*₅

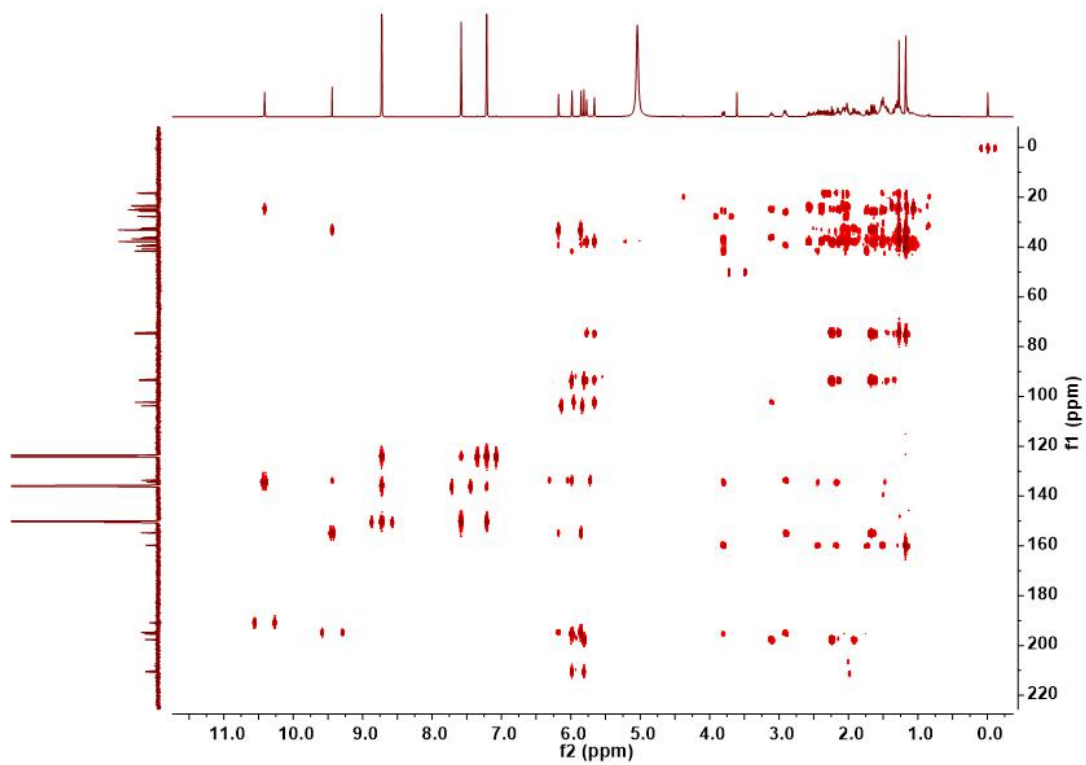


Figure S72. HMBC (600 MHz) spectrum of **3** in pyridine-*d*₅

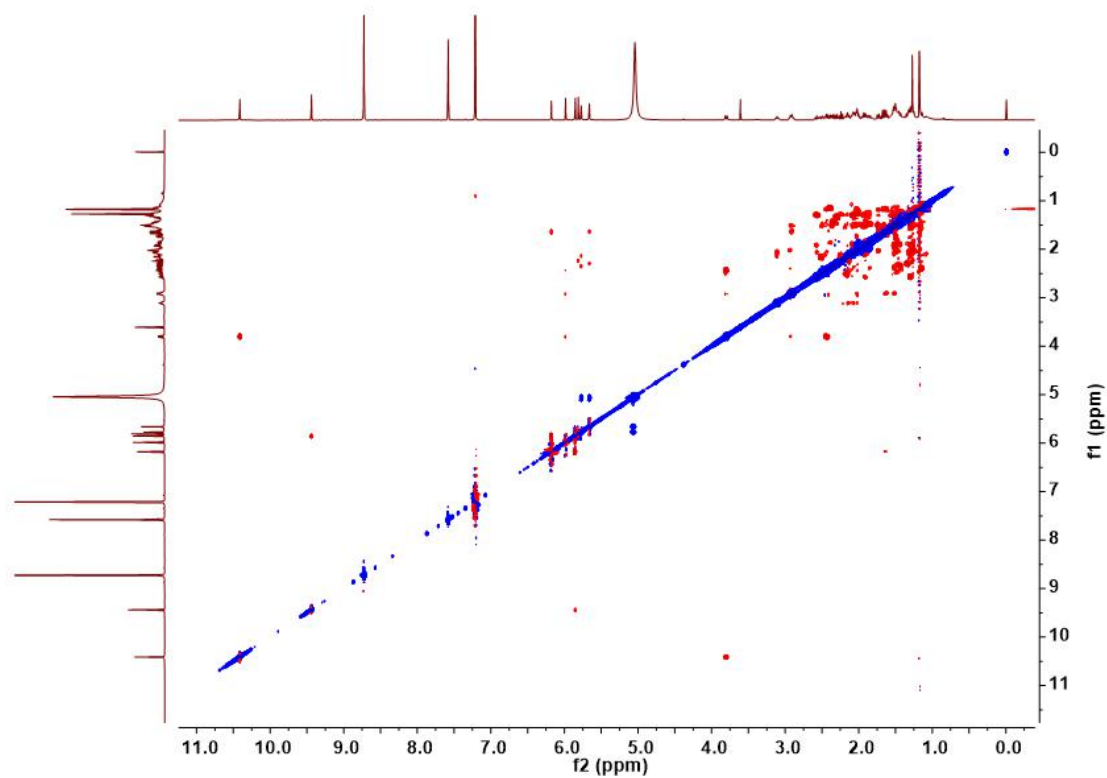


Figure S73. ROESY (600 MHz) spectrum of **3** in pyridine-*d*₅

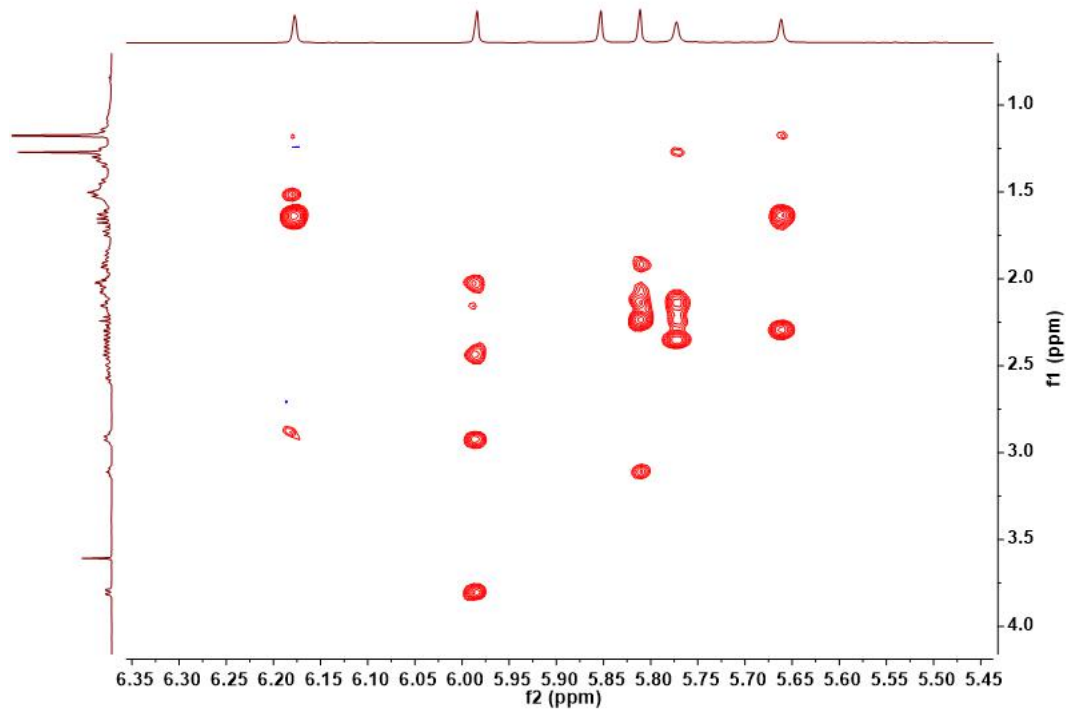


Figure S74. Enlarged ROESY (600 MHz) spectrum of **3** in pyridine-*d*₅

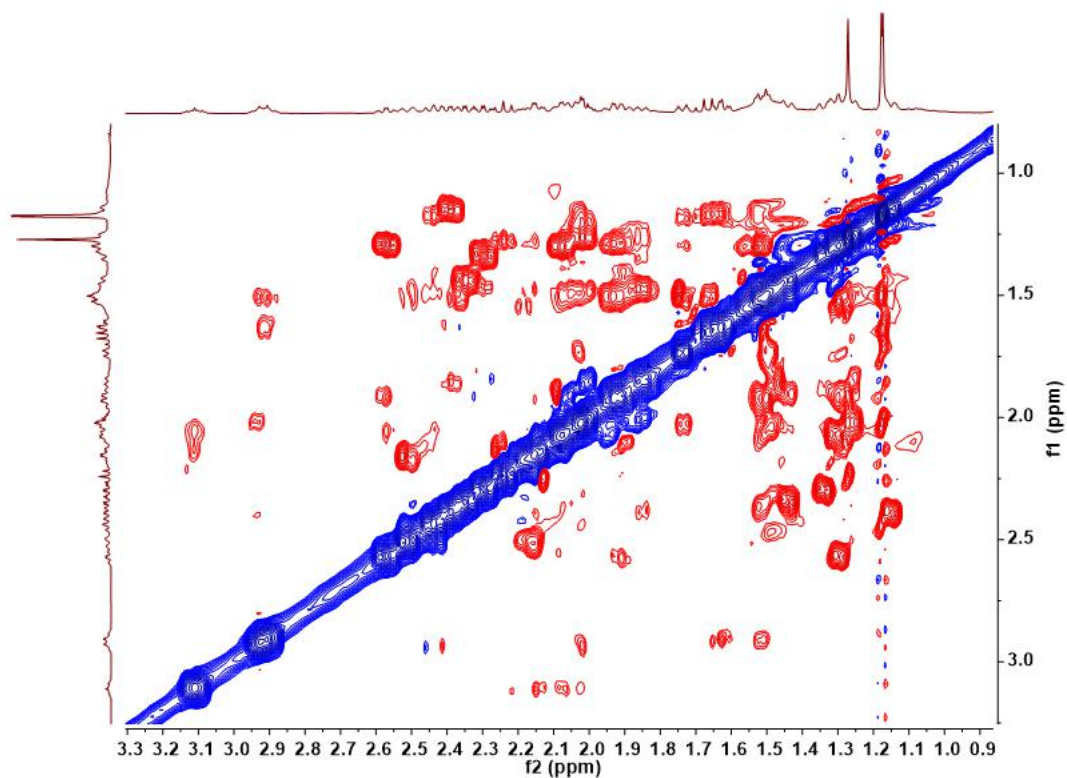


Figure S75. Enlarged ROESY (600 MHz) spectrum of **3** in pyridine-*d*₅

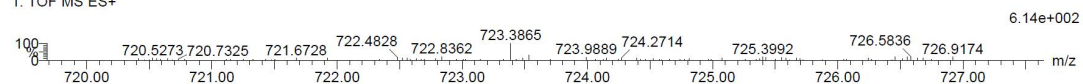
Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
 114 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
 Elements Used:
 C: 43-43 H: 0-80 N: 0-5 O: 0-10 Na: 0-1
 HCX-51 167 (0.941)
 1: TOF MS ES+



