

Synthesis and electronic properties of Polycyclic Aromatic Hydrocarbons doped with Phosphorus and Sulfur

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1. HRMS Measurements

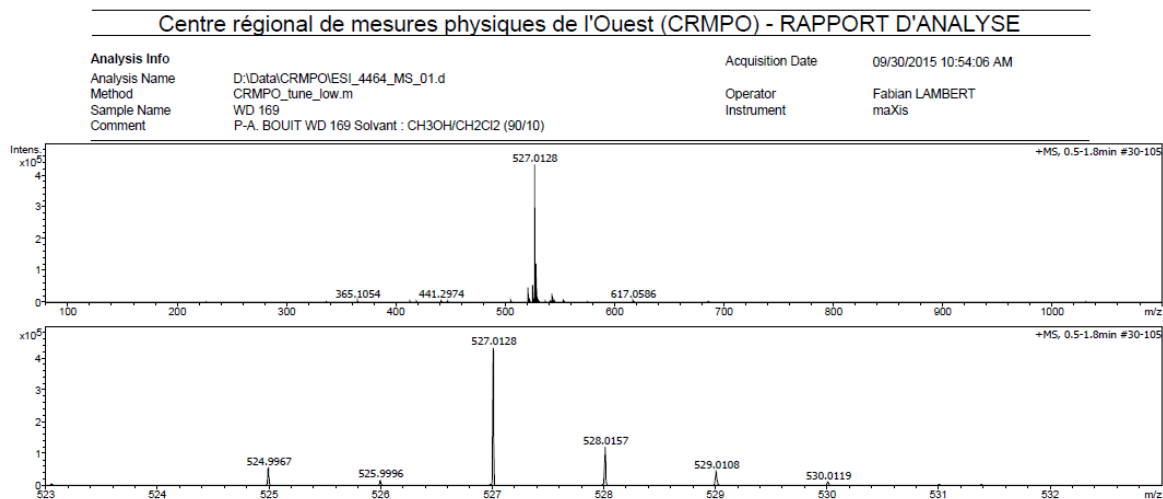


Figure S1 : HRMS spectra of the crude mixture of **5**.

2. Detailed information on crystallographic data

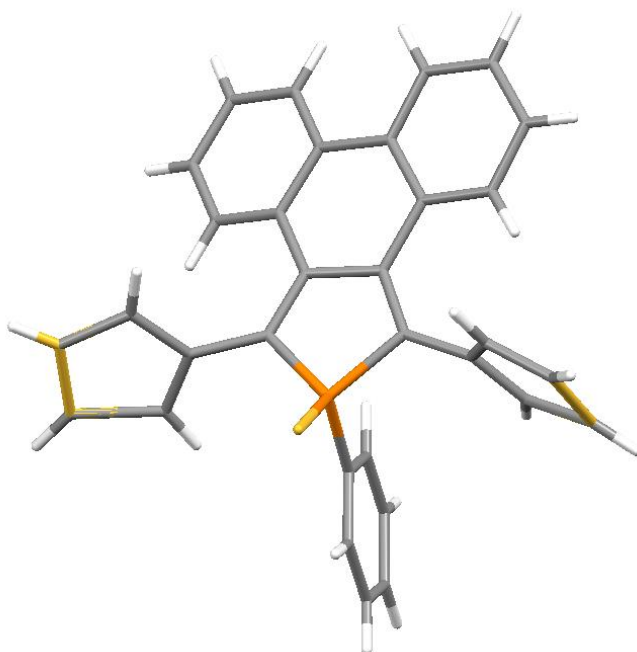


Figure S2: X-ray crystallographic structure of **3**

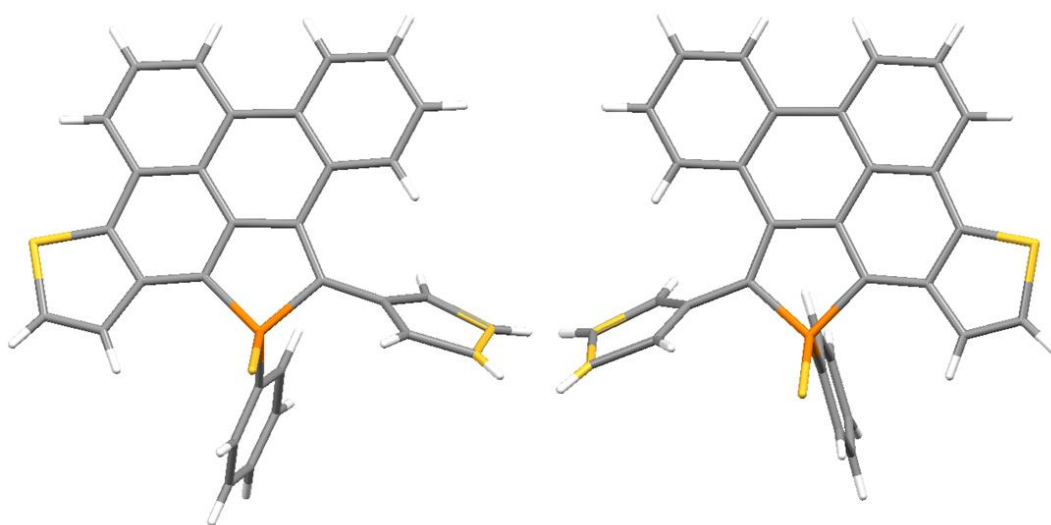


Figure S3: view of the two enantiomers of **5** in the crystallographic structure

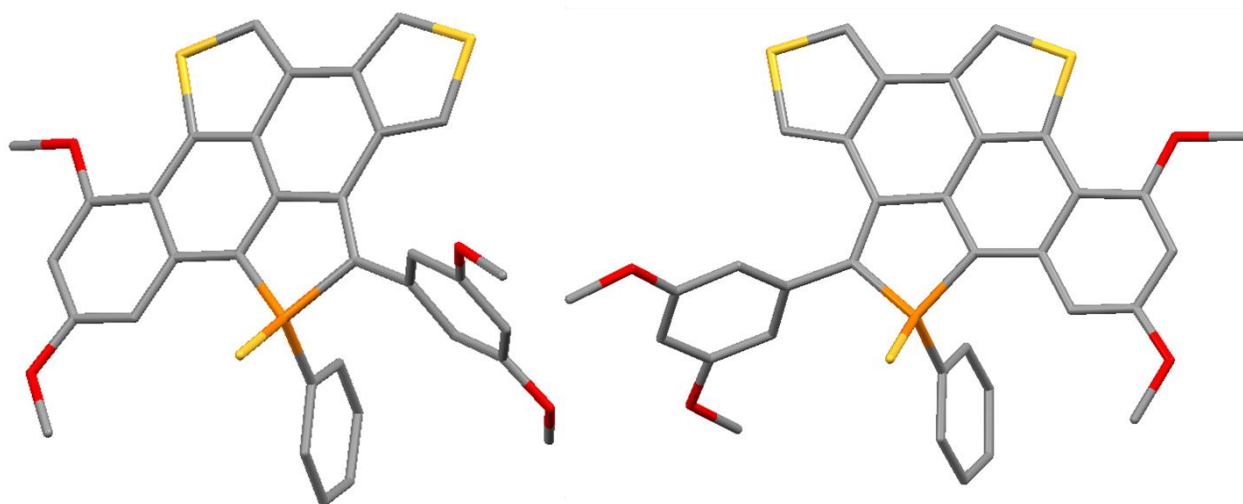


Figure S4: view of the two enantiomers of **6** in the crystallographic structure

Table S1 : Crystal data and structure refinement for **3**, **5** and **6**.

	3	5	6
Molecular formula	C ₃₀ H ₁₉ PS ₃	C ₃₀ H ₁₇ PS ₃	C ₃₄ H ₂₅ O ₄ PS ₃
CCDC number	1430204	1430205	1430206
Molecular weight	529.0	527.0	624.69
<i>a</i> (Å)	11.2994(10)	10.3219(4)	9.843(1)
<i>b</i> (Å)	9.1921(6)	14.7114(5)	11.691(1)
<i>c</i> (Å)	46.949(5)	15.3878(6)	13.887(1)
α (°)	90	90	101.061(2)
β (°)	92.111(4)	100.192(2)	101.113(2)
γ (°)	90	90	103.285(2)
<i>V</i> (Å ³)	4873.1(7)	2299.76(15)	1478.7(2)
Z	4	2	2
<i>D_c</i> (g cm ⁻³)	1.381	1.457	1.403
Crystal system	monoclinic	monoclinic	triclinic
Space group	P 1 21/c 1	P 1 2 ₁ 1	P-1
Temperature (K)	150	150	150
Wavelength Mo-K α (Å)	0.71073	0.71073	0.71073
Crystal size (mm)	0.2*0.16*0.12	0.48*0. 1*0.035	0.4*0.21*0.13
μ (mm ⁻¹)	0.388	0.411	0.344
<i>F</i> (000)	2096	1040	648
θ limit (°)	0.868-0.955	2.44-27.48	1.54-27.46
Index ranges <i>hkl</i>	-14< <i>h</i> <11 -9< <i>k</i> <11 -60< <i>k</i> <60	-13< <i>h</i> <13 -18< <i>k</i> <19 -19< <i>k</i> <19	-12< <i>h</i> <10 -13< <i>k</i> <15 -18< <i>k</i> <17
Reflections collected	31504	18324	18967
Independant reflections	11077	10239	6709
Reflections [<i>I</i> >2 σ (<i>I</i>)]	9026	8282	5332
Data/restraints/parameters	11077/0/615	10239/0/616	6709/0/380
Goodness-of-fit on <i>F</i> ²	1.093	1.028	1.099
Final <i>R</i> indices [<i>I</i> >2 σ (<i>I</i>)]	R1 = 0.0544 wR2= 0.1185	R1 = 0.0567 wR2= 0.1405	R1 = 0.0406 wR2= 0.1023

<i>R</i> indices (all data)	<i>R</i> 1 = 0.0712	<i>R</i> 1 = 0.0779	<i>R</i> 1 = 0.0561
	<i>wR</i> 2= 0.1251	<i>wR</i> 2= 0.1559	<i>wR</i> 2= 0.1206
Largest diff peak and hole (e Å ⁻³)	0.698 and -0.577	1.420 and -0.498	0.454 and -0.413

3. Theoretical Studies

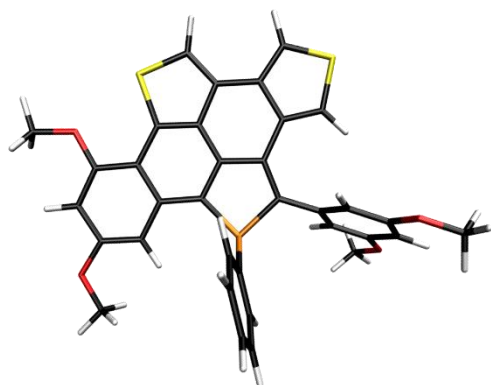


Figure S5: DFT optimized structure of **6** at the B3LYP/6-31+G* level



Figure S6: DFT optimized structure of **5** at the B3LYP/6-31+G* level

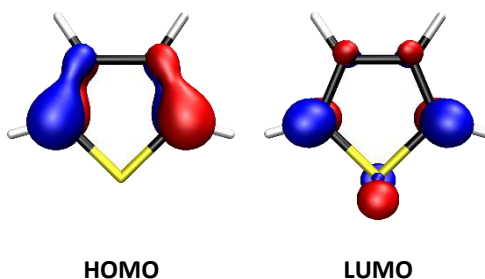


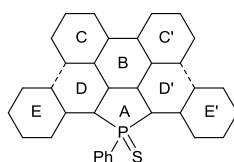
Figure S7: Frontier molecular orbitals of thiophene at the B3LYP/6-31+G* level

Table S2: Orbital composition analysis carried out on the B3LYP/6-31+G* level Kohn-Sham orbitals in order to study the participation of the different units.

Compounds		Hirshfeld method					Becke method				
		Phosphole	Thiophene I	Thiophene II	Phenyl I	Phenyl II	Phosphole	Thiophene I	Thiophene II	Phenyl I	Phenyl II
3	HOMO	39.17%	13.81%	11.96%	10.98%	11.40%	40.78%	13.62%	11.82%	11.11%	11.51%
	LUMO	45.31%	7.36%	7.28%	13.99%	14.83%	48.04%	6.99%	6.92%	14.20%	15.09%
4	HOMO	31.50%	10.09%	10.09%	6.35%	6.35%	32.56%	10.09%	10.09%	6.05%	6.04%

5	LUMO	53.38%	13.18%	13.18%	4.08%	4.08%	56.84%	13.16%	13.16%	3.51%	3.51%
	HOMO	33.78%	10.66%	14.36%	19.25%	11.62%	35.23%	10.38%	14.50%	19.51%	11.72%
6	LUMO	39.86%	5.89%	8.09%	19.52%	16.50%	42.18%	5.40%	7.93%	19.88%	16.81%
	HOMO	25.32%	28.26%	14.89%	14.70%	4.88%	26.42%	28.40%	14.79%	15.08%	4.51%
5f	LUMO	48.32%	8.87%	14.00%	11.09%	5.98%	51.35%	8.55%	14.04%	10.98%	5.40%
	HOMO	27.01%	15.47%	15.47%	17.85%	17.85%	28.21%	15.65%	15.65%	17.99%	17.99%
6f	LUMO	29.80%	8.19%	8.19%	22.59%	22.59%	31.49%	8.08%	8.08%	23.19%	23.19%
	HOMO	16.90%	24.91%	24.91%	13.20%	13.20%	17.61%	24.99%	24.99%	13.53%	13.53%
	LUMO	42.24%	10.51%	10.51%	13.66%	13.66%	44.83%	10.23%	10.23%	13.63%	13.63%

Table S3: NICS(0) and NICS(1)-indices for calculated geometries of **3-6** at the B3LYP/6-31+G* level



	3		4		5		6		5f		6f	
	NICS (0)	NICS (1)	NICS (0)	NICS (1)	NICS (0)	NICS (1)	NICS (0)	NICS (1)	NICS (0)	NICS (1)	NICS (0)	NICS (1)
A	1.5	0.6/ 0.9	0.6	-0.2/ 1	4.6	2.5/ 3.2	3.2	1.2/ 2.5	5.9	3/ 3.3	4.4	2.3/ 2.9
B	6.3	1.7/ 1.9	4.6	1/ 1.3	6.5	1.7/ 2.3	4.8	0.8/ 1.2	7.4	2.4/ 2.4	6.1	1.9/ 2
C	-5.3	-7.3/ -8	-10.4	-8.1/ -8.4	-5.8	-7.8/ -8.1	-9.0	-7.5/ -7.6	-5.6	-7.8/ -7.8	-9.1	-7.4/ -7.6
C'	-5.6	-7.6/ -8.1	-10.4	-8.1/ -8.4	-5.7	-7.8/ -8.2	-10.8	-8.4/ -8.4	-5.6	-7.8/ -7.8	-9.1	-7.4/ -7.6
D	-	-	-	-	-7.0	-8.2/ -8.6	-7.3	-8.4/ -8.7	-6.2	-7.9/ -8	-6.2	-7.5/ -7.6
D'	-	-	-	-	-	-	-	-	-6.2	-7.9/ -8	-6.2	-7.5/ -7.6
E	-11.4	-8.6/ -9	-9.3	-8.6/ -9	-10.2	-8.5/ -8.7	-9.6	-9.4/ -9.4	-10.3	-8.4/ -8.7	-9.5	-9.3/ -9.3
E'	-11.4	-8.5/ -9.5	-9.3	-8.6/ -9	-11.6	-8.8/ -9.5	-9.3	-8.6/ -9.1	-10.3	-8.4/ -8.7	-9.5	-9.3/ -9.3

4. XYZ coordinates for optimized structures

3-a

C	-0.9331080	0.8876330	-0.2003240
C	0.5435250	1.1293200	-0.1104240
C	-1.2870550	-0.4265900	-0.3499470
C	1.3196230	0.0570770	-0.4633380
P	0.2289870	-1.3971960	-0.6844220
C	2.7519990	-0.0272360	-0.7569470