Mass	Calc. Mass	nDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
723.3865	723.3873	-0.8	-1.1	15.5	271.3	n/a	n/a	C43 H56 O8 Na

Figure S76. HRESIMS of **3**

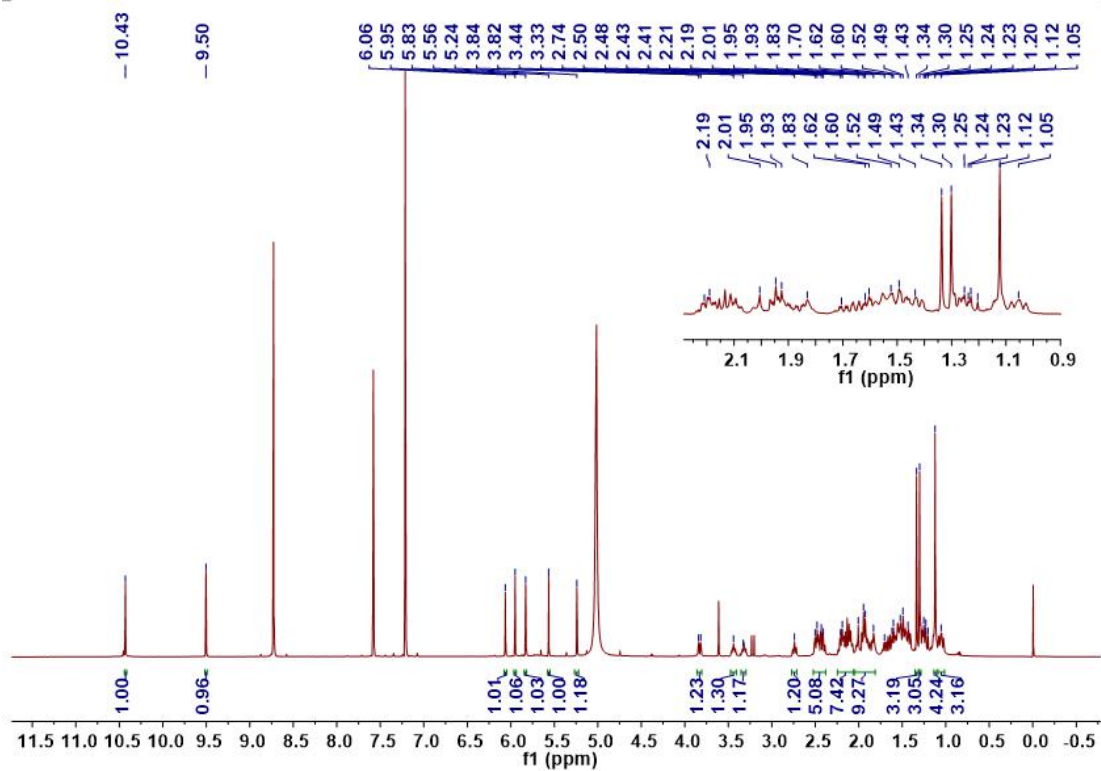


Figure S77. ^1H NMR (600 MHz) spectrum of **4** in pyridine- d_5

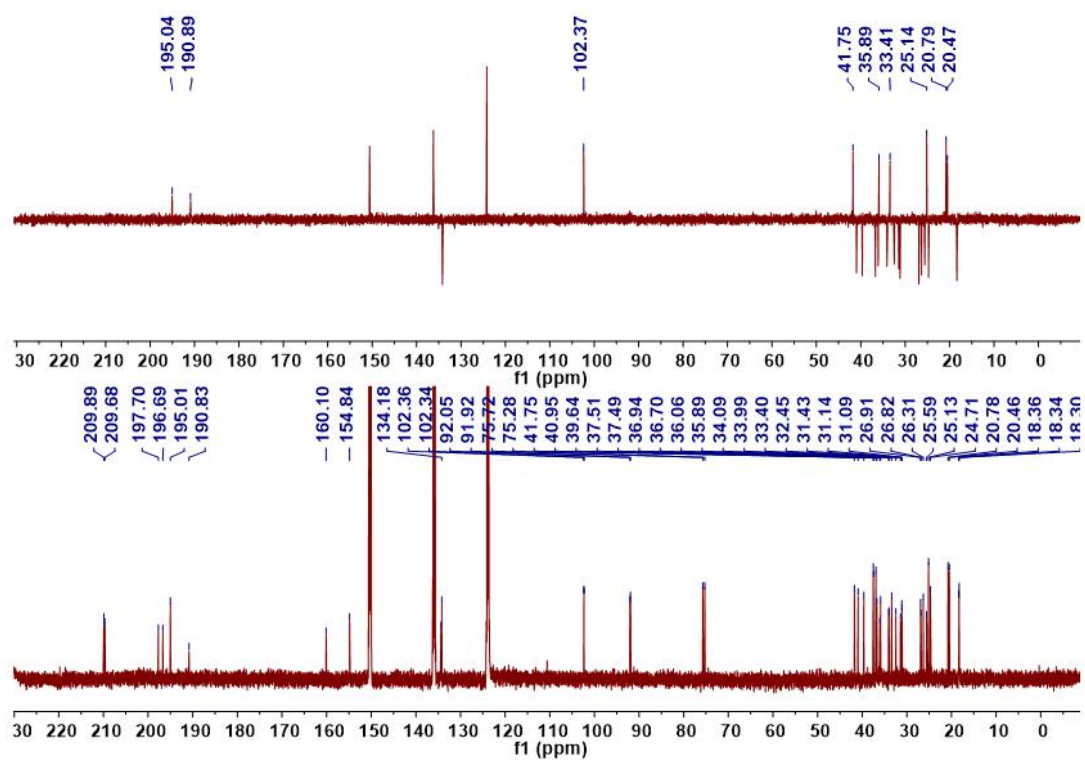


Figure S78. ^{13}C NMR and DEPT (150 MHz) spectra of **4** in pyridine- d_5

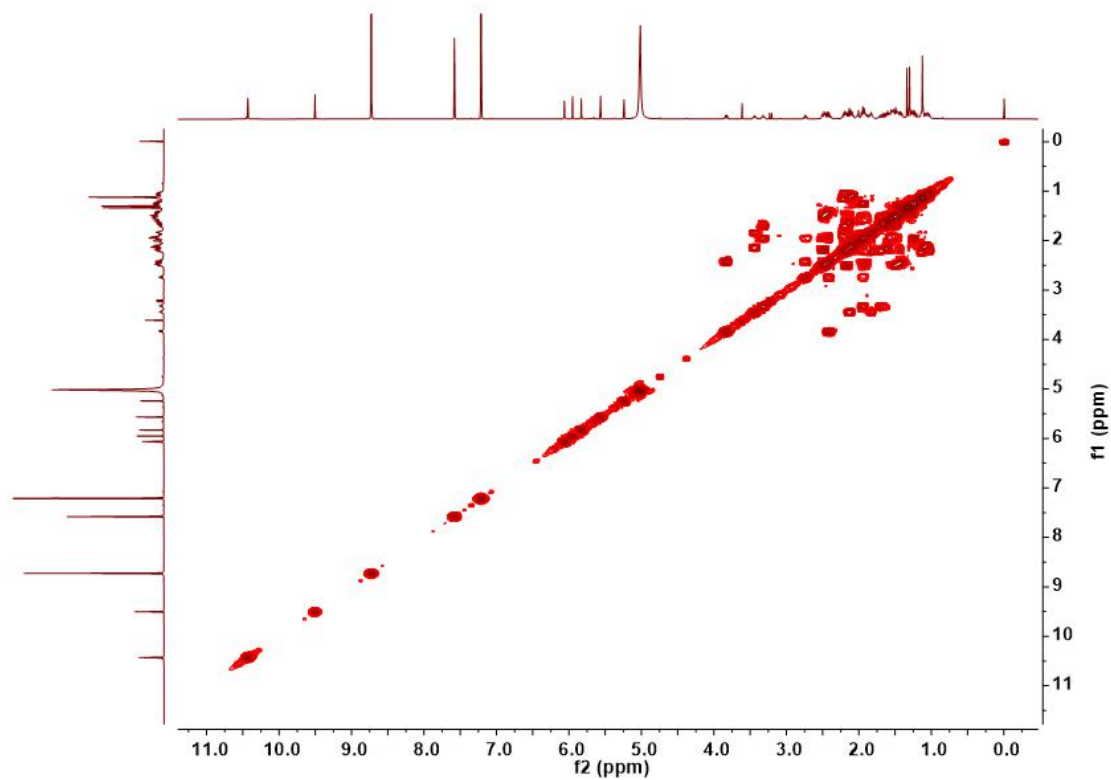


Figure S79. ^1H - ^1H COSY (600 MHz) spectrum of **4** in pyridine- d_5

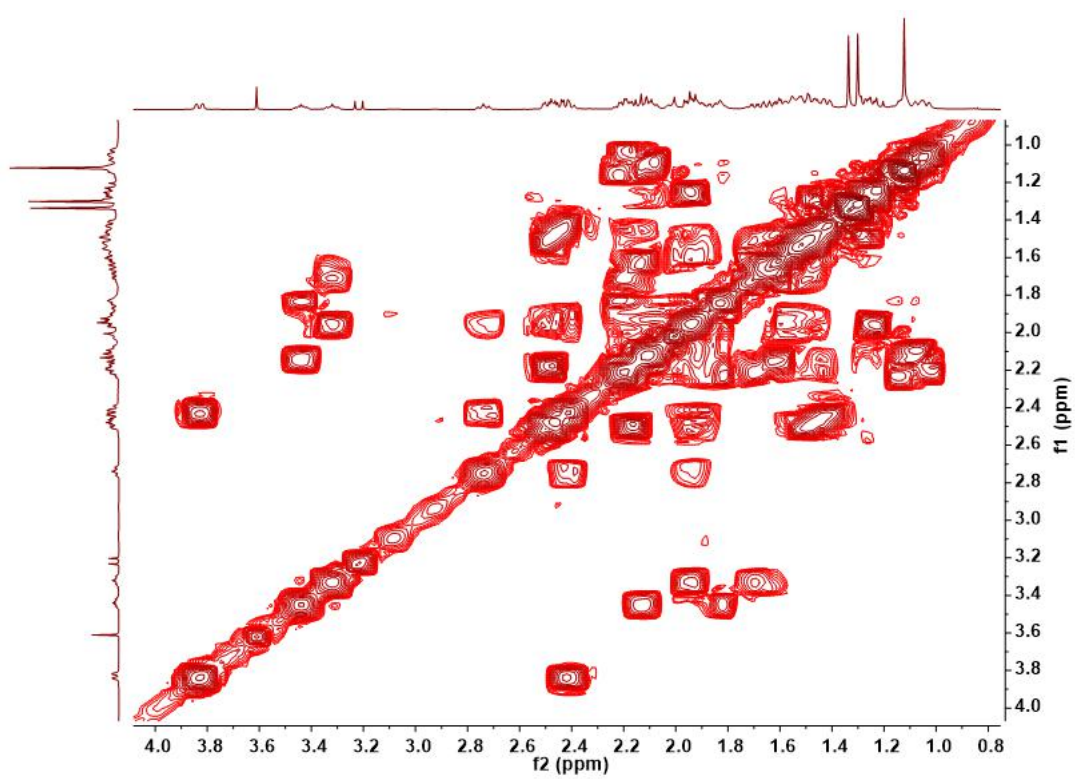


Figure S80. Enlarged ^1H - ^1H COSY (600 MHz) spectrum of **4** in pyridine- d_5

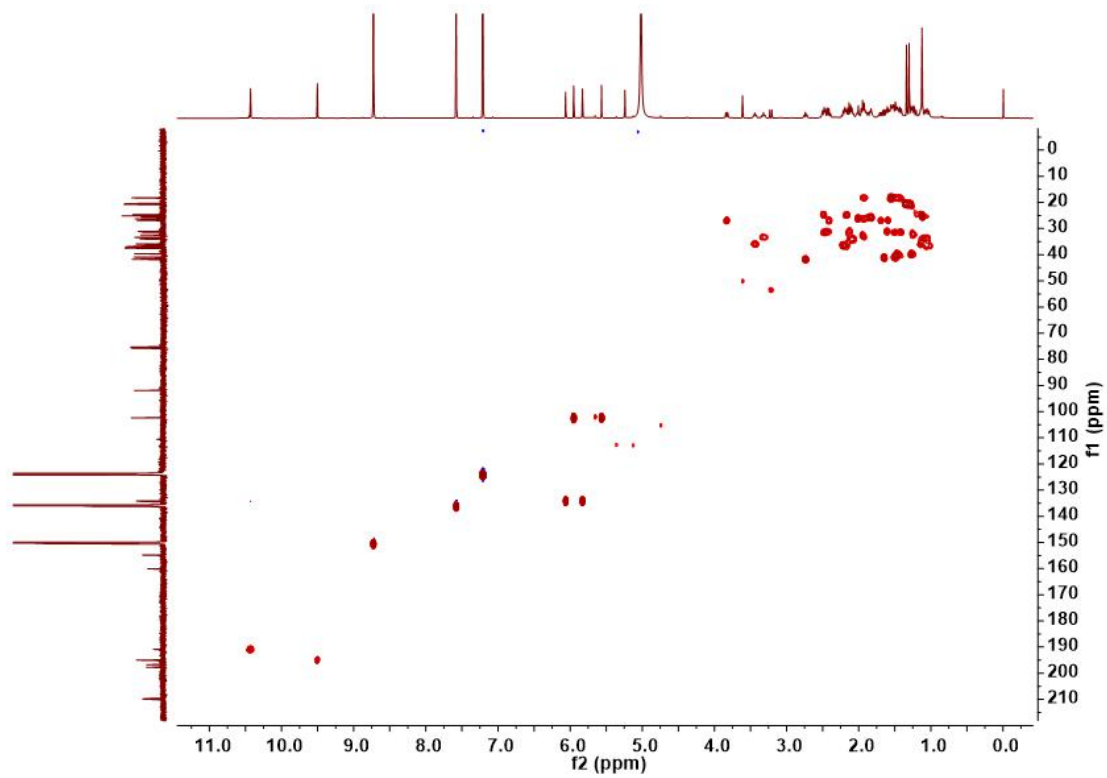


Figure S81. HSQC (600 MHz) spectrum of **4** in pyridine-*d*₅

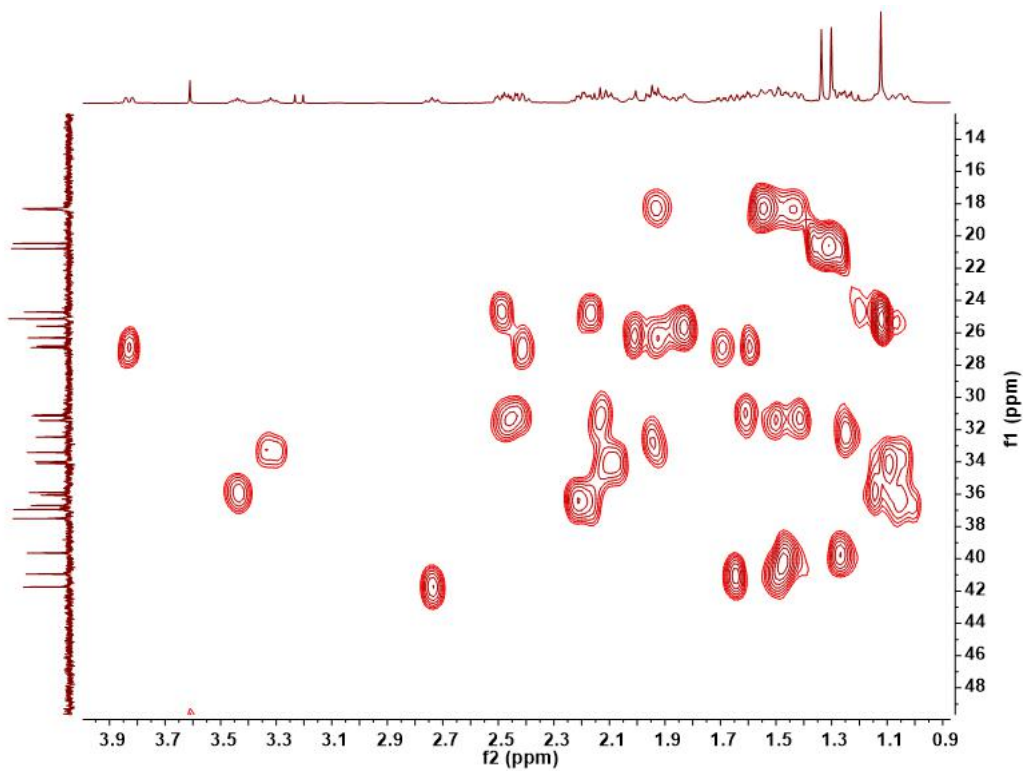


Figure S82. Enlarged HSQC (600 MHz) spectrum of **4** in pyridine-*d*₅

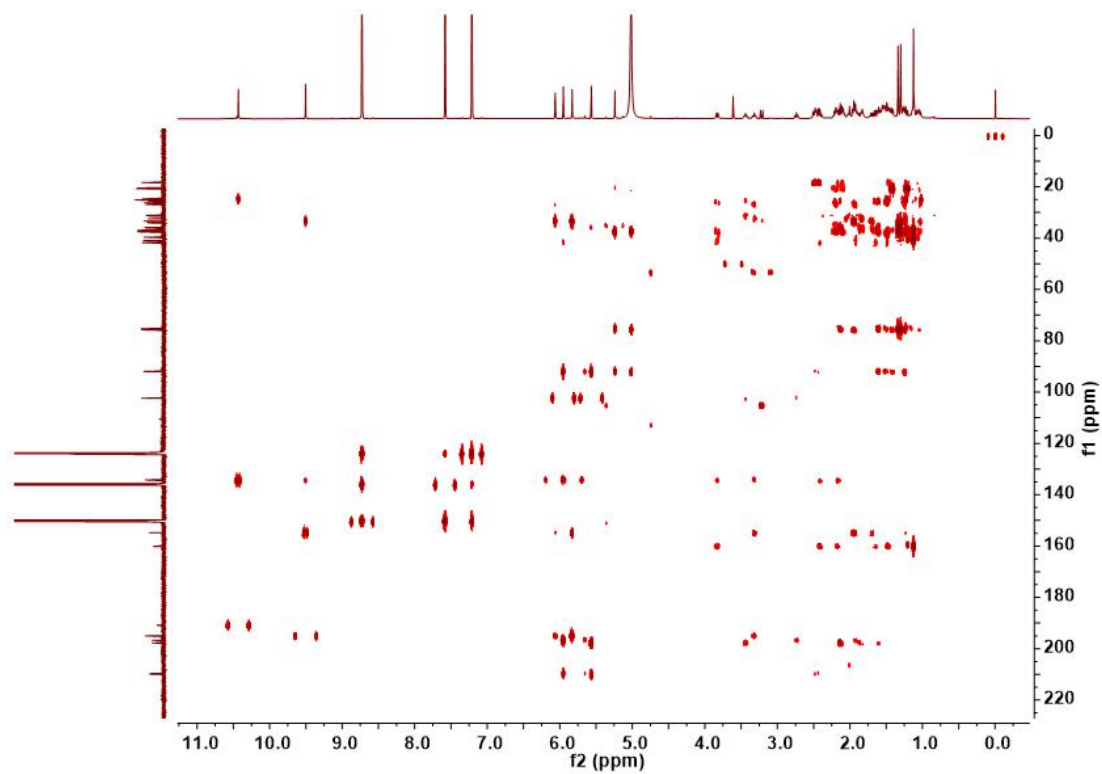


Figure S83. HMBC (600 MHz) spectrum of **4** in pyridine-*d*₅

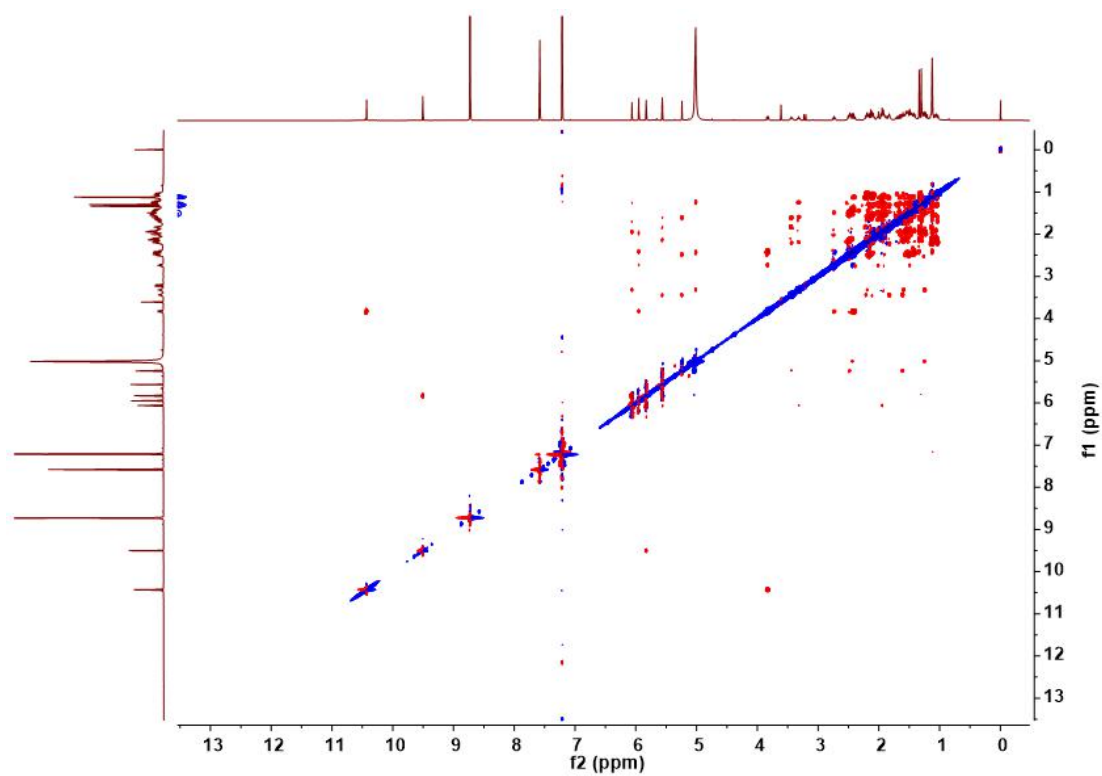


Figure S84. ROESY (600 MHz) spectrum of **4** in pyridine-*d*₅

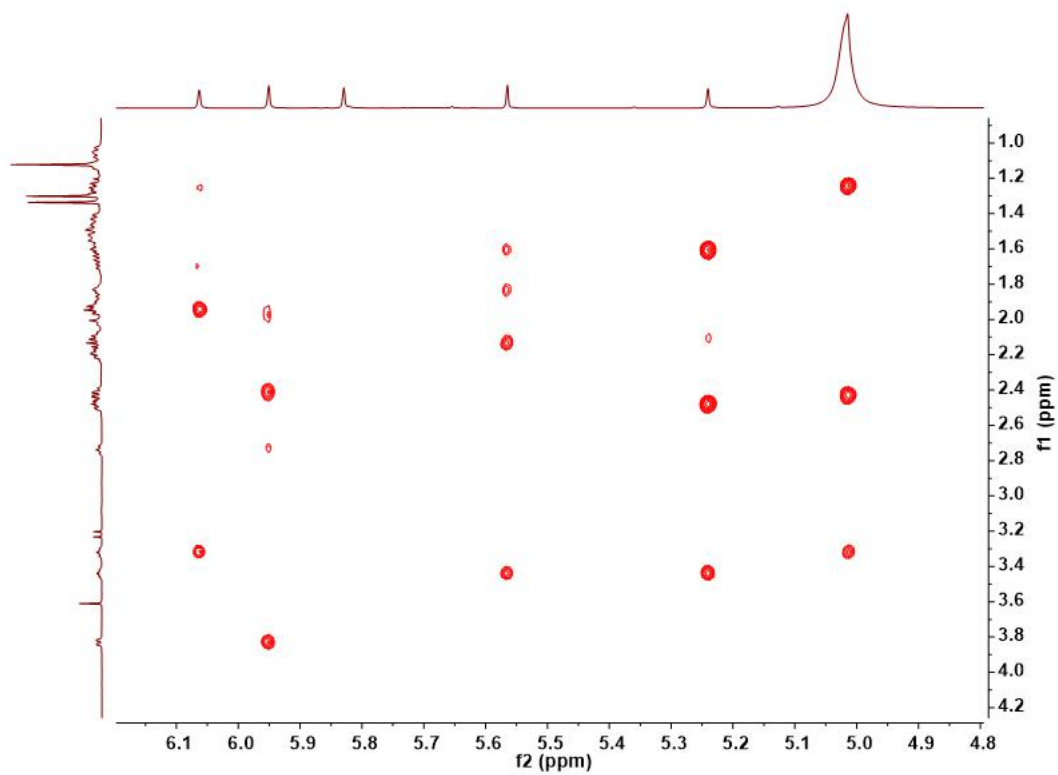