C	3.5702830	-1.0772140	-0.3912240
C	3.4637870	0.9319860	-1.5664290
S	5.1804980	-0.9012910	-0.9949190
C	4.7700250	0.5972610	-1.7740450
C	-2.5939320	-1.0799590	-0.2249240
C	-3.5137340	-0.8274290	0.8583400
C	-3.0663330	-2.0680980	-1.0656210
C	-4.6332950	-1.6063910	0.8059070
S	-4.6058660	-2.6748720	-0.5645680
C	-1.8177480	2.0654710	-0.2600260
C	-1.3110770	3.3432710	0.0937380
C	0.9931270	2.4119400	0.4628100
C	0.0672220	3.4777320	0.6130800
C	2.2901600	2.5602360	0.9945240
C	2.6877450	3.7314660	1.6293040
C	0.4859580	4.6474530	1.2738040
C	1.7793000	4.7849970	1.7678280
C	-3.1213200	1.9740090	-0.7877410
C	-3.9261840	3.0979550	-0.9358330
C	-2.1375250	4.4688250	-0.0784180
C	-3.4323530	4.3548870	-0.5746880
S	0.3181840	-2.3366850	-2.4204750
C	0.5069120	-2.4802170	0.7802090
C	0.7762800	-3.8410820	0.5975640
C	0.4480640	-1.9504150	2.0795480
C	0.9878210	-4.6675590	1.7058290
C	0.6605030	-2.7776750	3.1826420
C	0.9313050	-4.1383340	2.9970580
H	3.3113710	-1.9389770	0.2090710
H	2.9969960	1.8186830	-1.9806820
H	5.5121040	1.1304510	-2.3540070
H	-3.3246900	-0.0981080	1.6385330
H	-2.5833550	-2.4565930	-1.9523670
H	-5.4661000	-1.6258290	1.4968760
H	2.9888520	1.7358850	0.9306540
H	3.6939140	3.8127830	2.0316700
H	-0.2163330	5.4588650	1.4306470
H	2.0694910	5.7007380	2.2762780
H	-3.4977990	1.0125040	-1.1122650
H	-4.9247740	2.9957230	-1.3520190
H	-1.7565830	5.4580710	0.1505630
H	-4.0434250	5.2448360	-0.7007460
H	0.8173590	-4.2434840	-0.4111390
H	0.2380920	-0.8945430	2.2311300
H	1.1951860	-5.7241130	1.5564960
H	0.6139550	-2.3615840	4.1858030
H	1.0960310	-4.7817180	3.8576950

3-b

C	-0.6477740	1.0991340	-0.1821600
C	0.8392500	0.9125160	-0.0764870

C	-1.3556750	-0.0608560	-0.3462190
C	1.2792440	-0.3369600	-0.4129530
P	-0.1733650	-1.4169230	-0.6864330
C	2.6373680	-0.8467010	-0.6496530
C	3.4701980	-0.3462210	-1.6268430
C	3.2351950	-1.9652170	0.0323490
S	4.9724040	-1.1975210	-1.7071140
C	4.4921580	-2.2578370	-0.4199590
C	-2.7950140	-0.3227190	-0.2406590
C	-3.6195560	0.1667290	0.8380230
C	-3.5142790	-1.1343400	-1.0950980
C	-4.9107380	-0.2704050	0.7689560
S	-5.1670140	-1.2933600	-0.6123750
C	-1.1671590	2.4771390	-0.2379930
C	-0.3259540	3.5599720	0.1273390
C	1.6332540	2.0246020	0.4864590
C	1.0366420	3.3031010	0.6431980
C	2.9320960	1.8168330	0.9928960
C	3.6406850	2.8338760	1.6221320
C	1.7654260	4.3127000	1.2997920
C	3.0527400	4.0925970	1.7776250
C	-2.4424680	2.7567410	-0.7691600
C	-2.9032010	4.0610880	-0.9069370
C	-0.8064880	4.8723090	-0.0359380
C	-2.0805200	5.1276440	-0.5334200
S	-0.3149140	-2.2914410	-2.4538070
C	-0.2470530	-2.5724340	0.7446330
C	-0.3197780	-3.9518730	0.5229360
C	-0.2280130	-2.0774750	2.0589010
C	-0.3713980	-4.8325590	1.6080140
C	-0.2778200	-2.9591860	3.1390070
C	-0.3491450	-4.3389890	2.9143850
H	3.2652610	0.4690480	-2.3079360
H	2.7456280	-2.5085560	0.8329900
H	5.1608390	-3.0366440	-0.0771480
H	-3.2441040	0.8093960	1.6269980
H	-3.1489130	-1.6360690	-1.9813450
H	-5.7232200	-0.0631540	1.4533010
H	3.3869760	0.8387370	0.9082450
H	4.6387670	2.6388960	2.0051430
H	1.3123190	5.2839840	1.4646540
H	3.5866440	4.8931080	2.2830720
H	-3.0702470	1.9409930	-1.1035600
H	-3.8893020	4.2440060	-1.3252320
H	-0.1665040	5.7151310	0.2005180
H	-2.4191860	6.1536620	-0.6513100
H	-0.3375870	-4.3256360	-0.4973080
H	-0.1749080	-1.0065000	2.2388950
H	-0.4295480	-5.9031650	1.4291680
H	-0.2636650	-2.5706910	4.1541730
H	-0.3897420	-5.0248170	3.7569160

3-c

C	-1.0080680	0.7742500	-0.2272790
C	0.4354400	1.1634800	-0.1033000
C	-1.2197580	-0.5654330	-0.4048790
C	1.3241730	0.1830000	-0.4564400
P	0.3938300	-1.3692770	-0.7331120
C	2.7644760	0.2513790	-0.7146690
C	3.6765140	-0.7171260	-0.3462260
C	3.3942490	1.2955370	-1.4858980
S	5.2751450	-0.3644330	-0.9015680
C	4.7328810	1.1006660	-1.6634090
C	-2.4534440	-1.3579460	-0.3279460
C	-2.9028600	-2.2963600	-1.3251370
C	-3.2953650	-1.3386660	0.7653730
C	-4.0627010	-2.9297960	-0.9756170
S	-4.6304280	-2.4207830	0.5852080
C	-2.0075220	1.8598570	-0.2883830
C	-1.6331130	3.1789070	0.0767620
C	0.7417780	2.4752530	0.4970020
C	-0.2867690	3.4444180	0.6288010
C	2.0021090	2.7405620	1.0698940
C	2.2663780	3.9377830	1.7254330
C	-0.0018290	4.6424090	1.3097180
C	1.2575720	4.8984780	1.8427890
C	-3.2910280	1.6447640	-0.8291270
C	-4.1977260	2.6860450	-0.9881630
C	-2.5613740	4.2209210	-0.1073320
C	-3.8314880	3.9849010	-0.6222840
S	0.6003730	-2.2452470	-2.4912730
C	0.7551690	-2.4581280	0.7087410
C	1.1151040	-3.7938660	0.4986320
C	0.6617720	-1.9601630	2.0186210
C	1.3820180	-4.6266510	1.5900380
C	0.9301100	-2.7934810	3.1048950
C	1.2911330	-4.1288960	2.8918020
H	3.4921560	-1.6139060	0.2298760
H	2.8499250	2.1387240	-1.8963940
H	5.4308990	1.7198500	-2.2117510
H	-2.3727700	-2.4698360	-2.2543340
H	-3.1932690	-0.7417650	1.6620980
H	-4.6164640	-3.6678560	-1.5411700
H	2.7778210	1.9869520	1.0218570
H	3.2473520	4.1106070	2.1598480
H	-0.7836260	5.3801450	1.4526420
H	1.4433750	5.8326390	2.3663670
H	-3.5735470	0.6506600	-1.1497320
H	-5.1771590	2.4879910	-1.4151390
H	-2.2804730	5.2414890	0.1288400
H	-4.5232080	4.8123410	-0.7569330
H	1.1837500	-4.1719070	-0.5179810

H	0.3824770	-0.9237480	2.1913780
H	1.6601690	-5.6635220	1.4193670
H	0.8572750	-2.4017400	4.1162800
H	1.4994430	-4.7771580	3.7392210

3^α-A-ΔE₁-1

C	-0.2202530	1.2355510	-0.2584560
C	1.0482780	0.5080930	-0.2282560
C	-1.3213860	0.4293950	-0.4474900
C	0.9371510	-0.9071600	-0.5350360
P	-0.8165260	-1.3114940	-0.7718400
C	2.0500370	-1.6710920	-0.6989570
C	3.4047350	-0.9756420	-0.6206790
C	2.1861060	-3.0774940	-0.9739890
S	4.6500640	-2.3314350	-0.3578970
C	3.4566400	-3.5312910	-0.8334390
C	-2.7553970	0.7347380	-0.3330770
C	-3.3702510	1.3087540	0.8391920
C	-3.6957710	0.4204550	-1.2922420
C	-4.7272860	1.4203390	0.7342960
S	-5.3018810	0.8283520	-0.7947370
C	-0.1482920	2.6959580	-0.0771610
C	1.0852300	3.2987920	0.3106060
C	2.2289300	1.0719930	0.1687710
C	2.3133210	2.4860670	0.4644310
C	3.4217950	0.1462910	0.4184950
C	4.7277390	0.8862470	0.5252740
C	3.5434740	3.0136640	0.7751000
C	4.7514930	2.2166320	0.7462310
C	-1.2594460	3.5260400	-0.3324620
C	-1.1964650	4.9019550	-0.1578100
C	1.1157200	4.6957370	0.4942570
C	-0.0032660	5.4894150	0.2783240
S	-1.3373680	-2.1082140	-2.5086280
C	-1.3704260	-2.2987640	0.6806310
C	-2.2107860	-3.4032590	0.5011340
C	-0.9609380	-1.9416840	1.9755220
C	-2.6363520	-4.1468600	1.6060460
C	-1.3855840	-2.6866960	3.0763300
C	-2.2247280	-3.7911850	2.8924690
H	3.6276520	-0.5549410	-1.6155140
H	1.3468950	-3.7135430	-1.2338590
H	3.7830130	-4.5562880	-0.9722850
H	-2.8085220	1.6108550	1.7165200
H	-3.5166580	-0.0310520	-2.2587710
H	-5.4242380	1.8032600	1.4685120
H	3.2485330	-0.3430150	1.4029060
H	5.6490240	0.3085180	0.5024020
H	3.6568730	4.0708120	0.9871320
H	5.7008370	2.7276390	0.8890170
H	-2.1807370	3.0826430	-0.6867010

H	-2.0697120	5.5144190	-0.3656900
H	2.0371650	5.1791500	0.7992380
H	0.0592730	6.5639790	0.4293290
H	-2.5223730	-3.6740670	-0.5038890
H	-0.3099390	-1.0840720	2.1263440
H	-3.2891500	-5.0034890	1.4586050
H	-1.0618610	-2.4065070	4.0755860
H	-2.5553810	-4.3710490	3.7505950

3^α-A-ΔE₁-2

C	-0.1525890	1.2672820	-0.1735830
C	1.0839530	0.4827170	-0.1952730
C	-1.2920300	0.5149750	-0.3666290
C	0.8903810	-0.9298140	-0.4746070
P	-0.8677540	-1.2188310	-0.8144820
C	1.9255230	-1.8072950	-0.3993940
C	3.2463070	-1.3002840	0.1653280
C	1.9924160	-3.2047280	-0.7374310
S	4.5264800	-2.5504350	-0.3392550
C	3.2575550	-3.6949970	-0.7481950
C	-2.7098040	0.8789000	-0.2294830
C	-3.2848190	1.4345620	0.9717850
C	-3.6752250	0.6416190	-1.1862780
C	-4.6369420	1.6082120	0.8905060
S	-5.2556540	1.0990270	-0.6508440
C	-0.0103160	2.7265510	-0.0208190
C	1.2742990	3.2833700	0.2523790
C	2.3244770	1.0219790	0.0000860
C	2.4732260	2.4219030	0.3372370
C	3.5594910	0.1467550	-0.2201550
C	4.7881840	0.6928430	0.4600170
C	3.7048680	2.8654060	0.7537920
C	4.8402040	1.9757140	0.8729230
C	-1.1008590	3.6024530	-0.2034270
C	-0.9616300	4.9780620	-0.0755000
C	1.3863180	4.6820470	0.3808000
C	0.2906690	5.5221190	0.2314220
S	-1.3796110	-1.8358320	-2.6259930
C	-1.5081590	-2.2964720	0.5331090
C	-2.3372850	-3.3837800	0.2356660
C	-1.1717330	-2.0261290	1.8695800
C	-2.8229770	-4.1971490	1.2641250
C	-1.6573350	-2.8394530	2.8940280
C	-2.4839820	-3.9273810	2.5919210
H	3.1834310	-1.3728500	1.2641930
H	1.1258400	-3.7865110	-1.0330720
H	3.5421380	-4.7075470	-1.0129200
H	-2.6989020	1.6794210	1.8512750
H	-3.5282410	0.2219050	-2.1723830
H	-5.3072420	1.9930100	1.6481800
H	3.7596540	0.1490290	-1.3141450

H	5.6555590	0.0427420	0.5512010
H	3.8467890	3.8942210	1.0658590
H	5.7522630	2.3687580	1.3161140
H	-2.0691730	3.1972980	-0.4642010
H	-1.8222350	5.6243170	-0.2259320
H	2.3559590	5.1282310	0.5733930
H	0.4158460	6.5972490	0.3306190
H	-2.5951130	-3.5848510	-0.8005780
H	-0.5316260	-1.1811070	2.1116470
H	-3.4669220	-5.0396760	1.0250030
H	-1.3920120	-2.6247930	3.9261890
H	-2.8622780	-4.5604800	3.3906730

3^α-A'-ΔE₁-1

C	-1.0247860	0.5397670	-0.2347000
C	0.2769120	1.2064960	-0.2940950
C	-0.9874390	-0.8800950	-0.5380140
C	1.3320390	0.3480900	-0.5051550
P	0.7389910	-1.3690930	-0.8136260
C	2.7841640	0.5859570	-0.4461670
C	3.4493790	0.9887330	0.6923360
C	3.6952000	0.3526520	-1.5375890
S	5.1564240	1.1129610	0.4451250
C	4.9978910	0.6069890	-1.2085180
C	-2.1384440	-1.5911950	-0.6750470
C	-2.3465500	-2.9907800	-0.9402070
C	-3.4566970	-0.8323180	-0.5713400
C	-3.6336370	-3.3835110	-0.7696580
S	-4.7586510	-2.1266490	-0.2752470
C	-2.1686480	1.1596680	0.1856220
C	-2.1795470	2.5763480	0.4802800
C	0.2779850	2.6706150	-0.1119220
C	-0.9179300	3.3300140	0.2993050
C	1.4215120	3.4487110	-0.3873920
C	1.4246920	4.8261770	-0.2155050
C	-0.8807930	4.7273890	0.4813430
C	0.2682770	5.4688130	0.2417720
C	-3.3984480	0.2918140	0.4634280
C	-4.6654000	1.0927510	0.5967310
C	-3.3761600	3.1615100	0.8170910
C	-4.6211100	2.4228040	0.8160080
S	1.1857440	-2.1903720	-2.5586290
C	1.2785690	-2.3770430	0.6297320
C	2.0951240	-3.4972880	0.4378840
C	0.8866310	-2.0188040	1.9296830
C	2.5148750	-4.2547280	1.5355340
C	1.3054430	-2.7776380	3.0233860
C	2.1212960	-3.8973200	2.8271700
H	3.0200190	1.2190370	1.6584760
H	3.3709220	0.0112070	-2.5137020
H	5.8744090	0.5208410	-1.8373880

H	-1.5441320	-3.6668110	-1.2148800
H	-3.6809260	-0.4049060	-1.5630290
H	-4.0108020	-4.3925720	-0.8960240
H	2.3171980	2.9625460	-0.7499300
H	2.3214950	5.3973030	-0.4401290
H	-1.7727460	5.2526730	0.8041300
H	0.2580930	6.5452600	0.3919490
H	-3.2269770	-0.2029080	1.4455560
H	-5.6133120	0.5593280	0.5947940
H	-3.4346980	4.2227770	1.0305120
H	-5.5417070	2.9785110	0.9786210
H	2.3917160	-3.7698890	-0.5711970
H	0.2528560	-1.1501180	2.0899500
H	3.1488680	-5.1236830	1.3784990
H	0.9948100	-2.4967070	4.0266010
H	2.4473770	-4.4880280	3.6796230