Figure S85. Enlarged ROESY (600 MHz) spectrum of **4** in pyridine-*d*₅

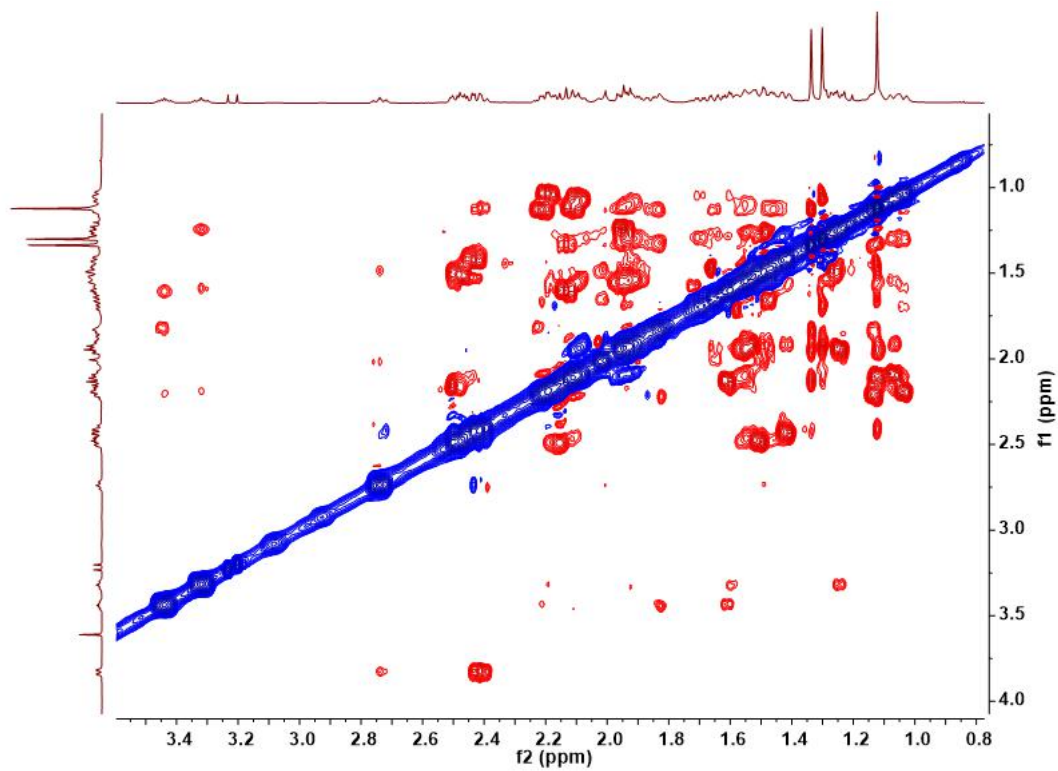


Figure S86. Enlarged ROESY (600 MHz) spectrum of **4** in pyridine-*d*₅

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

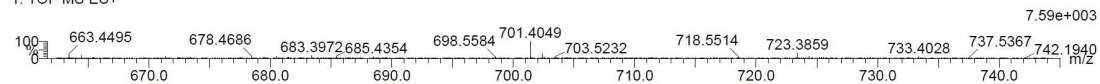
115 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 43-43 H: 0-80 N: 0-5 O: 0-10 Na: 0-1

HCX-52 281 (1.570)

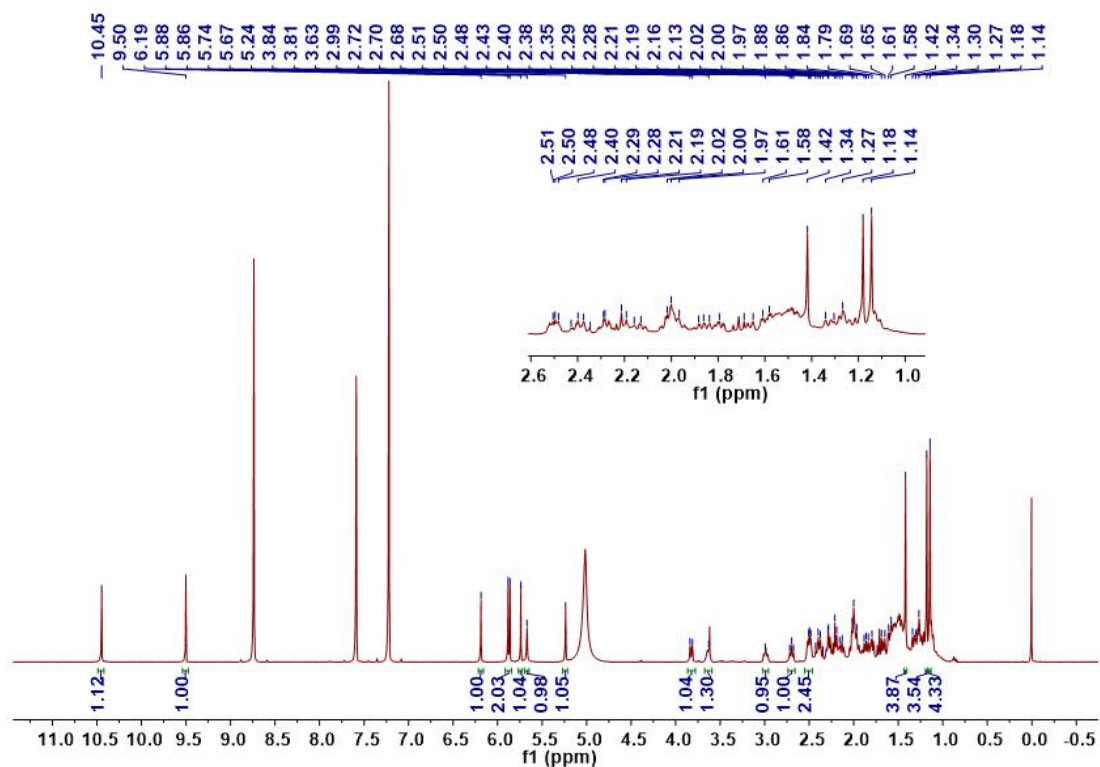
1: TOF MS ES+



Minimum: -1.5
Maximum: 20.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
701.4049	701.4053	-0.4	-0.6	15.5	314.1	n/a	n/a	C43 H57 O8

Figure S87. HRESIMS of 4

Figure S88. ^1H NMR (600 MHz) spectrum of 5 in pyridine- d_5

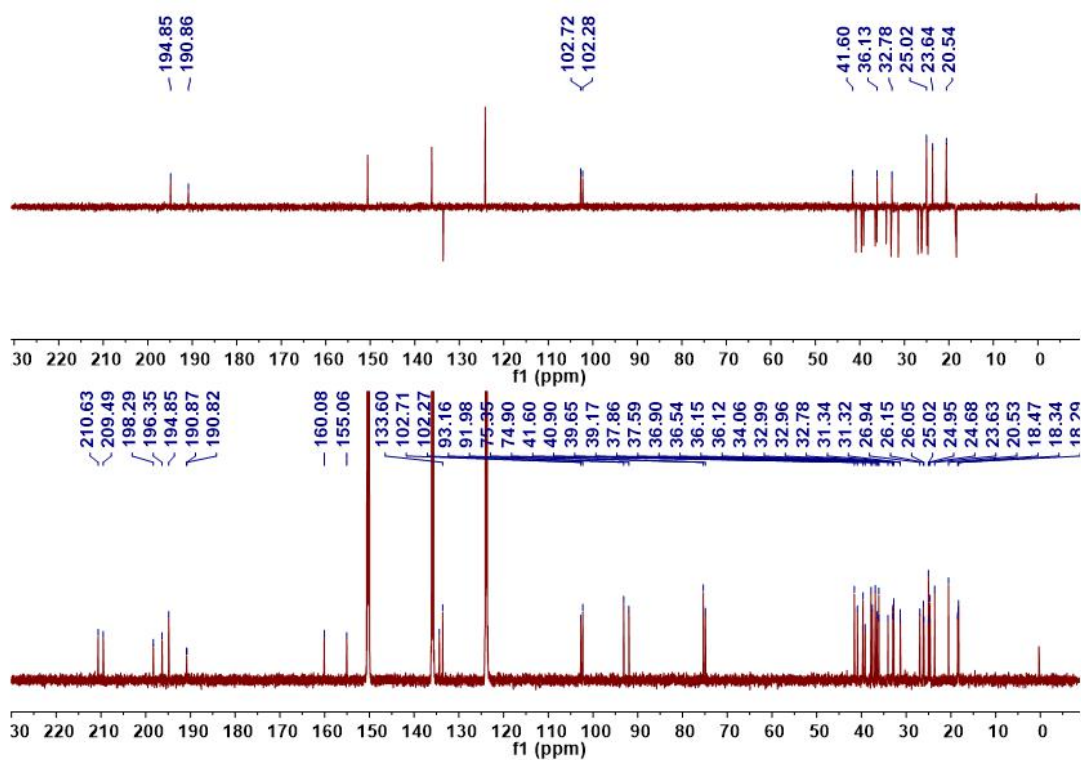


Figure S89. ^{13}C NMR and DEPT (150 MHz) spectra of **5** in pyridine- d_5

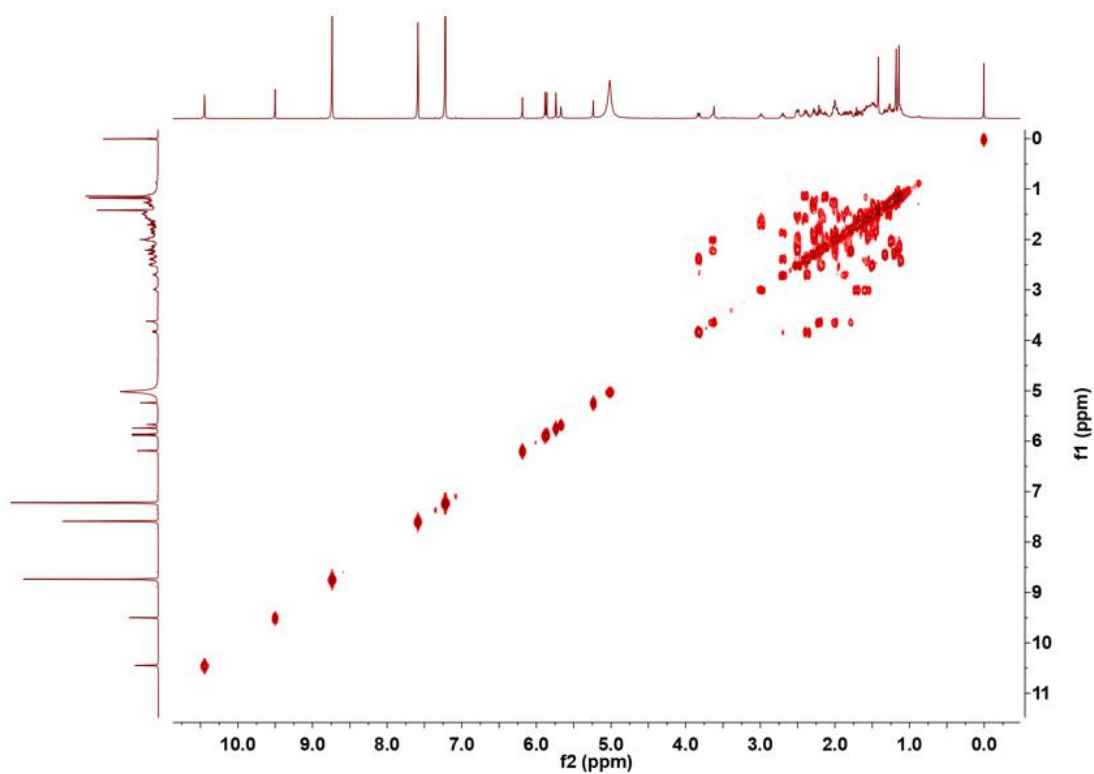


Figure S90. ^1H - ^1H COSY (600 MHz) spectrum of **5** in pyridine- d_5

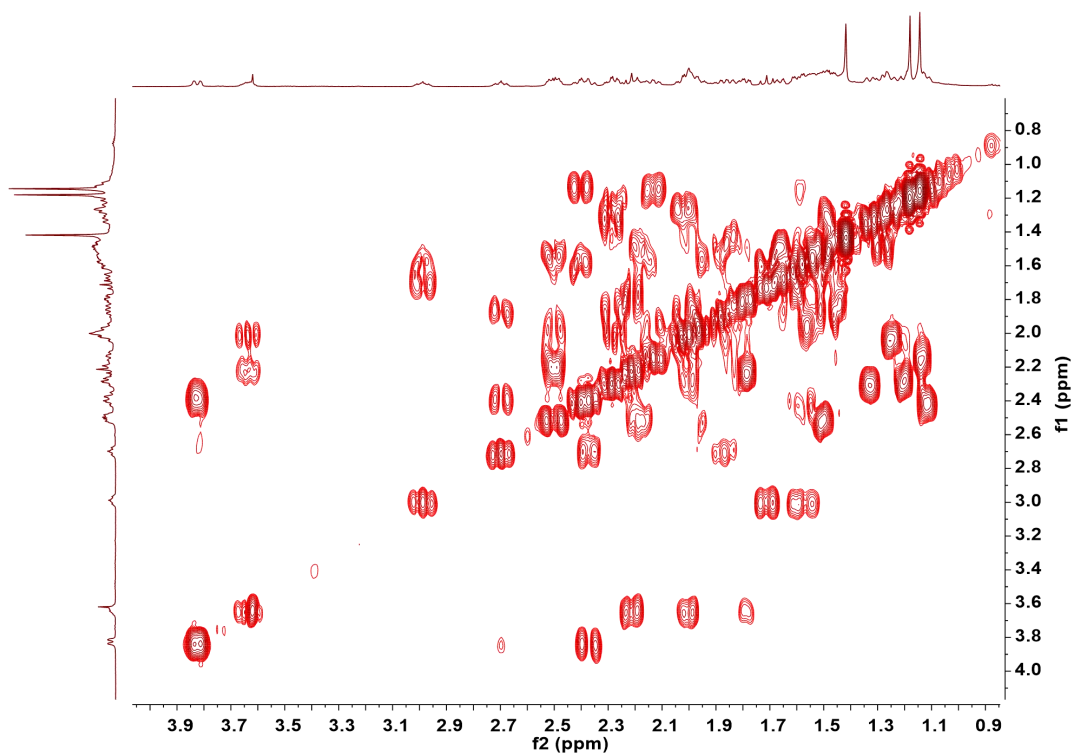


Figure S91. Enlarged ^1H - ^1H COSY (600 MHz) spectrum of **5** in pyridine- d_5

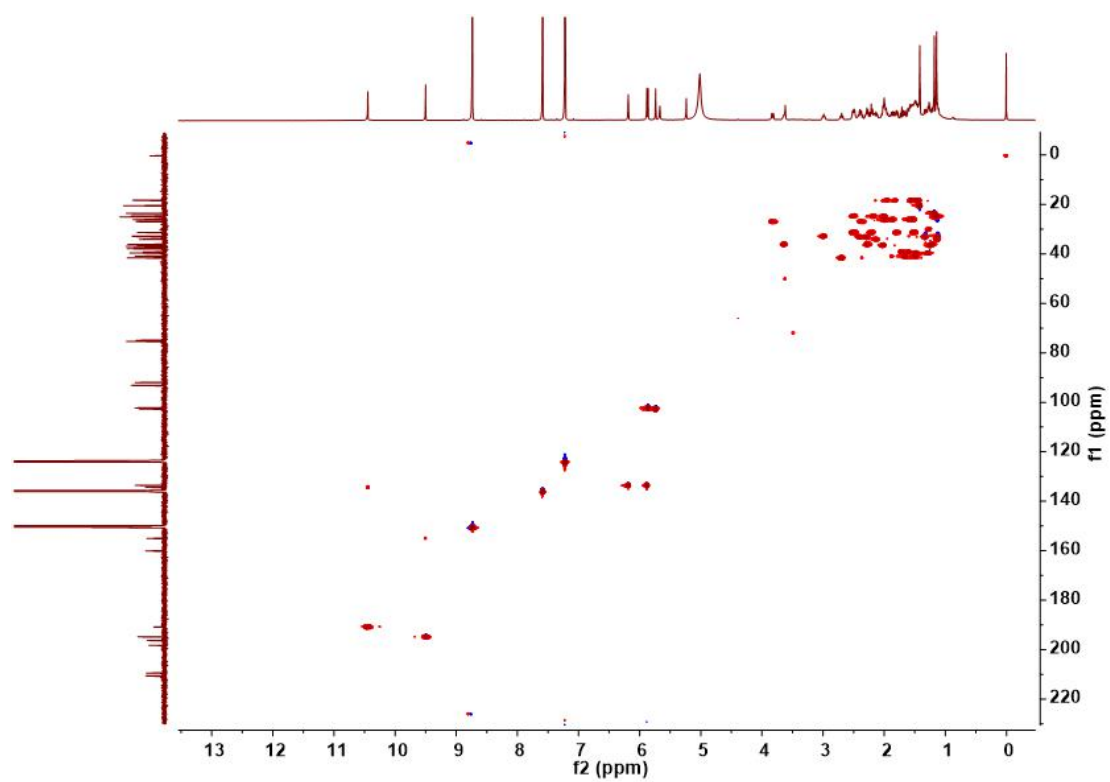


Figure S92. HSQC (600 MHz) spectrum of **5** in pyridine- d_5

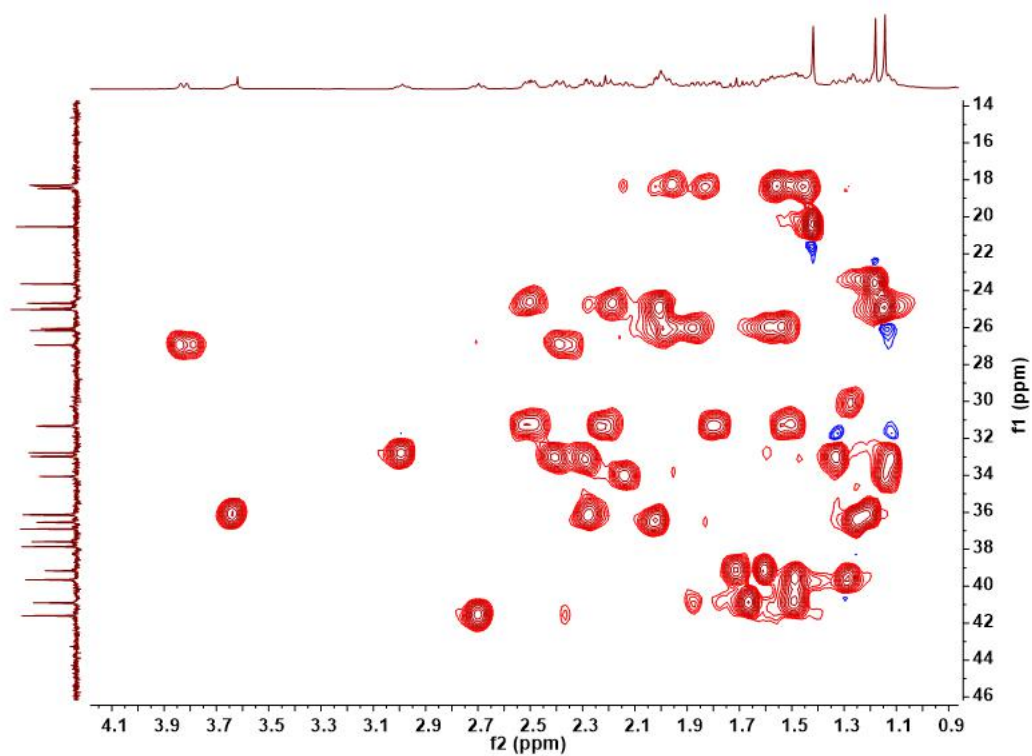


Figure S93. Enlarged HSQC (600 MHz) spectrum of **5** in pyridine-*d*₅

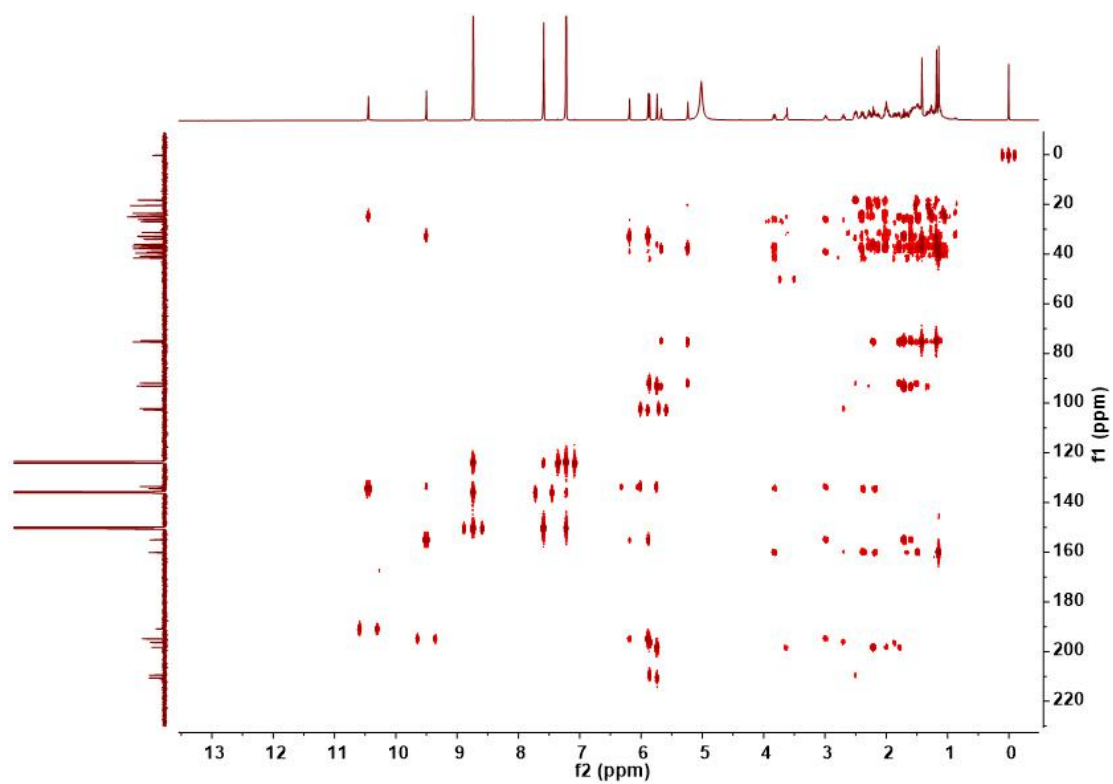


Figure S94. HMBC (600 MHz) spectrum of **5** in pyridine-*d*₅