3^α-A'-ΔE₁-2

C	-1.0624690	0.4777310	-0.1000120
C	0.2046660	1.2098800	-0.0445850
C	-0.9226840	-0.9441710	-0.3604040
C	1.3051360	0.4382370	-0.3402360
P	0.8239170	-1.3008820	-0.7067850
C	2.7127830	0.8275340	-0.5472270
C	3.7612880	0.3988350	0.2362930
C	3.1717840	1.6315180	-1.6508220
S	5.2887010	0.9781080	-0.3372590
C	4.5275200	1.8002710	-1.6637550
C	-2.0033430	-1.7685800	-0.3249850
C	-2.1183650	-3.1697050	-0.6330720
C	-3.3344170	-1.1719910	0.1217130
C	-3.4022470	-3.6009090	-0.7077820
S	-4.6373750	-2.3864970	-0.4129770
C	-2.2854480	1.0849820	-0.0351440
C	-2.3964590	2.5029530	0.2316250
C	0.1287570	2.6435880	0.2931580
C	-1.1455200	3.2753780	0.4051110
C	1.2881430	3.4051250	0.5484200
C	1.2192170	4.7560080	0.8626680
C	-1.1843320	4.6496370	0.7143290
C	-0.0277790	5.3867610	0.9324050
C	-3.5250470	0.2582240	-0.3844350
C	-4.8089070	0.9094520	0.0539270
C	-3.6516930	3.0381120	0.3919460
C	-4.8468410	2.2220000	0.3612840
S	1.2927370	-2.0083260	-2.4904800
C	1.4560210	-2.3346900	0.6827170
C	2.2788130	-3.4363240	0.4208820
C	1.1256670	-2.0161250	2.0104240
C	2.7652710	-4.2149510	1.4756180
C	1.6122420	-2.7949310	3.0614370

C	2.4334470	-3.8964930	2.7947250
H	3.7124430	-0.2195580	1.1227740
H	2.5039890	2.0448270	-2.3986610
H	5.1261830	2.3438450	-2.3831190
H	-1.2643950	-3.7996500	-0.8576200
H	-3.3589030	-1.1734910	1.2242750
H	-3.7189610	-4.6075320	-0.9582410
H	2.2566240	2.9251190	0.5074670
H	2.1318970	5.3138420	1.0542790
H	-2.1389720	5.1577010	0.7931800
H	-0.0982130	6.4455310	1.1679280
H	-3.5592580	0.1935370	-1.4946120
H	-5.7192600	0.3144950	0.0359850
H	-3.7823410	4.0918300	0.6110070
H	-5.7930700	2.6962010	0.6112440
H	2.5300940	-3.6747880	-0.6091250
H	0.4904890	-1.1601560	2.2252170
H	3.4037640	-5.0688880	1.2638390
H	1.3507590	-2.5435220	4.0862520
H	2.8121480	-4.5027970	3.6138090

3^β-A-ΔE₁-1

C	-0.2436270	1.2641320	-0.1945480
C	1.0579470	0.5761980	-0.1801070
C	-1.3141590	0.4200530	-0.3822510
C	0.9834910	-0.8297610	-0.4688680
P	-0.7342250	-1.2873180	-0.7576350
C	2.1181190	-1.6128030	-0.4553200
C	3.4098950	-1.0122940	0.1135970
C	2.3015890	-2.9434880	-0.8664230
C	4.5334720	-1.8911250	-0.3576090
S	3.9519660	-3.3531660	-0.9124170
C	-2.7583910	0.6699150	-0.2706410
C	-3.3929520	1.2145320	0.9053370
C	-3.6877560	0.3243710	-1.2297550
C	-4.7534800	1.2745710	0.8034310
S	-5.3076080	0.6679470	-0.7274930
C	-0.2257330	2.7334850	-0.0807070
C	0.9984050	3.3999060	0.2179980
C	2.2432280	1.2285610	0.0607250
C	2.2557370	2.6367580	0.3782440
C	3.5685410	0.4924980	-0.1232260
C	4.6714880	1.0979030	0.7087920
C	3.4199740	3.1881440	0.8655700
C	4.5956680	2.3847130	1.1105020
C	-1.3754420	3.5118250	-0.3286890
C	-1.3504430	4.8979820	-0.2436280
C	0.9958050	4.8058390	0.3006590
C	-0.1569670	5.5505770	0.0841780
S	-1.2173720	-2.0469580	-2.5265870
C	-1.2670990	-2.3485420	0.6510500

C	-2.0490790	-3.4864740	0.4249980
C	-0.8957340	-2.0119000	1.9629660
C	-2.4558320	-4.2828450	1.5000740
C	-1.3017010	-2.8088030	3.0341240
C	-2.0832950	-3.9464190	2.8034540
H	3.3244480	-1.1597800	1.2184450
H	1.5671480	-3.6026650	-1.3097790
H	-2.8408230	1.5340310	1.7826890
H	-3.4931150	-0.1147870	-2.1989950
H	-5.4631950	1.6274270	1.5404940
H	3.8597400	0.6231110	-1.1933120
H	5.5575960	0.5017860	0.9151410
H	3.4562190	4.2291960	1.1670220
H	5.4214970	2.8376300	1.6547410
H	-2.2984440	3.0212680	-0.6072160
H	-2.2538430	5.4676820	-0.4444920
H	1.9206730	5.3332270	0.5078180
H	-0.1205010	6.6350670	0.1478760
H	-2.3315490	-3.7399730	-0.5931240
H	-0.2902150	-1.1279920	2.1486470
H	-3.0644980	-5.1646870	1.3164210
H	-1.0094760	-2.5426530	4.0469240
H	-2.4000440	-4.5665490	3.6384360
H	5.5899540	-1.7517850	-0.1728270

3^β-A-ΔE₁-2

C	-0.2329290	1.2575990	-0.2476950
C	1.0640660	0.5681680	-0.2121000
C	-1.3034550	0.4159070	-0.4430750
C	0.9924500	-0.8425770	-0.4840430
P	-0.7284670	-1.3059070	-0.7537800
C	2.1449300	-1.5884790	-0.6105860
C	3.4917180	-0.8592630	-0.5301880
C	2.3095880	-2.9667310	-0.8362860
C	4.5373130	-1.9184010	-0.3040900
S	3.9321520	-3.4325820	-0.6521340
C	-2.7494620	0.6688780	-0.3500160
C	-3.4054880	1.2006050	0.8197850
C	-3.6600990	0.3368780	-1.3310630
C	-4.7636730	1.2652990	0.6918000
S	-5.2891300	0.6783640	-0.8568930
C	-0.2174510	2.7195700	-0.0689960
C	0.9915770	3.3700660	0.3157140
C	2.2306170	1.1921020	0.1622510
C	2.2530010	2.6056830	0.4563430
C	3.4647890	0.3284630	0.4349850
C	4.7393140	1.1303760	0.4556260
C	3.4632410	3.1949530	0.7455610
C	4.7071810	2.4622780	0.6691950
C	-1.3615180	3.5056180	-0.3189310
C	-1.3540960	4.8823180	-0.1384100

C	0.9663040	4.7661060	0.5051480
C	-0.1847370	5.5154850	0.2974480
S	-1.2000730	-2.1293580	-2.4954720
C	-1.2850990	-2.3084590	0.6896170
C	-2.1459580	-3.3959970	0.5026260
C	-0.8619910	-1.9749100	1.9863040
C	-2.5791790	-4.1446820	1.6012360
C	-1.2944910	-2.7245520	3.0811290
C	-2.1548010	-3.8113300	2.8896010
H	3.6673810	-0.4436190	-1.5527920
H	1.5414650	-3.7115670	-0.9925640
H	-2.8702250	1.5089200	1.7114080
H	-3.4473400	-0.0935250	-2.3004060
H	-5.4870090	1.6115170	1.4187000
H	3.3429020	-0.1010370	1.4586720
H	5.6876450	0.6026560	0.3880360
H	3.5284320	4.2559160	0.9572880
H	5.6349260	3.0229010	0.7604680
H	-2.2650970	3.0273570	-0.6729720
H	-2.2521870	5.4595510	-0.3414880
H	1.8680560	5.2854930	0.8095310
H	-0.1650190	6.5908950	0.4542960
H	-2.4657150	-3.6508990	-0.5040260
H	-0.1922900	-1.1326660	2.1411930
H	-3.2478270	-4.9879710	1.4475160
H	-0.9599420	-2.4620300	4.0817210
H	-2.4915130	-4.3950160	3.7428500
H	5.6031970	-1.7668740	-0.2021100

$3^B-\Delta E_2$

C	-1.0179900	0.5996070	-0.2243820
C	0.3363230	1.2070420	-0.2426620
C	-1.0793710	-0.7437700	-0.4974720
C	1.3372890	0.3001760	-0.4679800
P	0.6008960	-1.3601510	-0.7937940
C	2.8035330	0.4327330	-0.4438470
C	3.5311270	0.6780290	0.7007740
C	3.6593250	0.2441480	-1.5870600
S	5.2341390	0.7115890	0.3994290
C	4.9867940	0.3773750	-1.2864250
C	-2.3277230	-1.4395470	-0.5166630
C	-2.5787030	-2.7682790	-0.8112580
C	-3.5346010	-0.7031790	-0.1861030
S	-4.2563100	-3.1253250	-0.6937410
C	-4.6543450	-1.5099810	-0.2444080
C	-2.1943650	1.3642010	0.1049260
C	-2.0713720	2.7471440	0.4103020
C	0.4211880	2.6694240	-0.0613480
C	-0.7496080	3.4091370	0.2753160
C	1.6288490	3.3659210	-0.2664700
C	1.7145600	4.7440310	-0.1121630

C	-0.6323570	4.8041420	0.4309130
C	0.5757300	5.4679560	0.2511530
C	-3.4609860	0.7123690	0.1521900
C	-4.5920040	1.4567440	0.5303940
C	-3.2243740	3.4391390	0.7965600
C	-4.4683770	2.7997660	0.8566930
S	0.9718470	-2.1776420	-2.5548510
C	1.0449800	-2.4165920	0.6446390
C	1.8182410	-3.5654840	0.4442230
C	0.6362810	-2.0695540	1.9424890
C	2.1827220	-4.3621260	1.5338850
C	1.0011150	-2.8677970	3.0272330
C	1.7761120	-4.0151220	2.8241300
H	3.1496650	0.8436290	1.6997600
H	3.2811600	0.0193610	-2.5776020
H	5.8342620	0.2916740	-1.9539840
H	-1.8712710	-3.5290350	-1.1121110
H	2.5131430	2.8164980	-0.5587550
H	2.6616000	5.2493330	-0.2811970
H	-1.5058520	5.3957820	0.6789530
H	0.6229520	6.5464770	0.3772680
H	-5.5656940	0.9781560	0.5775680
H	-3.1783180	4.4891710	1.0606440
H	-5.3449480	3.3661220	1.1601210
H	2.1242720	-3.8307140	-0.5641390
H	0.0300240	-1.1823100	2.1068580
H	2.7835960	-5.2532130	1.3712080
H	0.6774130	-2.5971820	4.0290630
H	2.0584610	-4.6365820	3.6702420
H	-5.6866980	-1.2487820	-0.0558340

3^B-A'-ΔE₁-1

C	-1.0220100	0.6235970	-0.1811830
C	0.3212040	1.2283220	-0.2232670
C	-1.0430430	-0.7846220	-0.4672340
C	1.3290570	0.3179810	-0.4363840
P	0.6348670	-1.3507100	-0.7971820
C	2.7918160	0.4769640	-0.3864190
C	3.4836330	0.8163040	0.7568410
C	3.6832910	0.2235740	-1.4896060
S	5.1936740	0.8587370	0.5007750
C	4.9992620	0.4020260	-1.1635000
C	-2.2245120	-1.4942630	-0.4268560
C	-2.4993470	-2.8126870	-0.8266850
C	-3.4647400	-0.8113510	0.1633110
S	-4.1727570	-3.1173550	-0.8398660
C	-4.6503630	-1.6186740	-0.2834990
C	-2.1586680	1.3501710	0.0806080
C	-2.0763750	2.7567230	0.3944830
C	0.3988620	2.6976100	-0.1049110
C	-0.7765090	3.4388730	0.2103940

C	1.5923210	3.4034220	-0.3631100
C	1.6537440	4.7884280	-0.2815770
C	-0.6863550	4.8425310	0.2900550
C	0.5066030	5.5146070	0.0571120
C	-3.5313960	0.6998360	-0.0760650
C	-4.5781600	1.3753100	0.7742940
C	-3.1935260	3.3812260	0.9028840
C	-4.4133320	2.6549420	1.1717260
S	1.0298930	-2.1344930	-2.5761620
C	1.1352530	-2.4414340	0.6004720
C	1.8828930	-3.5998100	0.3618480
C	0.7802330	-2.1043400	1.9167710
C	2.2731270	-4.4148440	1.4289710
C	1.1695000	-2.9200470	2.9800680
C	1.9179060	-4.0771910	2.7369340
H	3.0714650	1.0452810	1.7307710
H	3.3361550	-0.0756480	-2.4717120
H	5.8664550	0.2862710	-1.8005100
H	-1.8167250	-3.5196460	-1.2791350
H	-3.3688640	-0.9609480	1.2672140
H	2.4826450	2.8562080	-0.6408000
H	2.5890580	5.3004440	-0.4915280
H	-1.5741850	5.4260370	0.5084300
H	0.5378930	6.5993900	0.1185600
H	-3.8335970	0.8466340	-1.1409720
H	-5.4963620	0.8370300	0.9983210
H	-3.1574660	4.4226060	1.2030240
H	-5.1981860	3.1602080	1.7303050
H	2.1507700	-3.8549670	-0.6598350
H	0.1989140	-1.2062420	2.1115630
H	2.8549650	-5.3125690	1.2356060
H	0.8893860	-2.6538410	3.9962950
H	2.2216520	-4.7120190	3.5656670
H	-5.6921510	-1.4129070	-0.0783430

3^β-A'-ΔE₁-2

C	-1.0611350	0.5749080	-0.1567830
C	0.2600780	1.2284590	-0.1825400
C	-1.0250710	-0.8399610	-0.4136660
C	1.2950430	0.3659680	-0.4467460
P	0.6785850	-1.3464540	-0.7166710
C	2.7462380	0.6051180	-0.5837110
C	3.6609030	0.4073790	0.4256290
C	3.3868840	0.9939740	-1.8129940
S	5.2845840	0.7161280	-0.0930420
C	4.7449700	1.1022390	-1.6972880
C	-2.1940650	-1.5597500	-0.5429770
C	-2.3905990	-2.9388710	-0.7292910
C	-3.5221410	-0.7957050	-0.5346920
S	-4.0296930	-3.3569450	-0.5664850
C	-4.6005510	-1.8146030	-0.2878460

C	-2.2220650	1.2455770	0.1456820
C	-2.2108750	2.6684810	0.3921140
C	0.3031070	2.6735250	0.1131470
C	-0.9059210	3.3680750	0.4109210
C	1.5162370	3.3932110	0.1254330
C	1.5598040	4.7480040	0.4281630
C	-0.8309280	4.7394360	0.7247790
C	0.3763140	5.4261790	0.7372230
C	-3.5095170	0.4468220	0.3578900
C	-4.7450340	1.2960720	0.2064550
C	-3.4165070	3.3219060	0.5129730
C	-4.6771990	2.6367230	0.3408690
S	1.0983300	-2.1927270	-2.4555500
C	1.2527400	-2.3376340	0.7295410
C	2.1183920	-3.4212980	0.5399500
C	0.8428430	-1.9979800	2.0291700
C	2.5702930	-4.1589520	1.6384900
C	1.2946180	-2.7363480	3.1243370
C	2.1605470	-3.8183460	2.9299660
H	3.4620200	0.1041690	1.4450190
H	2.8410570	1.1701340	-2.7331420
H	5.4614800	1.3693240	-2.4631810
H	-1.6399200	-3.7088930	-0.8424030
H	-3.6521410	-0.4382220	-1.5863190
H	2.4398850	2.8808120	-0.1038940
H	2.5126250	5.2706240	0.4278340
H	-1.7340940	5.2845850	0.9752220
H	0.3944510	6.4837860	0.9875660
H	-3.4960480	0.0826160	1.4136430
H	-5.7027470	0.8006550	0.0651010
H	-3.4541340	4.3958440	0.6545370
H	-5.5830450	3.2372530	0.2956260
H	2.4268580	-3.6815470	-0.4689720
H	0.1678670	-1.1602890	2.1860490
H	3.2422110	-4.9992340	1.4825790
H	0.9695250	-2.4696310	4.1269550
H	2.5118820	-4.3935040	3.7831100
H	-5.6624830	-1.6306260	-0.1992100