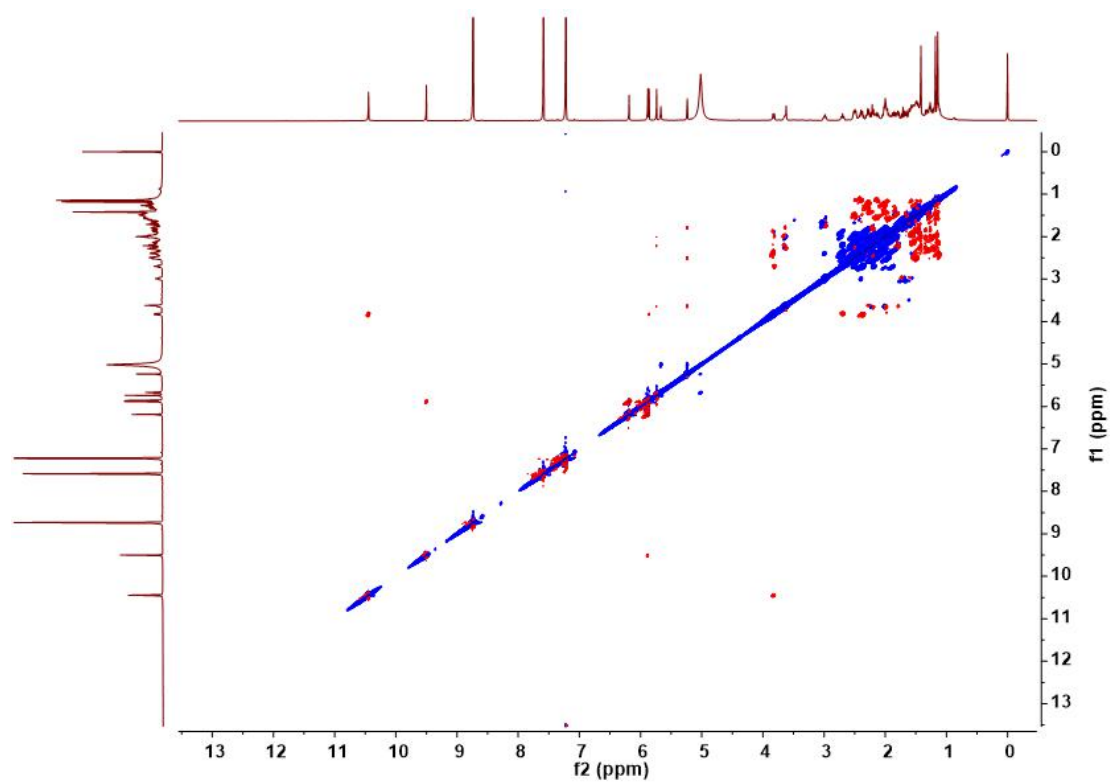


Figure S95. ROESY (600 MHz) spectrum of **5** in pyridine-*d*₅

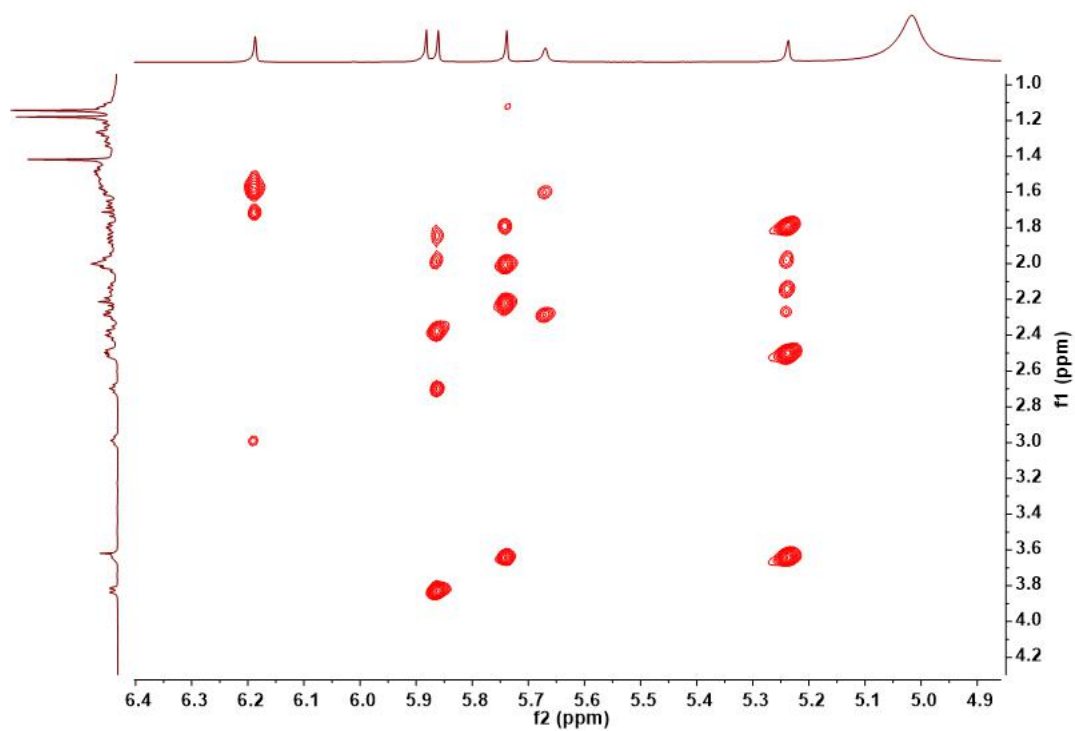


Figure S96. Enlarged ROESY (600 MHz) spectrum of **5** in pyridine-*d*₅

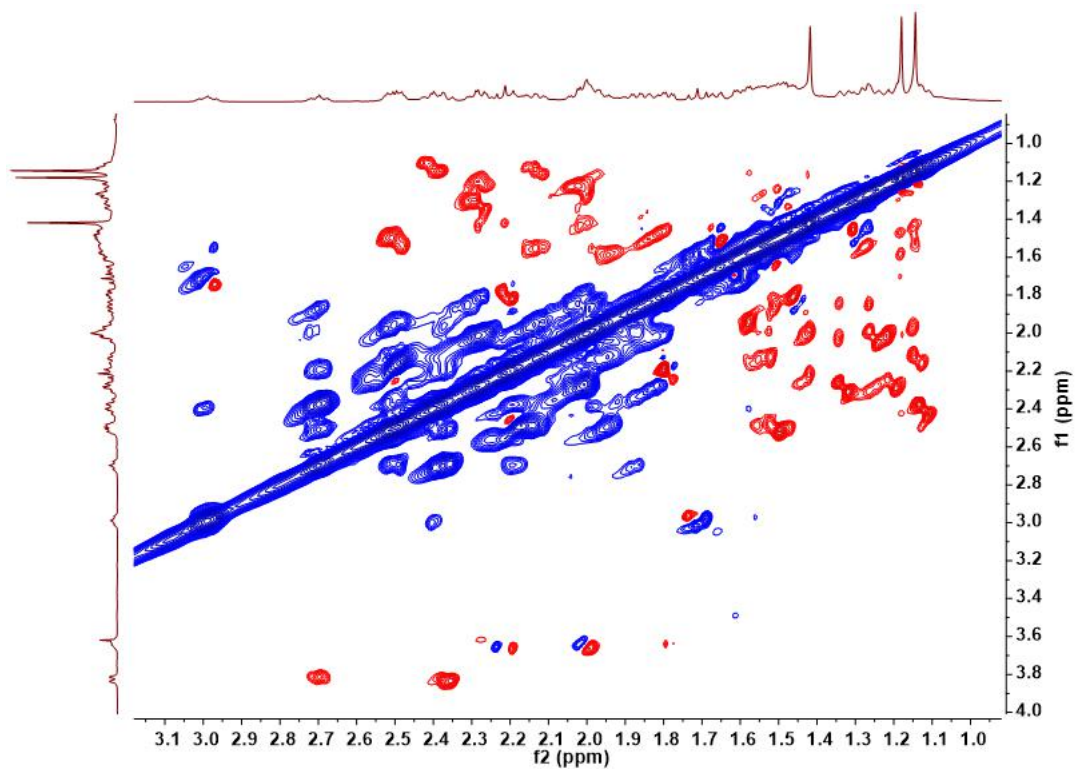


Figure S97. Enlarged ROESY (600 MHz) spectrum of **5** in pyridine-*d*₅

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

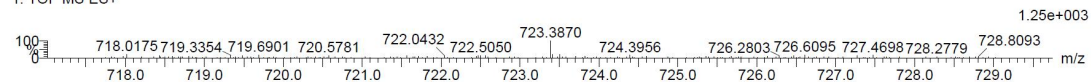
114 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 43-43 H: 0-80 N: 0-5 O: 0-10 Na: 0-1

HCX-53 115 (0.652)

1: TOF MS ES+



Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
723.3870	723.3873	-0.3	-0.4	15.5	316.1	n/a	n/a	C43 H56 O8 Na

Figure S98. HRESIMS of **5**