4-a

C	1.3218200	0.0173900	0.2391530
C	0.7580630	1.2434740	0.0624550
P	-0.0000240	-1.2148430	0.5188180
C	-0.7580500	1.2435030	0.0624820
C	-1.3218410	0.0174300	0.2391760
C	1.4605680	2.5242460	-0.0931190
C	0.7294830	3.7623040	-0.2623910
C	-1.4605000	2.5243200	-0.0930210
C	-0.7293610	3.7623420	-0.2623290
C	-2.8237390	2.7403870	-0.0816200
S	-3.2246870	4.4046230	-0.2815210

C	-1.5572480	4.8512690	-0.3802390
C	2.8238200	2.7402270	-0.0818560
S	3.2248470	4.4044380	-0.2818050
C	1.5574250	4.8511790	-0.3803910
C	-2.7479620	-0.3824130	0.2463440
C	-3.3709220	-0.7220880	1.4644990
C	-3.4544950	-0.4689730	-0.9548320
C	-4.7059140	-1.1320620	1.4544360
C	-4.7977610	-0.8800990	-0.9468010
C	-5.4301210	-1.2090420	0.2520080
C	2.7479360	-0.3824730	0.2463380
C	3.3709070	-0.7220330	1.4645200
C	3.4544590	-0.4691370	-0.9548360
C	4.7058970	-1.1320130	1.4544830
C	4.7977250	-0.8802640	-0.9467780
C	5.4300930	-1.2091040	0.2520550
C	-0.0000540	-2.3581940	-0.9184890
C	-0.0000280	-3.7418540	-0.7139690
C	-0.0001030	-1.8464530	-2.2260510
C	-0.0000490	-4.6097100	-1.8101770
C	-0.0001240	-2.7151380	-3.3173610
C	-0.0000970	-4.0991120	-3.1099920
S	-0.0000110	-2.1179070	2.2835180
O	5.4051840	-0.9271250	-2.1708600
C	6.7606600	-1.3497310	-2.2420770
O	5.4075030	-1.4856110	2.5719540
C	4.7359040	-1.4706520	3.8285420
O	-5.4075100	-1.4857610	2.5718810
C	-4.7358970	-1.4709240	3.8284640
O	-5.4052290	-0.9268530	-2.1708830
C	-6.7607050	-1.3494550	-2.2421280
H	-3.6135710	2.0134560	0.0273900
H	-1.2818530	5.8893430	-0.5102870
H	3.6136180	2.0132460	0.0270870
H	1.2820790	5.8892670	-0.5104360
H	-2.7969600	-0.6726760	2.3803510
H	-2.9858850	-0.2218240	-1.9014680
H	-6.4624810	-1.5340640	0.2979970
H	2.7969520	-0.6725340	2.3803720
H	2.9858410	-0.2220720	-1.9014900
H	6.4624520	-1.5341230	0.2980640
H	0.0000080	-4.1294340	0.3010120
H	-0.0001260	-0.7717670	-2.3918690
H	-0.0000280	-5.6841490	-1.6452590
H	-0.0001620	-2.3134040	-4.3274260
H	-0.0001140	-4.7754580	-3.9611460
H	6.8786560	-2.3753330	-1.8686910
H	7.0260050	-1.3148990	-3.3001790
H	7.4189690	-0.6761320	-1.6777810
H	5.4730480	-1.8092530	4.5587010
H	4.4021350	-0.4578040	4.0879310

H	3.8761070	-2.1514000	3.8282450
H	-5.4730350	-1.8095930	4.5585980
H	-3.8761020	-2.1516740	3.8280920
H	-4.4021220	-0.4581030	4.0879470
H	-6.8786950	-2.3750890	-1.8688280
H	-7.4190130	-0.6759060	-1.6777710
H	-7.0260560	-1.3145330	-3.3002260

4-b

C	1.2785200	0.0372020	0.2742370
C	0.6770710	1.2457210	0.0955940
P	-0.0066540	-1.2350610	0.5507240
C	-0.8379550	1.1972720	0.0863130
C	-1.3644490	-0.0439540	0.2686060
C	1.3368590	2.5505940	-0.0487320
C	0.5658120	3.7623100	-0.2336820
C	-1.5820080	2.4510710	-0.0905240
C	-0.8919890	3.7118090	-0.2621160
C	-2.9522900	2.6179400	-0.1055440
S	-3.4079970	4.2647610	-0.3329320
C	-1.7556740	4.7690680	-0.4085980
C	2.6908650	2.8154510	-0.0076080
S	3.0366760	4.4927300	-0.1994350
C	1.3570060	4.8798640	-0.3345030
C	-2.7799400	-0.4807690	0.2877550
C	-3.4087260	-0.7425320	1.5133050
C	-3.4652030	-0.6710730	-0.9240380
C	-4.7423270	-1.1808550	1.5194850
C	-4.7972260	-1.1081820	-0.8964060
C	-5.4374580	-1.3572390	0.3206000
C	2.7154910	-0.3209000	0.2788040
C	3.3350750	-0.7068700	1.4849720
C	3.4375720	-0.3265230	-0.9165810
C	4.6808810	-1.0800520	1.4696250
C	4.7912410	-0.7014720	-0.9138800
C	5.4197470	-1.0751540	0.2737420
C	0.0278650	-2.3738820	-0.8911440
C	-0.0370000	-3.7570100	-0.6933330
C	0.1103440	-1.8598980	-2.1952630
C	-0.0210130	-4.6216990	-1.7920700
C	0.1279960	-2.7253280	-3.2893050
C	0.0615610	-4.1088260	-3.0883670
S	0.0045200	-2.1442660	2.3109040
O	5.4122240	-0.6691240	-2.1316810
C	6.7788140	-1.0540210	-2.2088090
O	5.3794950	-1.4727750	2.5753750
C	4.6923370	-1.5486230	3.8216720
O	-5.4457050	-1.4625480	2.6554690
C	-4.7862610	-1.3449470	3.9125840
O	-5.5563330	-1.3218220	-2.0140930
C	-4.9651960	-1.1137420	-3.2903240

H	-3.7179480	1.8653640	0.0038160
H	-1.5151300	5.8147470	-0.5468570
H	3.5033630	2.1169200	0.1189180
H	1.0477160	5.9077300	-0.4692200
H	-2.8484900	-0.6132260	2.4300780
H	-2.9528460	-0.4761440	-1.8581000
H	-6.4671420	-1.6984150	0.3332560
H	2.7508360	-0.7205500	2.3955480
H	2.9737540	-0.0421970	-1.8550870
H	6.4598590	-1.3750090	0.3152280
H	-0.0972610	-4.1471480	0.3189130
H	0.1650420	-0.7858460	-2.3561170
H	-0.0715140	-5.6955840	-1.6316710
H	0.1985450	-2.3217400	-4.2963380
H	0.0773370	-4.7828820	-3.9411980
H	6.9186280	-2.0939820	-1.8862120
H	7.0538790	-0.9589560	-3.2606950
H	7.4141540	-0.3938750	-1.6038110
H	5.4301120	-1.9074890	4.5413850
H	4.3261410	-0.5622060	4.1336410
H	3.8527080	-2.2521150	3.7704100
H	-5.5240790	-1.6443120	4.6590140
H	-3.9145870	-2.0081880	3.9691720
H	-4.4738120	-0.3100580	4.1026950
H	-4.6548340	-0.0687850	-3.4222990
H	-4.1027810	-1.7750990	-3.4436640
H	-5.7425180	-1.3549750	-4.0176350

4-c

C	1.3644480	-0.0439540	0.2686100
C	0.8379540	1.1972720	0.0863170
P	0.0066530	-1.2350620	0.5507260
C	-0.6770720	1.2457210	0.0955990
C	-1.2785220	0.0372020	0.2742380
C	1.5820070	2.4510710	-0.0905200
C	0.8919870	3.7118090	-0.2621130
C	-1.3368600	2.5505940	-0.0487250
C	-0.5658140	3.7623100	-0.2336770
C	-2.6908660	2.8154510	-0.0076000
S	-3.0366770	4.4927320	-0.1994180
C	-1.3570070	4.8798640	-0.3344980
C	2.9522890	2.6179390	-0.1055380
S	3.4079960	4.2647590	-0.3329350
C	1.7556730	4.7690680	-0.4085940
C	-2.7154920	-0.3209000	0.2788030
C	-3.3350770	-0.7068760	1.4849690
C	-3.4375720	-0.3265190	-0.9165830
C	-4.6808830	-1.0800590	1.4696180
C	-4.7912410	-0.7014690	-0.9138850
C	-5.4197480	-1.0751570	0.2737350
C	2.7799390	-0.4807680	0.2877560

C	3.4087270	-0.7425340	1.5133050
C	3.4652010	-0.6710670	-0.9240390
C	4.7423280	-1.1808570	1.5194810
C	4.7972240	-1.1081750	-0.8964090
C	5.4374580	-1.3572370	0.3205960
C	-0.0278640	-2.3738810	-0.8911420
C	0.0370140	-3.7570100	-0.6933320
C	-0.1103510	-1.8598980	-2.1952610
C	0.0210310	-4.6216980	-1.7920700
C	-0.1279980	-2.7253270	-3.2893030
C	-0.0615510	-4.1088240	-3.0883670
S	-0.0045210	-2.1442670	2.3109050
O	5.5563310	-1.3218110	-2.0140980
C	4.9651910	-1.1137290	-3.2903270
O	5.4457070	-1.4625540	2.6554640
C	4.7862650	-1.3449550	3.9125800
O	-5.3794980	-1.4727860	2.5753670
C	-4.6923390	-1.5486410	3.8216620
O	-5.4122220	-0.6691160	-2.1316870
C	-6.7788110	-1.0540140	-2.2088180
H	-3.5033650	2.1169200	0.1189260
H	-1.0477170	5.9077300	-0.4692160
H	3.7179460	1.8653640	0.0038240
H	1.5151290	5.8147470	-0.5468530
H	-2.7508400	-0.7205600	2.3955460
H	-2.9737530	-0.0421890	-1.8550870
H	-6.4598600	-1.3750120	0.3152190
H	2.8484910	-0.6132330	2.4300790
H	2.9528440	-0.4761350	-1.8580990
H	6.4671420	-1.6984120	0.3332490
H	0.0972800	-4.1471480	0.3189130
H	-0.1650570	-0.7858460	-2.3561140
H	0.0715410	-5.6955820	-1.6316720
H	-0.1985540	-2.3217390	-4.2963360
H	-0.0773240	-4.7828800	-3.9411980
H	4.6548280	-0.0687720	-3.4222990
H	5.7425110	-1.3549600	-4.0176400
H	4.1027760	-1.7750870	-3.4436660
H	5.5240830	-1.6443220	4.6590090
H	4.4738180	-0.3100660	4.1026940
H	3.9145900	-2.0081940	3.9691670
H	-5.4301150	-1.9075130	4.5413730
H	-3.8527100	-2.2521310	3.7703960
H	-4.3261450	-0.5622260	4.1336380
H	-6.9186250	-2.0939760	-1.8862250
H	-7.4141530	-0.3938710	-1.6038190
H	-7.0538740	-0.9589460	-3.2607050

4-d

C	1.3298580	0.0281820	0.3197920
C	0.7588750	1.2445750	0.0982180

P	0.0097880	-1.2080280	0.6052460
C	-0.7550930	1.2259730	0.0431320
C	-1.3142790	0.0089560	0.2777470
C	1.4466530	2.5359470	-0.0365780
C	0.7079810	3.7526220	-0.3031730
C	-1.4637920	2.4756720	-0.2606200
C	-0.7432390	3.7164610	-0.4499970
C	-2.8235550	2.6493950	-0.4208730
S	-3.2338180	4.2814480	-0.7953440
C	-1.5750230	4.7683360	-0.7443370
C	2.7969660	2.7851710	0.1018960
S	3.1788090	4.4540560	-0.0955460
C	1.5193660	4.8584000	-0.3655380
C	-2.7435650	-0.3773050	0.3410530
C	-3.4365370	-0.2773270	1.5459250
C	-3.3844910	-0.8789410	-0.8123410
C	-4.7882990	-0.6611390	1.6055940
C	-4.7254880	-1.2587670	-0.7346890
C	-5.4381290	-1.1477740	0.4718870
C	2.7579770	-0.3605450	0.3475350
C	3.3422910	-0.7974890	1.5539890
C	3.5066440	-0.3458120	-0.8317070
C	4.6795100	-1.2005960	1.5558280
C	4.8509880	-0.7512080	-0.8116680
C	5.4447250	-1.1757870	0.3768770
C	0.0388460	-2.3692720	-0.8218360
C	-0.1052040	-3.7438870	-0.6062640
C	0.1942940	-1.8830420	-2.1300140
C	-0.0960950	-4.6269660	-1.6904950
C	0.2043990	-2.7666350	-3.2098610
C	0.0582970	-4.1413310	-2.9909440
S	-0.0353670	-2.0918480	2.3738070
O	5.4994610	-0.6961360	-2.0145610
C	6.8586820	-1.1087210	-2.0739310
O	5.3440690	-1.6429610	2.6637870
C	4.6262500	-1.7420640	3.8914030
O	-5.3840500	-0.5199870	2.8258210
C	-6.7408170	-0.9183270	2.9726640
O	-5.4476780	-1.7554400	-1.7847240
C	-4.7947030	-1.9297700	-3.0364150
H	-3.6049460	1.9094850	-0.3397110
H	-1.3080750	5.7998570	-0.9318300
H	3.5874610	2.0799830	0.3074110
H	1.2346930	5.8871390	-0.5415760
H	-2.9484530	0.0844070	2.4440780
H	-2.8246550	-0.9622240	-1.7355180
H	-6.4765160	-1.4562120	0.4807080
H	2.7380710	-0.8252960	2.4510080
H	3.0701930	-0.0214910	-1.7703840
H	6.4768110	-1.5003360	0.4310850
H	-0.2195160	-4.1129670	0.4093680

H	0.3119900	-0.8164700	-2.3057980
H	-0.2067670	-5.6940880	-1.5153830
H	0.3327370	-2.3840310	-4.2194020
H	0.0701300	-4.8297950	-3.8323170
H	6.9688990	-2.1611210	-1.7814290
H	7.1594480	-0.9870550	-3.1160310
H	7.4944700	-0.4821780	-1.4346060
H	5.3388360	-2.1404510	4.6156820
H	4.2750290	-0.7577680	4.2262680
H	3.7722910	-2.4235820	3.7984850
H	-6.9925280	-0.7295950	4.0176680
H	-7.4025280	-0.3282450	2.3249040
H	-6.8682360	-1.9861860	2.7524050
H	-4.4408420	-0.9713500	-3.4386000
H	-3.9507510	-2.6259460	-2.9519270
H	-5.5482130	-2.3482820	-3.7060530

4-e

C	1.3142790	0.0089560	0.2777470
C	0.7550940	1.2259730	0.0431320
P	-0.0097880	-1.2080280	0.6052460
C	-0.7588750	1.2445760	0.0982180
C	-1.3298580	0.0281820	0.3197920
C	1.4637920	2.4756720	-0.2606190
C	0.7432400	3.7164620	-0.4499960
C	-1.4466530	2.5359470	-0.0365780
C	-0.7079800	3.7526230	-0.3031720
C	-2.7969660	2.7851710	0.1018960
S	-3.1788090	4.4540570	-0.0955450
C	-1.5193650	4.8584000	-0.3655360
C	2.8235550	2.6493950	-0.4208720
S	3.2338180	4.2814480	-0.7953430
C	1.5750240	4.7683370	-0.7443350
C	-2.7579770	-0.3605450	0.3475350
C	-3.3422910	-0.7974900	1.5539890
C	-3.5066430	-0.3458110	-0.8317070
C	-4.6795100	-1.2005960	1.5558270
C	-4.8509880	-0.7512070	-0.8116680
C	-5.4447250	-1.1757870	0.3768760
C	2.7435650	-0.3773050	0.3410520
C	3.4365370	-0.2773280	1.5459250
C	3.3844910	-0.8789400	-0.8123410
C	4.7882990	-0.6611400	1.6055940
C	4.7254880	-1.2587670	-0.7346900
C	5.4381290	-1.1477750	0.4718860
C	-0.0388460	-2.3692720	-0.8218360
C	0.1052030	-3.7438870	-0.6062630
C	-0.1942950	-1.8830430	-2.1300140
C	0.0960930	-4.6269670	-1.6904930
C	-0.2044000	-2.7666360	-3.2098600
C	-0.0582990	-4.1413320	-2.9909430