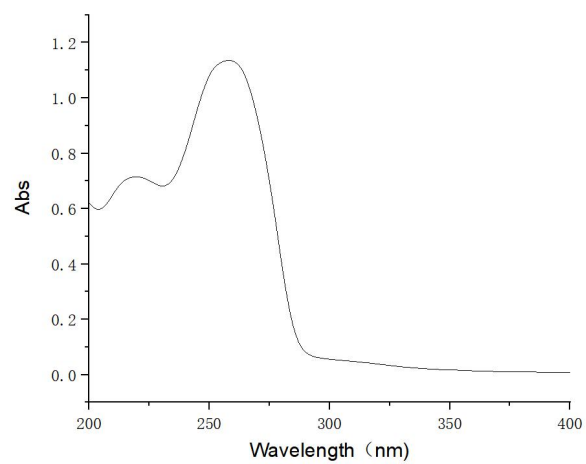


Figure S99. The UV spectrum of **1**

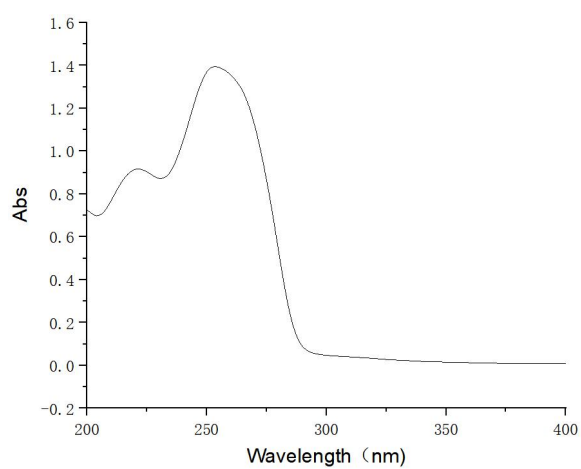


Figure S100. The UV spectrum of **2**

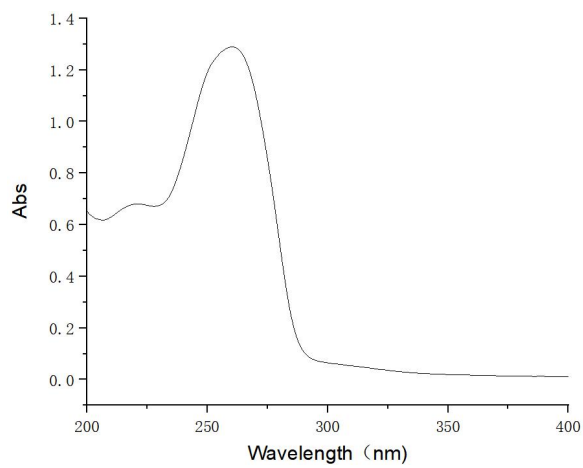


Figure S101. The UV spectrum of **3**

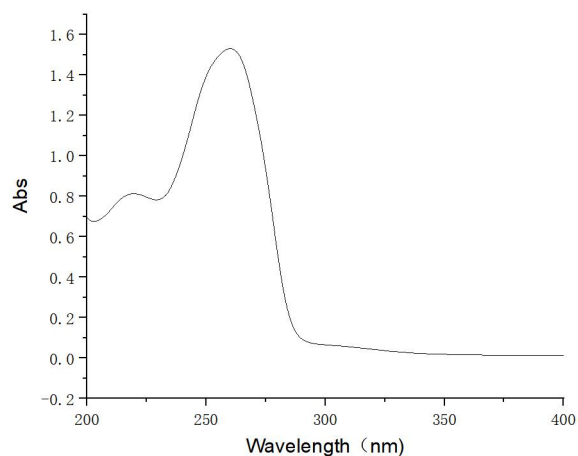


Figure S102. The UV spectrum of **4**

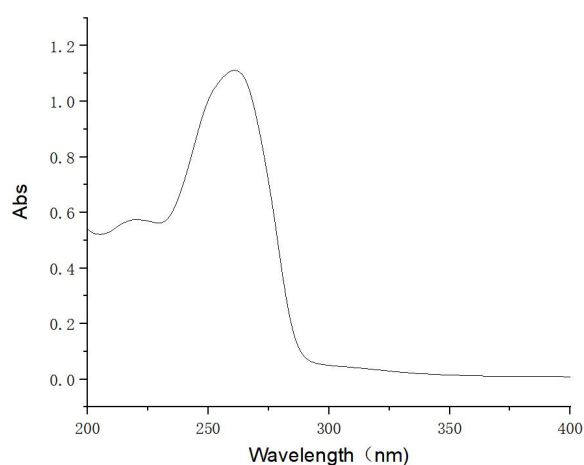


Figure S103. The UV spectrum of **5**

Biological Assays

Cell culture

RAW264.7, a mouse macrophage line (Procell life science & technology Co., Wuhan, China), was cultured in high-glucose DMEM (C11995500BT, Gibco) supplemented with 10% fetal bovine serum (FBS) (2094468CP, Gibco), 100 U/mL penicillin and 100 μ g/mL streptomycin at 37 °C in a humidified environment containing 5% CO₂.