S	0.0353670	-2.0918480	2.3738070
O	5.4476780	-1.7554390	-1.7847260
C	4.7947040	-1.9297660	-3.0364170
O	5.3840500	-0.5199900	2.8258200
C	6.7408170	-0.9183300	2.9726640
O	-5.3440690	-1.6429610	2.6637860
C	-4.6262510	-1.7420650	3.8914020
O	-5.4994610	-0.6961350	-2.0145610
C	-6.8586810	-1.1087200	-2.0739320
H	-3.5874610	2.0799840	0.3074110
H	-1.2346920	5.8871400	-0.5415740
H	3.6049470	1.9094840	-0.3397110
H	1.3080760	5.7998580	-0.9318280
H	-2.7380720	-0.8252960	2.4510070
H	-3.0701930	-0.0214900	-1.7703850
H	-6.4768110	-1.5003360	0.4310840
H	2.9484520	0.0844050	2.4440790
H	2.8246550	-0.9622220	-1.7355190
H	6.4765160	-1.4562120	0.4807070
H	0.2195150	-4.1129670	0.4093690
H	-0.3119900	-0.8164710	-2.3057980
H	0.2067650	-5.6940890	-1.5153820
H	-0.3327370	-2.3840320	-4.2194020
H	-0.0701320	-4.8297970	-3.8323150
H	4.4408430	-0.9713460	-3.4386000
H	5.5482140	-2.3482770	-3.7060550
H	3.9507520	-2.6259430	-2.9519300
H	6.9925280	-0.7295990	4.0176680
H	6.8682350	-1.9861890	2.7524030
H	7.4025270	-0.3282480	2.3249040
H	-5.3388370	-2.1404520	4.6156810
H	-3.7722920	-2.4235830	3.7984840
H	-4.2750300	-0.7577690	4.2262670
H	-6.9688990	-2.1611200	-1.7814310
H	-7.4944700	-0.4821770	-1.4346070
H	-7.1594480	-0.9870540	-3.1160320

4-f

C	1.3223510	-0.0297190	0.2876530
C	0.7578690	1.1928960	0.0909450
P	-0.0000090	-1.2605100	0.5718600
C	-0.7578500	1.1929020	0.0909160
C	-1.3223470	-0.0297020	0.2876340
C	1.4603960	2.4706110	-0.0851840
C	0.7296030	3.7052240	-0.2794930
C	-1.4603620	2.4706110	-0.0853150
C	-0.7295530	3.7052210	-0.2795830
C	-2.8239120	2.6858700	-0.0758810
S	-3.2256360	4.3460300	-0.3072790
C	-1.5583550	4.7911060	-0.4180070
C	2.8239440	2.6858770	-0.0755820

S	3.2256860	4.3460550	-0.3068170
C	1.5584170	4.7911190	-0.4177790
C	-2.7507520	-0.4209830	0.3230730
C	-3.3665260	-0.6816680	1.5554890
C	-3.4633140	-0.5699480	-0.8788530
C	-4.7131060	-1.0777900	1.5792460
C	-4.8076820	-0.9657680	-0.8338400
C	-5.4341730	-1.2140010	0.3904540
C	2.7507490	-0.4210200	0.3230690
C	3.3664880	-0.6819410	1.5554520
C	3.4633470	-0.5697600	-0.8788650
C	4.7130650	-1.0780790	1.5791720
C	4.8077080	-0.9656020	-0.8338900
C	5.4341630	-1.2140740	0.3903760
C	-0.0000100	-2.3990690	-0.8724500
C	-0.0001040	-3.7833430	-0.6740080
C	0.0000730	-1.8828690	-2.1784750
C	-0.0001140	-4.6474940	-1.7735670
C	0.0000630	-2.7474050	-3.2734930
C	-0.0000300	-4.1326600	-3.0715800
S	-0.0000380	-2.1685150	2.3305970
O	5.5928250	-1.1376660	-1.9408120
C	5.0176920	-0.9308780	-3.2243070
O	5.4046970	-1.3550930	2.7231030
C	4.7196060	-1.2793530	3.9699620
O	-5.4047720	-1.3545850	2.7232090
C	-4.7197130	-1.2786270	3.9700710
O	-5.5927680	-1.1380330	-1.9407520
C	-5.0176030	-0.9314710	-3.2242690
H	-3.6130530	1.9612380	0.0538310
H	-1.2838660	5.8268100	-0.5676770
H	3.6130740	1.9612440	0.0541980
H	1.2839390	5.8268270	-0.5674410
H	-2.7869010	-0.5843960	2.4640630
H	-2.9621090	-0.3760110	-1.8191210
H	-6.4734940	-1.5237460	0.4162280
H	2.7868420	-0.5848310	2.4640300
H	2.9621730	-0.3756320	-1.8191100
H	6.4734810	-1.5238340	0.4161200
H	-0.0001660	-4.1748450	0.3395250
H	0.0001450	-0.8071870	-2.3392870
H	-0.0001850	-5.7223990	-1.6124070
H	0.0001290	-2.3423150	-4.2825890
H	-0.0000360	-4.8061030	-3.9250410
H	4.6747770	0.1049700	-3.3474970
H	5.8152890	-1.1355310	-3.9407890
H	4.1808390	-1.6185340	-3.4022870
H	5.4537370	-1.5665030	4.7247340
H	4.3701230	-0.2583830	4.1703570
H	3.8694270	-1.9714890	4.0003760
H	-5.4538660	-1.5656290	4.7248780

H	-3.8695450	-1.9707710	4.0006330
H	-4.3702190	-0.2576260	4.1702890
H	-4.6746860	0.1043560	-3.3476310
H	-4.1807450	-1.6191580	-3.4021080
H	-5.8151820	-1.1362500	-3.9407350

4-g

C	1.3742800	-0.0566030	0.3212190
C	0.8445060	1.1781480	0.1052140
P	0.0171100	-1.2495290	0.6082000
C	-0.6702650	1.2183240	0.0901950
C	-1.2688670	0.0175010	0.3137170
C	1.5819410	2.4358250	-0.0729980
C	0.8863470	3.6843430	-0.3043030
C	-1.3368410	2.5065960	-0.1394590
C	-0.5718380	3.7178880	-0.3483440
C	-2.6945200	2.7508240	-0.1855730
S	-3.0504050	4.4112120	-0.4826940
C	-1.3705180	4.8164600	-0.5491920
C	2.9494540	2.6189290	-0.0292970
S	3.3969400	4.2657850	-0.2719930
C	1.7443170	4.7483340	-0.4348760
C	-2.7091660	-0.3266880	0.3693420
C	-3.3509970	-0.4377080	1.6011500
C	-3.4126360	-0.5817330	-0.8285810
C	-4.7133120	-0.7864820	1.6473650
C	-4.7619440	-0.9311090	-0.7641770
C	-5.4231680	-1.0311490	0.4726030
C	2.7918180	-0.4829350	0.3762640
C	3.3854160	-0.7497280	1.6182260
C	3.5165450	-0.6555670	-0.8151830
C	4.7221220	-1.1761520	1.6624970
C	4.8507870	-1.0814870	-0.7497320
C	5.4554890	-1.3360090	0.4841760
C	-0.0123010	-2.3864910	-0.8394700
C	-0.0922460	-3.7684260	-0.6407990
C	0.0426100	-1.8736010	-2.1456070
C	-0.1169390	-4.6332720	-1.7396270
C	0.0181550	-2.7386690	-3.2401440
C	-0.0617670	-4.1216110	-3.0377740
S	-0.0178070	-2.1588540	2.3620410
O	5.6464770	-1.2784110	-1.8452410
C	5.0933610	-1.0656350	-3.1372070
O	5.3917440	-1.4611150	2.8174890
C	4.6909090	-1.3618640	4.0541690
O	-5.2565520	-0.8607800	2.8971710
C	-6.6215250	-1.2365190	3.0263260
O	-5.5426040	-1.1988540	-1.8554650
C	-4.9490060	-1.1420920	-3.1463780
H	-3.5035540	2.0475840	-0.0611380
H	-1.0677510	5.8402530	-0.7240850

H	3.7171100	1.8780130	0.1333680
H	1.4988510	5.7880900	-0.6054090
H	-2.8153660	-0.2685580	2.5284180
H	-2.8922310	-0.5020350	-1.7748840
H	-6.4709440	-1.3061300	0.4694310
H	2.7962480	-0.6332810	2.5183830
H	3.0328650	-0.4548840	-1.7631690
H	6.4872060	-1.6686740	0.5254810
H	-0.1332320	-4.1573240	0.3730020
H	0.1049380	-0.7998670	-2.3073770
H	-0.1778570	-5.7063740	-1.5776500
H	0.0623690	-2.3356930	-4.2491700
H	-0.0793340	-4.7955720	-3.8906880
H	4.7770360	-0.0226370	-3.2709430
H	5.8950700	-1.2936450	-3.8420010
H	4.2425840	-1.7340870	-3.3224090
H	5.4072110	-1.6620570	4.8208930
H	4.3631620	-0.3317030	4.2438960
H	3.8239800	-2.0331640	4.0760380
H	-6.8269560	-1.2390500	4.0980950
H	-7.2827390	-0.5149150	2.5286190
H	-6.7985390	-2.2396980	2.6171120
H	-4.5771210	-0.1336070	-3.3704280
H	-4.1288010	-1.8652190	-3.2398630
H	-5.7442220	-1.3996860	-3.8482610

4-h

C	1.2688480	0.0174560	0.3138780
C	0.6702220	1.2182960	0.0905070
P	-0.0171040	-1.2496750	0.6080450
C	-0.8445450	1.1780350	0.1052720
C	-1.3742950	-0.0567510	0.3211240
C	1.3367680	2.5066810	-0.1386020
C	0.5717290	3.7179270	-0.3476320
C	-1.5820340	2.4356610	-0.0730990
C	-0.8864740	3.6842350	-0.3042080
C	-2.9495760	2.6186380	-0.0298510
S	-3.3971310	4.2654460	-0.2727860
C	-1.7444960	4.7481410	-0.4351180
C	2.6944410	2.7510850	-0.1839100
S	3.0502830	4.4115770	-0.4805160
C	1.3703810	4.8166280	-0.5478710
C	-2.7918240	-0.4831180	0.3761560
C	-3.3855830	-0.7493150	1.6181640
C	-3.5163680	-0.6563740	-0.8153100
C	-4.7222900	-1.1757360	1.6624570
C	-4.8506120	-1.0822900	-0.7498380
C	-5.4554890	-1.3361850	0.4841140
C	2.7091510	-0.3267340	0.3694190
C	3.3506850	-0.4393900	1.6012280
C	3.4129150	-0.5801680	-0.8286810

C	4.7130040	-0.7881860	1.6472960
C	4.7622080	-0.9296080	-0.7644280
C	5.4231390	-1.0312830	0.4723800
C	0.0125330	-2.3863310	-0.8398690
C	0.0924160	-3.7683080	-0.6414680
C	-0.0421720	-1.8731750	-2.1459090
C	0.1172400	-4.6329330	-1.7404670
C	-0.0175940	-2.7380240	-3.2406170
C	0.0622590	-4.1210090	-3.0385170
S	0.0176080	-2.1593550	2.3616910
O	5.5431380	-1.1958710	-1.8558860
C	4.9499070	-1.1371990	-3.1468740
O	5.2559690	-0.8640620	2.8971260
C	6.6208300	-1.2402310	3.0261400
O	-5.3920550	-1.4601600	2.8174990
C	-4.6914640	-1.3600360	4.0542320
O	-5.6461290	-1.2798220	-1.8453610
C	-5.0929720	-1.0672980	-3.1373470
H	-3.7172200	1.8776630	0.1325940
H	-1.4990710	5.7879120	-0.6056250
H	3.5034970	2.0479260	-0.0591560
H	1.0675840	5.8404230	-0.7227010
H	-2.7965370	-0.6324460	2.5183480
H	-3.0325490	-0.4561650	-1.7633250
H	-6.4872100	-1.6688330	0.5254410
H	2.8148320	-0.2715060	2.5285950
H	2.8927180	-0.4992080	-1.7749930
H	6.4709280	-1.3062100	0.4690970
H	0.1332550	-4.1574090	0.3722610
H	-0.1044410	-0.7994070	-2.3074750
H	0.1781080	-5.7060690	-1.5787000
H	-0.0616550	-2.3348440	-4.2495680
H	0.0799320	-4.7947990	-3.8915630
H	4.5781170	-0.1283760	-3.3695660
H	5.7453060	-1.3938010	-3.8489130
H	4.1297060	-1.8601620	-3.2416480
H	6.8259710	-1.2442800	4.0979600
H	6.7977760	-2.2428760	2.6155840
H	7.2823280	-0.5180680	2.5296170
H	-5.4078830	-1.6597620	4.8210310
H	-3.8244960	-2.0312700	4.0767180
H	-4.3638090	-0.3297310	4.2433380
H	-4.7767280	-0.0243030	-3.2713050
H	-4.2421270	-1.7357140	-3.3223650
H	-5.8946220	-1.2955420	-3.8421320

4-i

C	1.2666310	0.0481190	0.2492720
C	0.6763170	1.2565200	0.0471650
P	-0.0258310	-1.2126710	0.5385830
C	-0.8388750	1.2276770	0.0715670

C	-1.3759060	-0.0076110	0.2665820
C	1.3518330	2.5421740	-0.1714040
C	0.5955400	3.7640590	-0.3464950
C	-1.5666570	2.4957170	-0.0724770
C	-0.8618800	3.7430330	-0.2817230
C	-2.9313420	2.6914190	-0.0073520
S	-3.3655380	4.3477600	-0.2039780
C	-1.7104390	4.8183880	-0.3746770
C	2.7106370	2.7741440	-0.2382520
S	3.0777470	4.4358620	-0.5132140
C	1.4011300	4.8584960	-0.5417830
C	-2.7939490	-0.4333110	0.2978390
C	-3.3849230	-0.7961300	1.5252390
C	-3.5246760	-0.5200800	-0.8889070
C	-4.7123090	-1.2296260	1.5395970
C	-4.8597980	-0.9554380	-0.8563830
C	-5.4605980	-1.3076790	0.3520680
C	2.7039860	-0.3103920	0.2891960
C	3.3546050	-0.4483050	1.5216560
C	3.3985480	-0.5558750	-0.9045440
C	4.7049630	-0.8146480	1.5534530
C	4.7464560	-0.9236550	-0.8593920
C	5.4155800	-1.0540310	0.3673720
C	-0.0110820	-2.3480050	-0.9073010
C	0.0738420	-3.7300180	-0.7095890
C	-0.0822600	-1.8340360	-2.2120030
C	0.0874810	-4.5936900	-1.8091020
C	-0.0682160	-2.6983530	-3.3068380
C	0.0166380	-4.0807230	-3.1060690
S	0.0146100	-2.1241500	2.2941760
O	5.3423010	-1.1372810	-2.0730620
C	6.7050670	-1.5354260	-2.1110610
O	5.2589280	-0.9161570	2.7988790
C	6.6164190	-1.3145350	2.9202950
O	-5.3828890	-1.6065960	2.6683720
C	-4.6836840	-1.5912930	3.9101460
O	-5.4927500	-1.0011390	-2.0678530
C	-6.8412450	-1.4484480	-2.1141840
H	-3.7045750	1.9538000	0.1419460
H	-1.4564470	5.8594480	-0.5231950
H	3.5145020	2.0602630	-0.1465360
H	1.1052010	5.8876820	-0.6952970
H	-2.7923820	-0.7457780	2.4290700
H	-3.0815570	-0.2540090	-1.8426480
H	-6.4859010	-1.6513850	0.4164440
H	2.8255060	-0.2866880	2.4538530
H	2.9085300	-0.4663530	-1.8680700
H	6.4582080	-1.3388830	0.3977810
H	0.1269310	-4.1194630	0.3033940
H	-0.1495180	-0.7607750	-2.3733900
H	0.1524200	-5.6669060	-1.6487890

H	-0.1247010	-2.2944120	-4.3144930
H	0.0263590	-4.7537870	-3.9597950
H	6.8575010	-2.4927200	-1.5950320
H	6.9494930	-1.6520690	-3.1684040
H	7.3588300	-0.7711860	-1.6696170
H	6.8233290	-1.3355670	3.9916810
H	6.7791560	-2.3155430	2.4989240
H	7.2904910	-0.5962000	2.4343080
H	-5.3981220	-1.9505760	4.6528770
H	-3.8116540	-2.2556790	3.8839670
H	-4.3629730	-0.5749370	4.1721430
H	-6.9320700	-2.4796840	-1.7487680
H	-7.4997570	-0.7930030	-1.5290810
H	-7.1301740	-1.4083230	-3.1659310

4-j

C	1.3759060	-0.0076140	0.2665740
C	0.8388760	1.2276740	0.0715560
P	0.0258310	-1.2126700	0.5385850
C	-0.6763170	1.2565210	0.0471660
C	-1.2666310	0.0481210	0.2492760
C	1.5666600	2.4957110	-0.0725040
C	0.8618850	3.7430280	-0.2817470
C	-1.3518310	2.5421770	-0.1713910
C	-0.5955360	3.7640600	-0.3464940
C	-2.7106350	2.7741530	-0.2382130
S	-3.0777440	4.4358730	-0.5131650
C	-1.4011250	4.8585010	-0.5417640
C	2.9313470	2.6914070	-0.0074050
S	3.3655470	4.3477450	-0.2040490
C	1.7104470	4.8183790	-0.3747230
C	-2.7039870	-0.3103900	0.2891990
C	-3.3545990	-0.4483360	1.5216590
C	-3.3985550	-0.5558420	-0.9045440
C	-4.7049570	-0.8146780	1.5534530
C	-4.7464620	-0.9236220	-0.8593940
C	-5.4155810	-1.0540290	0.3673690
C	2.7939480	-0.4333130	0.2978350
C	3.3849320	-0.7960850	1.5252450
C	3.5246660	-0.5201270	-0.8889130
C	4.7123180	-1.2295800	1.5396090
C	4.8597900	-0.9554820	-0.8563820
C	5.4605980	-1.3076770	0.3520780
C	0.0110720	-2.3480100	-0.9072940
C	-0.0738360	-3.7300240	-0.7095750
C	0.0822300	-1.8340460	-2.2119990
C	-0.0874810	-4.5937000	-1.8090850
C	0.0681810	-2.6983670	-3.3068300
C	-0.0166580	-4.0807370	-3.1060550
S	-0.0145990	-2.1241410	2.2941830
O	5.4927330	-1.0012270	-2.0678550

C	6.8412280	-1.4485370	-2.1141780
O	5.3829060	-1.6065070	2.6683930
C	4.6837080	-1.5911640	3.9101710
O	-5.2589160	-0.9162200	2.7988790
C	-6.6164070	-1.3146020	2.9202920
O	-5.3423140	-1.1372150	-2.0730680
C	-6.7050790	-1.5353600	-2.1110700
H	-3.5145020	2.0602760	-0.1464830
H	-1.1051950	5.8876850	-0.6952800
H	3.7045800	1.9537860	0.1418830
H	1.4564560	5.8594390	-0.5232450
H	-2.8254960	-0.2867440	2.4538580
H	-2.9085410	-0.4662950	-1.8680690
H	-6.4582090	-1.3388820	0.3977750
H	2.7923960	-0.7457000	2.4290770
H	3.0815400	-0.2540930	-1.8426610
H	6.4859020	-1.6513800	0.4164590
H	-0.1269100	-4.1194650	0.3034090
H	0.1494760	-0.7607850	-2.3733910
H	-0.1524080	-5.6669160	-1.6487670
H	0.1246500	-2.2944300	-4.3144880
H	-0.0263840	-4.7538050	-3.9597780
H	6.9320560	-2.4797590	-1.7487240
H	7.1301500	-1.4084510	-3.1659290
H	7.4997440	-0.7930690	-1.5291050
H	5.3981500	-1.9504210	4.6529100
H	4.3629980	-0.5747990	4.1721360
H	3.8116790	-2.2555510	3.8840190
H	-6.8233120	-1.3356620	3.9916780
H	-7.2904820	-0.5962550	2.4343260
H	-6.7791450	-2.3155990	2.4988960
H	-6.8575090	-2.4926680	-1.5950650
H	-7.3588410	-0.7711320	-1.6696030
H	-6.9495100	-1.6519770	-3.1684150

4-k

C	1.3217280	-0.0062120	0.3505580
C	0.7576170	1.2095580	0.1182050
P	-0.0000480	-1.2365350	0.6463980
C	-0.7575910	1.2095510	0.1179980
C	-1.3217500	-0.0061830	0.3503860
C	1.4601310	2.4805760	-0.1006140
C	0.7296830	3.7084110	-0.3351150
C	-1.4600680	2.4804750	-0.1014740
C	-0.7295700	3.7083330	-0.3356890
C	-2.8237280	2.6933280	-0.1088750
S	-3.2263160	4.3441370	-0.4001220
C	-1.5588010	4.7875650	-0.5166890
C	2.8237710	2.6935930	-0.1068320
S	3.2264080	4.3445120	-0.3973790
C	1.5589370	4.7877820	-0.5151770

C	-2.7520890	-0.3880870	0.4142010
C	-3.3782320	-0.5395560	1.6498620
C	-3.4618150	-0.6366750	-0.7815430
C	-4.7313070	-0.9219190	1.7023910
C	-4.8012300	-1.0204720	-0.7108150
C	-5.4472110	-1.1607810	0.5301030
C	2.7520460	-0.3881890	0.4142390
C	3.3779780	-0.5411530	1.6498270
C	3.4619890	-0.6353500	-0.7816800
C	4.7310470	-0.9235790	1.7021250
C	4.8013790	-1.0192480	-0.7111830
C	5.4471520	-1.1610440	0.5296790
C	0.0000210	-2.3740500	-0.8033260
C	-0.0002310	-3.7579490	-0.6024790
C	0.0003100	-1.8614130	-2.1106730
C	-0.0001970	-4.6248950	-1.7000000
C	0.0003440	-2.7284030	-3.2041270
C	0.0000900	-4.1133490	-2.9993920
S	-0.0002140	-2.1450830	2.3975590
O	5.5867620	-1.2835180	-1.8002820
C	5.0084290	-1.1835530	-3.0952830
O	5.2593290	-1.0364990	2.9554260
C	6.6137370	-1.4462590	3.0904830
O	-5.2598070	-1.0333470	2.9557350
C	-6.6142300	-1.4429760	3.0910380
O	-5.5864300	-1.2860230	-1.7997310
C	-5.0078440	-1.1877480	-3.0947500
H	-3.6121840	1.9722940	0.0428670
H	-1.2847700	5.8176350	-0.7018750
H	3.6121850	1.9726200	0.0454200
H	1.2849370	5.8178740	-0.7002840
H	-2.8376070	-0.3752050	2.5750730
H	-2.9535520	-0.5254020	-1.7312500
H	-6.4881220	-1.4607490	0.5318190
H	2.8372060	-0.3778970	2.5751440
H	2.9538840	-0.5229590	-1.7313420
H	6.4880620	-1.4610140	0.5312160
H	-0.0004510	-4.1462570	0.4124050
H	0.0005040	-0.7861190	-2.2742720
H	-0.0003900	-5.6994710	-1.5360750
H	0.0005730	-2.3253450	-4.2141380
H	0.0001250	-4.7887810	-3.8513790
H	4.6637080	-0.1614830	-3.3005190
H	5.8043490	-1.4452580	-3.7948910
H	4.1717010	-1.8839120	-3.2131380
H	6.8079620	-1.4747250	4.1639790
H	6.7720020	-2.4450510	2.6631480
H	7.2966570	-0.7305930	2.6138580
H	-6.8086370	-1.4702050	4.1645330
H	-7.2970810	-0.7278720	2.6134700
H	-6.7724040	-2.4422630	2.6648290

H	-4.6630380	-0.1659580	-3.3012340
H	-4.1711250	-1.8882940	-3.2115460
H	-5.8036440	-1.4503120	-3.7941730

4-I

C	1.2232010	0.0589730	0.2729630
C	0.5979000	1.2487920	0.0637470
P	-0.0329960	-1.2368320	0.5703060
C	-0.9154860	1.1760900	0.0894730
C	-1.4170150	-0.0711690	0.2993560
C	1.2341970	2.5535810	-0.1597760
C	0.4411300	3.7500310	-0.3497480
C	-1.6818410	2.4184910	-0.0732940
C	-1.0156050	3.6842750	-0.2961430
C	-3.0527550	2.5705570	-0.0199870
S	-3.5382130	4.2094130	-0.2439450
C	-1.8976470	4.7302170	-0.4112240
C	2.5855180	2.8279730	-0.2165370
S	2.9025620	4.4984180	-0.5000420
C	1.2137760	4.8677900	-0.5461150
C	-2.8242490	-0.5299620	0.3529050
C	-3.4130630	-0.8159300	1.5929020
C	-3.5429360	-0.7141930	-0.8404230
C	-4.7395030	-1.2735390	1.6330820
C	-4.8670420	-1.1710510	-0.7788820
C	-5.4674210	-1.4448750	0.4530590
C	2.6701800	-0.2583620	0.3145790
C	3.3185750	-0.3946980	1.5483560
C	3.3775790	-0.4677380	-0.8785960
C	4.6785270	-0.7239210	1.5823590
C	4.7349710	-0.7983640	-0.8314330
C	5.4013190	-0.9273370	0.3969370
C	0.0053230	-2.3701810	-0.8783960
C	0.0388410	-3.7543680	-0.6814680
C	-0.0036410	-1.8526710	-2.1837400
C	0.0617350	-4.6169150	-1.7819340
C	0.0208490	-2.7156500	-3.2796690
C	0.0529330	-4.1005710	-3.0793880
S	0.0290890	-2.1474560	2.3238670
O	5.3425160	-0.9783150	-2.0448030
C	6.7166390	-1.3359360	-2.0808140
O	5.2287200	-0.8270450	2.8290370
C	6.5950600	-1.1936520	2.9527290
O	-5.4040180	-1.5795680	2.7860110
C	-4.7067600	-1.4708790	4.0237100
O	-5.6561860	-1.3817700	-1.8765150
C	-5.1055890	-1.1508450	-3.1666390
H	-3.8029080	1.8114220	0.1401980
H	-1.6764460	5.7767040	-0.5735740
H	3.4105260	2.1403540	-0.1126360
H	0.8871750	5.8862990	-0.7083030

H	-2.8278230	-0.6898560	2.4943560
H	-3.0620060	-0.4987630	-1.7865900
H	-6.4913040	-1.8012770	0.4914280
H	2.7806730	-0.2612700	2.4799440
H	2.8905910	-0.3785060	-1.8436310
H	6.4511990	-1.1838930	0.4289880
H	0.0469500	-4.1465000	0.3318250
H	-0.0265230	-0.7772740	-2.3441360
H	0.0866260	-5.6917960	-1.6219370
H	0.0186470	-2.3090110	-4.2879960
H	0.0726580	-4.7726480	-3.9337290
H	6.8942740	-2.2957000	-1.5776160
H	6.9698860	-1.4301270	-3.1383050
H	7.3452570	-0.5592940	-1.6248000
H	6.7967240	-1.2239100	4.0248670
H	6.7843200	-2.1846480	2.5190150
H	7.2537560	-0.4525550	2.4800570
H	-5.4160820	-1.7929430	4.7880940
H	-3.8237390	-2.1210340	4.0423490
H	-4.4040750	-0.4342640	4.2200170
H	-4.8141570	-0.1000610	-3.2956870
H	-4.2385510	-1.7977760	-3.3524790
H	-5.9001850	-1.3953850	-3.8739510

4-m

C	1.4170150	-0.0711690	0.2993560
C	0.9154860	1.1760910	0.0894740
P	0.0329960	-1.2368320	0.5703070
C	-0.5979000	1.2487920	0.0637490
C	-1.2232010	0.0589730	0.2729640
C	1.6818410	2.4184910	-0.0732940
C	1.0156040	3.6842750	-0.2961420
C	-1.2341970	2.5535820	-0.1597730
C	-0.4411300	3.7500320	-0.3497460
C	-2.5855180	2.8279740	-0.2165320
S	-2.9025630	4.4984190	-0.5000360
C	-1.2137770	4.8677900	-0.5461110
C	3.0527550	2.5705570	-0.0199880
S	3.5382120	4.2094140	-0.2439460
C	1.8976470	4.7302180	-0.4112240
C	-2.6701800	-0.2583620	0.3145790
C	-3.3185750	-0.3947030	1.5483560
C	-3.3775790	-0.4677340	-0.8785960
C	-4.6785270	-0.7239260	1.5823580
C	-4.7349710	-0.7983600	-0.8314340
C	-5.4013190	-0.9273390	0.3969350
C	2.8242490	-0.5299620	0.3529040
C	3.4130640	-0.8159290	1.5929020
C	3.5429350	-0.7141930	-0.8404240
C	4.7395030	-1.2735390	1.6330810
C	4.8670410	-1.1710510	-0.7788830

C	5.4674210	-1.4448750	0.4530580
C	-0.0053230	-2.3701800	-0.8783960
C	-0.0388390	-3.7543680	-0.6814680
C	0.0036390	-1.8526700	-2.1837400
C	-0.0617330	-4.6169150	-1.7819340
C	-0.0208510	-2.7156500	-3.2796690
C	-0.0529330	-4.1005700	-3.0793880
S	-0.0290880	-2.1474560	2.3238680
O	5.6561850	-1.3817710	-1.8765160
C	5.1055880	-1.1508440	-3.1666400
O	5.4040190	-1.5795670	2.7860100
C	4.7067610	-1.4708810	4.0237090
O	-5.2287190	-0.8270560	2.8290360
C	-6.5950600	-1.1936590	2.9527260
O	-5.3425160	-0.9783070	-2.0448050
C	-6.7166390	-1.3359290	-2.0808170
H	-3.4105260	2.1403540	-0.1126300
H	-0.8871760	5.8862990	-0.7082990
H	3.8029080	1.8114220	0.1401960
H	1.6764460	5.7767040	-0.5735740
H	-2.7806730	-0.2612780	2.4799440
H	-2.8905910	-0.3784980	-1.8436310
H	-6.4511980	-1.1838950	0.4289850
H	2.8278240	-0.6898540	2.4943560
H	3.0620050	-0.4987640	-1.7865910
H	6.4913040	-1.8012770	0.4914260
H	-0.0469470	-4.1465000	0.3318250
H	0.0265200	-0.7772730	-2.3441350
H	-0.0866220	-5.6917960	-1.6219380
H	-0.0186500	-2.3090110	-4.2879960
H	-0.0726580	-4.7726470	-3.9337290
H	4.8141560	-0.1000600	-3.2956860
H	5.9001840	-1.3953830	-3.8739520
H	4.2385490	-1.7977740	-3.3524810
H	5.4160830	-1.7929460	4.7880930
H	4.4040750	-0.4342660	4.2200170
H	3.8237410	-2.1210360	4.0423470
H	-6.7967250	-1.2239190	4.0248640
H	-7.2537550	-0.4525590	2.4800560
H	-6.7843240	-2.1846530	2.5190100
H	-6.8942730	-2.2956960	-1.5776220
H	-7.3452570	-0.5592890	-1.6248000
H	-6.9698860	-1.4301170	-3.1383080

4-n

C	1.2781950	0.0395860	0.3063780
C	0.6864170	1.2443950	0.0855830
P	-0.0138550	-1.2200340	0.6093590
C	-0.8284480	1.2111960	0.0973390
C	-1.3639020	-0.0175240	0.3276650
C	1.3581370	2.5326030	-0.1307780