Cell viability assay

RAW264.7 (2×10^4 cells/mL) were seeded into 96-well plates with completed DMEM. After overnight culture, cells were treated with various concentrations of compound or DMSO for 24 h. Then Cell Count Kit-8 (CCK-8, Beyotime, Shanghai, China) was added into each well for 1 h at 37 °C. The absorbance of each well was recorded at 450 nm using a microplate reader (BioTek, USA).

ELISA of TNF- α and IL-6

The culture supernatants were collected and centrifuged from treated cells. The concentrations of TNF- α and IL-6 were measured using the ELISA Kit (Proteintech, USA) according to the manufacturer's instructions.

Determination of nitrite oxide

The production of nitrite oxide was measured using the Griess Kit (Beyotime, Shanghai, China) according to the manufacturer's instructions. In short, 50 μ L of the cell supernatants were mixed with 50 μ L Griess reagent I and II, then the absorbance at 560 nm wavelength was measured using a microplate reader (BioTek, USA).

Western blot

After lipopolysaccharide (LPS) treatment, total protein was extracted from the cell lines using radioimmunoprecipitation assay (RIPA) buffer (Beyotime, China) containing protease cocktail (Roche, Germany) and quantified protein samples using the BCA assay (Thermo Scientific, USA). Equal amounts of protein extracts were separated by 10% SDS-PAGE and transferred to PVDF membranes. The membranes were blocked with 5% BSA, then with the indicated antibodies overnight at 4 °C, and followed the incubation with horseradish peroxidase (HRP)-conjugated secondary antibody at room temperature. The bands were visualized and measured via the ECL kit (Pierce, USA) and analysis system (Bio-Rad, CA, USA). The densitometry analysis of the immunoblots results was performed using ImageJ software (NIH, USA).

Statistical analysis

All experimental data obtained from this study were performed in triplicate. The results were represented Mean \pm SEM. Statistical analyses were performed by Graphpad prism 6 (GraphPad Software, San Diego, CA, USA) and Excel (Microsoft) with Student's *t*-test, one-way ANOVA test. Differences were considered significant when $*P \leq 0.05$, $**P \leq 0.01$, and $***P \leq 0.001$.

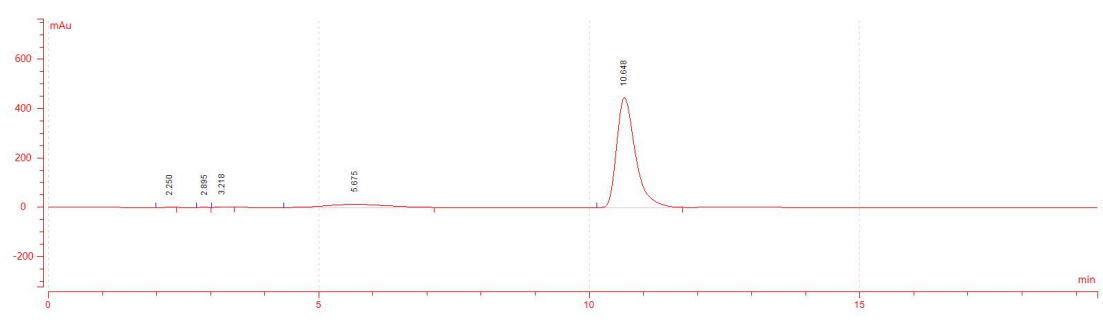


Figure S104. The chiral HPLC analysis of **1** by Lux Cellulose-1 column. (250 mm × 4.6 mm, i.d., 5 μm) Analysis condition: aqueous MeCN 75% (flow rate: 1 mL/min).

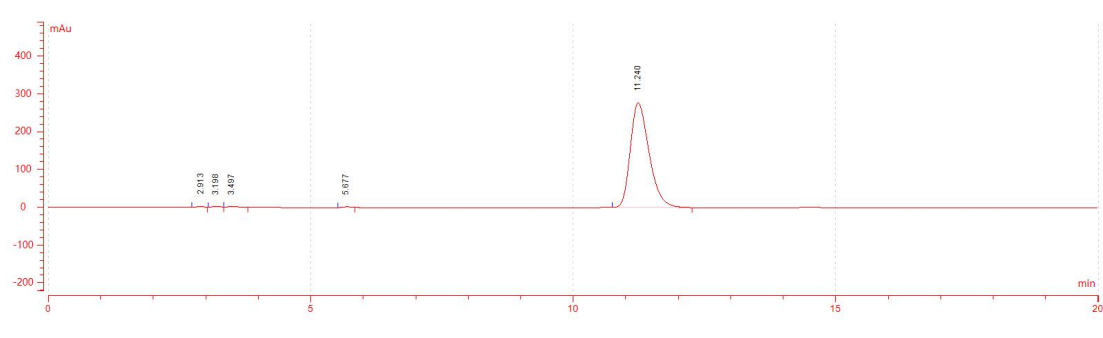


Figure S105. The chiral HPLC analysis of **2** by Lux Cellulose-1 column. (250 mm × 4.6 mm, i.d., 5 μm) Analysis condition: aqueous MeCN 75% (flow rate: 1 mL/min).

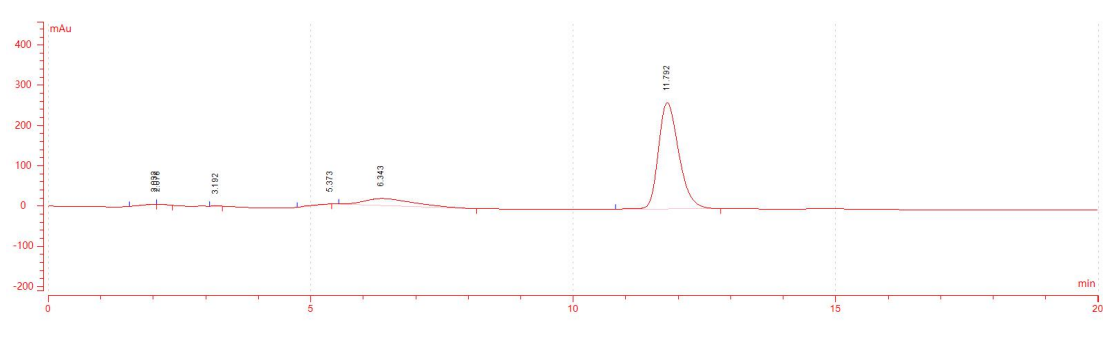


Figure S106. The chiral HPLC analysis of **3** by Lux Cellulose-1 column. (250 mm × 4.6 mm, i.d., 5 μm) Analysis condition: aqueous MeCN 80% (flow rate: 1 mL/min).

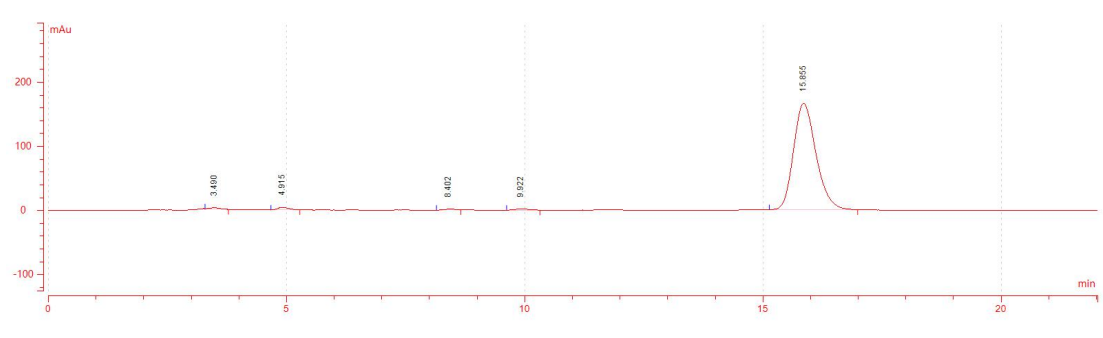


Figure S107. The chiral HPLC analysis of **4** by Lux Cellulose-1 column. (250 mm × 4.6 mm, i.d., 5 μm) Analysis condition: aqueous MeCN 80% (flow rate: 1 mL/min).

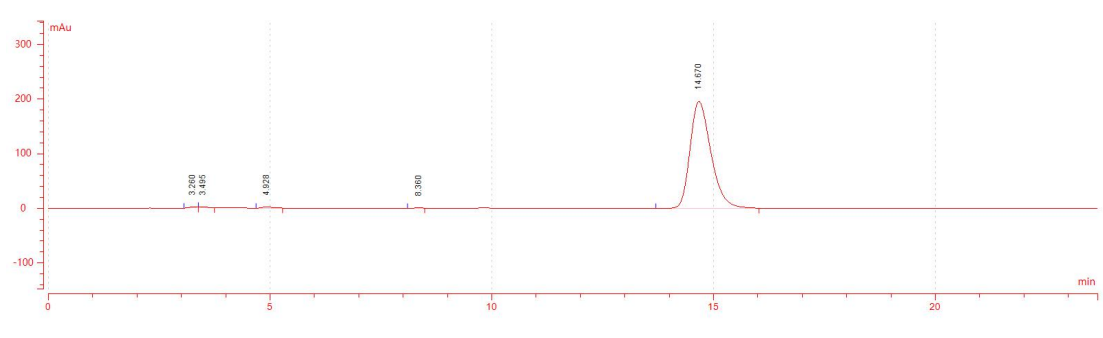


Figure S108. The chiral HPLC analysis of **5** by Lux Cellulose-1 column. (250 mm × 4.6 mm, i.d., 5 μm) Analysis condition: aqueous MeCN 80% (flow rate: 1 mL/min).