C	0.5979970	3.7457110	-0.3480930
C	-1.5613410	2.4667900	-0.1101620
C	-0.8607910	3.7127760	-0.3387040
C	-2.9295570	2.6478010	-0.1092740
S	-3.3718280	4.2910640	-0.3858300
C	-1.7155910	4.7739700	-0.5069720
C	2.7163050	2.7764780	-0.1499350
S	3.0788750	4.4382420	-0.4304210
C	1.4008520	4.8450420	-0.5265310
C	-2.7848340	-0.4323170	0.3940740
C	-3.4086370	-0.5921000	1.6299340
C	-3.4867970	-0.7038110	-0.8011550
C	-4.7524640	-1.0055030	1.6827380
C	-4.8169630	-1.1184030	-0.7300120
C	-5.4611920	-1.2669130	0.5109060
C	2.7160890	-0.3149760	0.3575980
C	3.3480640	-0.4880170	1.5953950
C	3.4308910	-0.5221900	-0.8317060
C	4.6991710	-0.8509580	1.6374140
C	4.7789040	-0.8874010	-0.7764730
C	5.4291850	-1.0527260	0.4561490
C	-0.0067270	-2.3573940	-0.8387900
C	-0.0583430	-3.7404590	-0.6378470
C	0.0425290	-1.8457650	-2.1454980
C	-0.0619580	-4.6073460	-1.7351820
C	0.0406920	-2.7129870	-3.2385500
C	-0.0122440	-4.0966870	-3.0340480
S	0.0150070	-2.1274390	2.3620070
O	5.3945320	-1.0628980	-1.9867120
C	6.7598400	-1.4531550	-2.0145500
O	5.2336710	-0.9878270	2.8876360
C	6.5890600	-1.3901010	3.0191920
O	-5.2800720	-1.1229250	2.9362340
C	-6.6249140	-1.5625430	3.0716300
O	-5.5940340	-1.4082870	-1.8184880
C	-5.0149630	-1.3053360	-3.1131570
H	-3.7002360	1.9075530	0.0412440
H	-1.4664430	5.8113620	-0.6863420
H	3.5222450	2.0712900	-0.0178600
H	1.1018120	5.8700300	-0.7007940
H	-2.8731840	-0.4100040	2.5548490
H	-2.9795120	-0.5862330	-1.7506350
H	-6.4949450	-1.5907120	0.5129930
H	2.8041350	-0.3564530	2.5237230
H	2.9567130	-0.4047270	-1.8000940
H	6.4721110	-1.3354760	0.4946700
H	-0.0936480	-4.1280170	0.3767060
H	0.0859550	-0.7715570	-2.3095010
H	-0.1019240	-5.6812810	-1.5716040
H	0.0852430	-2.3106980	-4.2476940
H	-0.0116060	-4.7722520	-3.8859210

H	6.9092200	-2.4245600	-1.5246590
H	7.0217650	-1.5372150	-3.0708090
H	7.4023730	-0.6991560	-1.5402410
H	6.7785480	-1.4426040	4.0927050
H	6.7585490	-2.3784250	2.5713500
H	7.2709810	-0.6581520	2.5654830
H	-6.8202950	-1.5892070	4.1449910
H	-7.3232780	-0.8654690	2.5898050
H	-6.7598980	-2.5671540	2.6499070
H	-4.6931560	-0.2773340	-3.3256330
H	-4.1621910	-1.9872230	-3.2235950
H	-5.8031310	-1.5905980	-3.8123400

4-o

C	1.3638910	-0.0174680	0.3278590
C	0.8284140	1.2112710	0.0976710
P	0.0138630	-1.2200370	0.6094200
C	-0.6864540	1.2444370	0.0858900
C	-1.2782140	0.0395870	0.3065320
C	1.5612840	2.4669070	-0.1096850
C	0.8607130	3.7128820	-0.3382190
C	-1.3581920	2.5326580	-0.1303550
C	-0.5980750	3.7457840	-0.3476420
C	-2.7163650	2.7765270	-0.1494520
S	-3.0789620	4.4382970	-0.4298380
C	-1.4009460	4.8451230	-0.5259750
C	2.9294940	2.6479750	-0.1086490
S	3.3717280	4.2912710	-0.3850630
C	1.7154860	4.7741200	-0.5063530
C	-2.7160950	-0.3150480	0.3575910
C	-3.3481030	-0.4885860	1.5952990
C	-3.4308580	-0.5218390	-0.8318140
C	-4.6991990	-0.8515960	1.6371360
C	-4.7788570	-0.8871230	-0.7767660
C	-5.4291680	-1.0529370	0.4557760
C	2.7848250	-0.4322870	0.3940720
C	3.4086970	-0.5925370	1.6298230
C	3.4867200	-0.7033560	-0.8013100
C	4.7525320	-1.0059730	1.6823950
C	4.8168790	-1.1179840	-0.7303990
C	5.4611870	-1.2669360	0.5104310
C	0.0068010	-2.3572670	-0.8388200
C	0.0586420	-3.7403400	-0.6379910
C	-0.0425590	-1.8455430	-2.1454870
C	0.0623420	-4.6071420	-1.7353940
C	-0.0406230	-2.7126800	-3.2386070
C	0.0125090	-4.0963890	-3.0342180
S	-0.0149430	-2.1276210	2.3619830
O	5.5938860	-1.4075150	-1.8190180
C	5.0148600	-1.3036830	-3.1136350
O	5.2802230	-1.1238040	2.9358170

C	6.6248150	-1.5642590	3.0709970
O	-5.2337300	-0.9889670	2.8872910
C	-6.5891400	-1.3912320	3.0186390
O	-5.3944450	-1.0621750	-1.9870920
C	-6.7596800	-1.4526670	-2.0151130
H	-3.5222840	2.0713170	-0.0173800
H	-1.1019240	5.8701230	-0.7001900
H	3.7001870	1.9077520	0.0419110
H	1.4663140	5.8115130	-0.6856740
H	-2.8042220	-0.3573500	2.5237010
H	-2.9566600	-0.4039920	-1.8001450
H	-6.4720870	-1.3357360	0.4941640
H	2.8733040	-0.4107910	2.5548410
H	2.9793630	-0.5854670	-1.7507100
H	6.4949540	-1.5906920	0.5123250
H	0.0940270	-4.1279760	0.3765290
H	-0.0861200	-0.7713300	-2.3094080
H	0.1024750	-5.6810830	-1.5718980
H	-0.0852570	-2.3103170	-4.2477180
H	0.0119430	-4.7718840	-3.8861450
H	4.6931590	-0.2755150	-3.3254640
H	5.8030160	-1.5885940	-3.8129770
H	4.1620200	-1.9854140	-3.2245260
H	6.8201540	-1.5916230	4.1443480
H	6.7592320	-2.5687030	2.6487000
H	7.3235860	-0.8673050	2.5895820
H	-6.7786710	-1.4441270	4.0921260
H	-7.2710090	-0.6590870	2.5651670
H	-6.7586460	-2.3793830	2.5704190
H	-6.9088960	-2.4242720	-1.5255640
H	-7.4023650	-0.6989520	-1.5405560
H	-7.0215530	-1.5364000	-3.0714110

4-p

C	1.3210510	0.0284430	0.2824350
C	0.7577150	1.2474620	0.0668820
P	0.0000010	-1.2041740	0.5709740
C	-0.7577190	1.2474610	0.0668880
C	-1.3210520	0.0284400	0.2824390
C	1.4602250	2.5217550	-0.1331570
C	0.7295370	3.7542870	-0.3404280
C	-1.4602310	2.5217550	-0.1331340
C	-0.7295470	3.7542870	-0.3404130
C	-2.8237260	2.7343620	-0.1426440
S	-3.2259590	4.3904800	-0.4022900
C	-1.5582480	4.8369280	-0.5019740
C	2.8237190	2.7343590	-0.1427030
S	3.2259490	4.3904780	-0.4023540
C	1.5582360	4.8369250	-0.5020170
C	-2.7503640	-0.3587870	0.3342410
C	-3.3781600	-0.5509800	1.5714220

C	-3.4601440	-0.5772900	-0.8560410
C	-4.7208070	-0.9439500	1.6117070
C	-4.7997390	-0.9723200	-0.8023540
C	-5.4462740	-1.1567190	0.4295920
C	2.7503640	-0.3587810	0.3342390
C	3.3781680	-0.5509320	1.5714230
C	3.4601360	-0.5773230	-0.8560400
C	4.7208150	-0.9439000	1.6117140
C	4.7997330	-0.9723500	-0.8023470
C	5.4462750	-1.1567070	0.4296010
C	0.0000020	-2.3423140	-0.8749020
C	0.0000280	-3.7260820	-0.6719540
C	-0.0000200	-1.8303440	-2.1823260
C	0.0000310	-4.5935160	-1.7686800
C	-0.0000170	-2.6982710	-3.2745180
C	0.0000090	-4.0824990	-3.0683440
S	0.0000070	-2.1097680	2.3260640
O	5.4113850	-1.1566690	-2.0132870
C	6.7675670	-1.5769830	-2.0429230
O	5.2523100	-1.0981220	2.8615040
C	6.5984670	-1.5305580	2.9909150
O	-5.2522940	-1.0982150	2.8614960
C	-6.5984500	-1.5306560	2.9909010
O	-5.4113980	-1.1566000	-2.0132960
C	-6.7675810	-1.5769100	-2.0429380
H	-3.6125250	2.0094100	-0.0142550
H	-1.2836790	5.8703370	-0.6665090
H	3.6125200	2.0094060	-0.0143300
H	1.2836640	5.8703330	-0.6665560
H	-2.8373020	-0.4107660	2.5002930
H	-2.9879270	-0.4461280	-1.8236880
H	-6.4828300	-1.4621920	0.4669510
H	2.8373150	-0.4106880	2.5002920
H	2.9879140	-0.4461930	-1.8236880
H	6.4828310	-1.4621780	0.4669640
H	0.0000440	-4.1134690	0.3432350
H	-0.0000400	-0.7555610	-2.3479100
H	0.0000510	-5.6680930	-1.6041330
H	-0.0000340	-2.2957080	-4.2843530
H	0.0000110	-4.7583540	-3.9199640
H	6.8955230	-2.5533050	-1.5567120
H	7.0273660	-1.6628890	-3.0995730
H	7.4268800	-0.8392560	-1.5659800
H	6.7868040	-1.5925970	4.0641520
H	6.7464560	-2.5201050	2.5381150
H	7.2964150	-0.8115400	2.5408520
H	-6.7867810	-1.5927310	4.0641370
H	-7.2964020	-0.8116240	2.5408660
H	-6.7464410	-2.5201880	2.5380690
H	-6.8955360	-2.5532490	-1.5567590
H	-7.4268900	-0.8391990	-1.5659670

H	-7.0273870	-1.6627820	-3.0995890
4-ΔE₁-1			
C	-1.3634900	0.0963920	-0.2901240
C	-0.6223370	1.2385590	-0.1403150
P	-0.2610040	-1.3791950	-0.4300220
C	0.8188630	0.9962860	-0.0624320
C	1.2423680	-0.3741770	-0.2224640
C	-1.0344600	2.6500030	-0.0515140
C	-0.0438710	3.7112020	0.1166740
C	1.7137530	1.9850840	0.1698280
C	1.3794630	3.3802030	0.2007080
C	3.1610800	1.6632100	0.4115590
S	4.0284970	3.2953450	0.1271750
C	2.4937080	4.1672300	0.1904560
C	-2.3104020	3.1613330	-0.1423660
S	-2.3387330	4.8818350	-0.0207370
C	-0.6194600	4.9574000	0.1517930
C	2.5692910	-0.6998010	-0.3627870
C	3.0403460	-2.0332460	-0.5856930
C	3.6013400	0.4557090	-0.4316980
C	4.3797960	-2.3138550	-0.5459990
C	5.0141300	-0.0093460	-0.1465340
C	5.3805310	-1.3059570	-0.2537150
C	-2.8355820	-0.0592860	-0.3175450
C	-3.4724350	-0.4983270	-1.4970200
C	-3.5867200	0.1866230	0.8347100
C	-4.8577500	-0.6718140	-1.5005700
C	-4.9800410	0.0113880	0.8126590
C	-5.6226950	-0.4140910	-0.3498160
C	-0.5094730	-2.3608940	1.1108880
C	-1.0257580	-3.6603250	1.0473610
C	-0.2070910	-1.7966110	2.3605740
C	-1.2381970	-4.3890530	2.2215880
C	-0.4176460	-2.5267580	3.5311420
C	-0.9350730	-3.8248380	3.4630060
S	-0.4196830	-2.4806140	-2.0754160
O	-5.6257320	0.2823370	1.9884040
C	-7.0342180	0.1023570	2.0468710
O	-5.5738840	-1.0941850	-2.5852650
C	-4.8671640	-1.4123470	-3.7810810
O	4.9229170	-3.5416150	-0.7275680
C	4.0514010	-4.6370610	-1.0157700
O	5.8444030	1.0212250	0.1297640
C	7.2303590	0.7503520	0.3369560
H	3.3115810	1.4285960	1.4783950
H	2.5230020	5.2510970	0.1604810
H	-3.2347370	2.6175240	-0.2696490
H	-0.1286200	5.9144020	0.2712560
H	2.3062740	-2.8123040	-0.7488550
H	3.5967120	0.7809440	-1.4926200

H	6.4014520	-1.6444150	-0.1254190
H	-2.8719280	-0.7041260	-2.3729400
H	-3.1119640	0.5071060	1.7561020
H	-6.6942030	-0.5638190	-0.4042940
H	-1.2520080	-4.0933450	0.0768800
H	0.1943750	-0.7881780	2.4205880
H	-1.6404630	-5.3974650	2.1637430
H	-0.1791690	-2.0831470	4.4946090
H	-1.1007060	-4.3926800	4.3752920
H	-7.3118980	-0.9406210	1.8454380
H	-7.3242590	0.3656860	3.0656740
H	-7.5515290	0.7621250	1.3377790
H	-5.6261770	-1.7500420	-4.4890230
H	-4.3552430	-0.5300020	-4.1859750
H	-4.1368690	-2.2125010	-3.6108290
H	4.7033600	-5.5006420	-1.1535060
H	3.3643570	-4.8184930	-0.1810310
H	3.4785650	-4.4489410	-1.9308430
H	7.3694710	0.0762090	1.1906380
H	7.6757500	0.3084210	-0.5623240
H	7.6916170	1.7161200	0.5457450

4- ΔE_1 -2

C	-1.3703960	0.1137440	-0.3269280
C	-0.6322640	1.2597690	-0.1867770
P	-0.2632620	-1.3450780	-0.5771220
C	0.8126070	1.0322780	-0.2177800
C	1.2345750	-0.3416390	-0.3384670
C	-1.0501930	2.6672110	-0.0645990
C	-0.0599080	3.7334420	0.0733150
C	1.7138740	2.0402600	-0.1583310
C	1.3680540	3.4116450	0.0842320
C	3.1803670	1.7703540	-0.3423130
S	3.9982620	3.2841200	0.3922650
C	2.4676830	4.1662180	0.3715760
C	-2.3329030	3.1694220	-0.0751490
S	-2.3673150	4.8871230	0.0819660
C	-0.6418850	4.9736390	0.1658950
C	2.5529570	-0.7003050	-0.2080110
C	3.0237140	-2.0457070	-0.3407700
C	3.5619410	0.3947870	0.2294320
C	4.3655080	-2.3166870	-0.3591960
C	5.0008770	0.0005440	-0.0282210
C	5.3728750	-1.2798700	-0.2497500
C	-2.8410390	-0.0520940	-0.2946110
C	-3.5274820	-0.4700470	-1.4538780
C	-3.5412540	0.1629510	0.8953760
C	-4.9105360	-0.6531540	-1.3989760
C	-4.9326620	-0.0240280	0.9326730
C	-5.6243690	-0.4278650	-0.2091180
C	-0.4630000	-2.4078370	0.9156930

C	-0.9103040	-3.7281850	0.7913650
C	-0.1869600	-1.8877480	2.1904650
C	-1.0800460	-4.5219420	1.9299620
C	-0.3547700	-2.6823390	3.3253970
C	-0.8026190	-4.0016480	3.1963050
S	-0.4506710	-2.3598480	-2.2736050
O	-5.5258500	0.2136570	2.1427800
C	-6.9276710	0.0136670	2.2632650
O	-5.6725820	-1.0545480	-2.4599180
C	-5.0202290	-1.3335060	-3.6957980
O	4.9095190	-3.5461960	-0.5264980
C	4.0349680	-4.6633160	-0.6960940
O	5.8413230	1.0541830	0.0784040
C	7.2435860	0.8324960	-0.0680520
H	3.4231610	1.7935130	-1.4175750
H	2.4835820	5.2190280	0.6324120
H	-3.2589350	2.6199920	-0.1587140
H	-0.1515750	5.9336220	0.2608530
H	2.2938360	-2.8244370	-0.5241580
H	3.4601970	0.4653060	1.3319770
H	6.4064080	-1.5813410	-0.3686020
H	-2.9657650	-0.6518060	-2.3603760
H	-3.0276410	0.4669430	1.8014000
H	-6.6962610	-0.5844200	-0.2187010
H	-1.1192580	-4.1245490	-0.1985830
H	0.1593580	-0.8626980	2.2972370
H	-1.4304950	-5.5457980	1.8249930
H	-0.1381560	-2.2723990	4.3087130
H	-0.9354060	-4.6196600	4.0809420
H	-7.2020480	-1.0272920	2.0474300
H	-7.1717260	0.2464440	3.3013940
H	-7.4864690	0.6848180	1.5976570
H	-5.8096370	-1.6545800	-4.3777510
H	-4.5312760	-0.4367960	-4.0974280
H	-4.2794880	-2.1342800	-3.5833250
H	4.6869630	-5.5315170	-0.8006250
H	3.3868480	-4.7863570	0.1795250
H	3.4217980	-4.5459420	-1.5968490
H	7.6095960	0.1502270	0.7085320
H	7.4686340	0.4226180	-1.0598870
H	7.7104380	1.8113840	0.0453900

5-a

C	0.9550300	-0.8777390	-0.5280270
C	1.0505970	0.4714390	-0.2362790
P	-0.7956010	-1.2943230	-0.7780140
C	-0.2235900	1.2233770	-0.2124920
C	-1.3274970	0.4362710	-0.4158990
C	2.3013880	1.0795330	0.0633780
C	2.3605510	2.4681200	0.3902450
C	-0.1340550	2.6823510	-0.0196910

C	1.1216610	3.2791630	0.2992140
C	3.4866350	0.2730650	0.0623180
C	4.7197920	0.8746840	0.4146990
C	3.5961030	3.0023680	0.7463110
C	4.7618210	2.2106720	0.7583770
C	-1.2555600	3.5166690	-0.1993180
C	-1.1787350	4.8930760	-0.0254350
C	1.1688070	4.6755100	0.4755260
C	0.0415850	5.4757020	0.3284220
C	3.3513830	-1.1029260	-0.2868530
C	2.1083270	-1.6949800	-0.5875700
C	2.2265710	-3.0928210	-0.9079180
C	3.5128900	-3.5325020	-0.8465750
S	4.6444980	-2.2790860	-0.3973390
C	-2.7639550	0.7320520	-0.3128780
C	-3.6817230	0.4801770	-1.3108710
C	-3.4044540	1.2296160	0.8801060
S	-5.2988510	0.8565080	-0.8241350
C	-4.7590470	1.3495630	0.7518400
C	-1.3104690	-2.3102690	0.6666170
C	-2.1955280	-3.3782340	0.4820180
C	-0.8373440	-2.0121570	1.9547690
C	-2.6053930	-4.1440770	1.5776820
C	-1.2475080	-2.7796320	3.0452920
C	-2.1328480	-3.8470660	2.8578220
H	5.6290310	0.2796660	0.4226990
H	3.6904380	4.0460970	1.0231310
H	5.7072440	2.6666900	1.0400680
H	-2.1999010	3.0781390	-0.4927950
H	-2.0628190	5.5071950	-0.1738580
H	2.1099770	5.1578720	0.7132230
H	0.1203460	6.5504520	0.4699030
H	1.3861780	-3.7185000	-1.1863520
H	3.8827280	-4.5301160	-1.0465660
H	-3.4810130	0.0893210	-2.2992770
H	-2.8617920	1.4755740	1.7865950
H	-5.4725300	1.6867070	1.4925920
H	-2.5521700	-3.6063680	-0.5186900
H	-0.1460990	-1.1869470	2.1067980
H	-3.2924960	-4.9728270	1.4272510
H	-0.8737670	-2.5475180	4.0393010
H	-2.4502970	-4.4451480	3.7083390
S	-1.3101250	-2.0525140	-2.5304720

5-b

C	0.9934190	-0.8596020	-0.5242920
C	1.0381350	0.4933110	-0.2374640
P	-0.7352900	-1.3342490	-0.8196660
C	-0.2615230	1.2031550	-0.2446360
C	-1.3317350	0.3789970	-0.4731030
C	2.2621840	1.1432080	0.0843840

C	2.2700540	2.5349060	0.4024150
C	-0.2240630	2.6659670	-0.0478780
C	1.0067030	3.3039390	0.2867030
C	3.4728200	0.3757760	0.1129260
C	4.6788810	1.0193890	0.4842110
C	3.4806930	3.1114970	0.7774630
C	4.6711170	2.3584850	0.8177670
C	-1.3710700	3.4629130	-0.2358940
C	-1.3407230	4.8413450	-0.0658250
C	1.0066780	4.7019330	0.4594240
C	-0.1433950	5.4649690	0.2971070
C	3.3897160	-1.0062110	-0.2284960
C	2.1734570	-1.6397030	-0.5524720
C	2.3434610	-3.0348180	-0.8613150
C	3.6415040	-3.4325190	-0.7687690
S	4.7221040	-2.1406580	-0.3028980
C	-2.7826070	0.6255150	-0.4323010
C	-3.4732130	0.9495580	0.7159400
C	-3.6668660	0.4765550	-1.5594990
S	-5.1731690	1.1032550	0.4362560
C	-4.9760590	0.7154900	-1.2448890
C	-1.2568190	-2.3655810	0.6114360
C	-2.1069900	-3.4573880	0.4037680
C	-0.8261500	-2.0554460	1.9115500
C	-2.5244190	-4.2348880	1.4882400
C	-1.2439210	-2.8344430	2.9911050
C	-2.0945320	-3.9255120	2.7804980
H	5.6065140	0.4541860	0.5139450
H	3.5361710	4.1595000	1.0483810
H	5.5956420	2.8472090	1.1136100
H	-2.3000780	2.9918050	-0.5263560
H	-2.2437060	5.4253780	-0.2217590
H	1.9288750	5.2147040	0.7072810
H	-0.1010400	6.5420790	0.4362010
H	1.5301400	-3.6888620	-1.1544550
H	4.0474990	-4.4188850	-0.9539170
H	-3.0660710	1.1066240	1.7061460
H	-3.3201960	0.2023760	-2.5490190
H	-5.8371840	0.6802350	-1.8994050
H	-2.4309640	-3.6939770	-0.6060780
H	-0.1619170	-1.2118430	2.0818740
H	-3.1843910	-5.0820360	1.3198990
H	-0.9029060	-2.5929030	3.9946060
H	-2.4181070	-4.5323760	3.6224310
S	-1.1787690	-2.1047380	-2.5850460
5-c			
C	1.0333090	-0.7806610	-0.5082420
C	1.0412810	0.5634770	-0.2319490
P	-0.6816580	-1.3165850	-0.7593750
C	-0.2806200	1.2347340	-0.2241110

C	-1.3316360	0.3768960	-0.4192720
C	2.2570400	1.2697150	0.0847930
C	2.2030290	2.6546120	0.4019610
C	-0.2911210	2.6991070	-0.0574060
C	0.9155080	3.3818750	0.2739460
C	3.4909150	0.5572910	0.1142340
C	4.6591990	1.2429440	0.4905230
C	3.3904860	3.2864620	0.7869290
C	4.6023220	2.5868510	0.8319350
C	-1.4604990	3.4537220	-0.2778430
C	-1.4782380	4.8352950	-0.1297830
C	0.8674730	4.7812970	0.4224860
C	-0.3066720	5.5029590	0.2371840
C	3.4925300	-0.8569760	-0.2381430
C	2.2470750	-1.5337930	-0.5544540
C	2.4313250	-2.8700060	-0.8640370
S	4.0924810	-3.3052560	-0.7785640
C	4.5723610	-1.7142310	-0.3224040
C	-2.7835070	0.5801890	-0.3178330
C	-3.6870810	0.2378660	-1.3019420
C	-3.4505740	1.0703050	0.8637890
S	-5.3235310	0.5204480	-0.8161960
C	-4.8105680	1.0956180	0.7408770
C	-1.1364900	-2.3470190	0.6945980
C	-1.9548960	-3.4681570	0.5179250
C	-0.6891240	-2.0067180	1.9814200
C	-2.3247730	-4.2446500	1.6203170
C	-1.0591290	-2.7850200	3.0786430
C	-1.8785220	-3.9051560	2.8993100
H	5.6090760	0.7177450	0.5261930
H	3.3965620	4.3348190	1.0617730
H	5.5072480	3.1068180	1.1352060
H	-2.3666660	2.9483200	-0.5839350
H	-2.3969820	5.3870240	-0.3094510
H	1.7696330	5.3301410	0.6665530
H	-0.3008160	6.5831050	0.3579080
H	1.6843740	-3.5945190	-1.1586950
H	-3.4654160	-0.1670570	-2.2801970
H	-2.9214500	1.3787010	1.7590800
H	-5.5415800	1.4063710	1.4760670
H	-2.2918470	-3.7283170	-0.4818270
H	-0.0495200	-1.1398950	2.1272850
H	-2.9607370	-5.1143140	1.4761170
H	-0.7056260	-2.5197710	4.0717750
H	-2.1649660	-4.5111100	3.7552490
S	-1.1363050	-2.1251750	-2.5064200
H	5.6188440	-1.5025280	-0.1503080

5-d

C	1.0793420	-0.7438160	-0.4977870
C	1.0180630	0.5995500	-0.2245830

P	-0.6009670	-1.3600850	-0.7939900
C	-0.3362070	1.2070720	-0.2427690
C	-1.3372430	0.3002790	-0.4680760
C	2.1944750	1.3639840	0.1049060
C	2.0715970	2.7469290	0.4103400
C	-0.4209380	2.6694630	-0.0614920
C	0.7499370	3.4090730	0.2751110
C	3.4610130	0.7119880	0.1523420
C	4.5920440	1.4562000	0.5308330
C	3.2246080	3.4387430	0.7969240
C	4.4685120	2.7992060	0.8572560
C	-1.6285150	3.3660770	-0.2667190
C	-1.7140570	4.7442200	-0.1126560
C	0.6328710	4.8041450	0.4303750
C	-0.5751210	5.4680800	0.2504780
C	3.5345440	-0.7035130	-0.1860820
C	2.3276130	-1.4397370	-0.5168930
C	2.5784840	-2.7684730	-0.8115240
S	4.2560070	-3.1257170	-0.6937670
C	4.6541920	-1.5104660	-0.2443130
C	-2.8034630	0.4328930	-0.4437400
C	-3.5308190	0.6787600	0.7009210
C	-3.6595160	0.2436730	-1.5866550
S	-5.2338790	0.7121970	0.3999430
C	-4.9869100	0.3771450	-1.2858180
C	-1.0451020	-2.4163900	0.6445690
C	-1.8196120	-3.5644820	0.4443780
C	-0.6353450	-2.0699800	1.9422470
C	-2.1843020	-4.3609410	1.5341050
C	-1.0003920	-2.8680490	3.0270590
C	-1.7766400	-4.0145630	2.8241860
H	5.5656660	0.9774930	0.5781750
H	3.1786200	4.4887430	1.0611420
H	5.3450930	3.3654100	1.1609430
H	-2.5128750	2.8167030	-0.5588990
H	-2.6610390	5.2496030	-0.2817700
H	1.5064640	5.3957190	0.6782210
H	-0.6221940	6.5466390	0.3763210
H	1.8710530	-3.5291510	-1.1125750
H	-3.1491050	0.8449210	1.6997210
H	-3.2815620	0.0183520	-2.5771570
H	-5.8345270	0.2911130	-1.9531420
H	-2.1264200	-3.8292630	-0.5638660
H	-0.0281350	-1.1833640	2.1064590
H	-2.7861510	-5.2514020	1.3716060
H	-0.6758570	-2.5979310	4.0287540
H	-2.0591420	-4.6358890	3.6703460
S	-0.9721680	-2.1776960	-2.5549540
H	5.6865430	-1.2494140	-0.0555090

5^α-ΔE₁-1

C	1.3232820	-0.3906200	-0.5281420
C	0.6937090	0.8061210	-0.2315130
P	0.0774670	-1.7173840	-0.7737890
C	-0.7466880	0.7697460	-0.1873860
C	-1.3018090	-0.5347080	-0.4893370
C	1.3896820	2.0103790	0.0635230
C	0.6514810	3.1895100	0.3983520
C	-1.4843390	1.8594040	0.1689920
C	-0.8338430	3.1346040	0.4218060
C	2.8173380	1.9994560	0.0294370
C	3.5031480	3.1975030	0.3313670
C	1.3828860	4.3407230	0.6960100
C	2.7882580	4.3393940	0.6581720
C	-2.9828100	1.6735510	0.3842400
C	-3.7294670	2.9820420	0.3310680
C	-1.6362430	4.2366400	0.5955160
C	-3.0783110	4.1555010	0.4838390
C	3.4530760	0.7584460	-0.3092200
C	2.7442130	-0.4293850	-0.5864050
C	3.6165030	-1.5292110	-0.8967880
C	4.9325120	-1.1819410	-0.8509150
S	5.1783160	0.4943420	-0.4322270
C	-2.6488190	-0.6693270	-0.6286000
C	-3.4970040	0.6050620	-0.5883410
C	-3.4586070	-1.8334760	-0.8694970
S	-5.2392590	0.0353360	-0.2839410
C	-4.7881760	-1.6054570	-0.7205620
C	0.1853250	-2.8059560	0.7110960
C	0.2121450	-4.1969930	0.5592190
C	0.2322320	-2.2472670	1.9986260
C	0.2829830	-5.0237650	1.6846560
C	0.3033450	-3.0749570	3.1197760
C	0.3283570	-4.4652380	2.9640510
H	4.5893820	3.2236580	0.3119980
H	0.8748250	5.2595950	0.9708210
H	3.3227330	5.2555900	0.8954750
H	-3.1188120	1.2595850	1.4084970
H	-4.8134780	2.9563840	0.2439130
H	-1.2016410	5.2193810	0.7475130
H	-3.6406860	5.0861990	0.5068470
H	3.2619080	-2.5195730	-1.1593470
H	5.7920930	-1.8098380	-1.0476500
H	-3.4975020	1.0217180	-1.6099490
H	-3.0402820	-2.8054800	-1.1077160
H	-5.5740290	-2.3449080	-0.8304180
H	0.1792310	-4.6216850	-0.4404940
H	0.2160980	-1.1682050	2.1291240
H	0.3036510	-6.1032950	1.5584560
H	0.3408610	-2.6355640	4.1133180
H	0.3845460	-5.1089440	3.8383250
S	0.0942520	-2.7060860	-2.4838390

5^α-ΔE₁-2

C	1.3255490	-0.4287130	-0.4279440
C	0.7327650	0.7910220	-0.1481640
P	0.0390970	-1.6883510	-0.7899940
C	-0.7085540	0.8106440	-0.1573420
C	-1.3020600	-0.4790550	-0.4475070
C	1.4643540	1.9868550	0.0896240
C	0.7615760	3.2097910	0.3302680
C	-1.4135830	1.9656560	0.0082880
C	-0.7249000	3.2068930	0.3209900
C	2.8910470	1.9300010	0.0665150
C	3.6123250	3.1214950	0.3051360
C	1.5267790	4.3560670	0.5521990
C	2.9317050	4.3056670	0.5421160
C	-2.9158010	1.9374610	-0.2535490
C	-3.6236040	3.1043970	0.3866530
C	-1.4943060	4.2944240	0.6592390
C	-2.9372970	4.2082720	0.7542200
C	3.4894690	0.6555630	-0.2101820
C	2.7452350	-0.5140380	-0.4711380
C	3.5849210	-1.6480280	-0.7464270
C	4.9110450	-1.3443050	-0.6858010
S	5.2066010	0.3311640	-0.2977940
C	-2.6548600	-0.6182730	-0.3995960
C	-3.4693310	0.5623200	0.1390670
C	-3.4975950	-1.7323400	-0.7404950
S	-5.2234290	0.2431000	-0.3860640
C	-4.8184330	-1.4212780	-0.7717560
C	0.0490250	-2.8765850	0.6201700
C	0.0049180	-4.2544560	0.3785320
C	0.0982450	-2.4048310	1.9421220
C	0.0058440	-5.1542220	1.4489860
C	0.0995470	-3.3051850	3.0082190
C	0.0527150	-4.6819970	2.7626410
H	4.6989660	3.1123330	0.2956090
H	1.0460370	5.3133780	0.7264830
H	3.4931500	5.2197490	0.7170580
H	-3.0545850	2.0328950	-1.3536970
H	-4.7074630	3.0703280	0.4726250
H	-1.0310700	5.2360330	0.9359450
H	-3.4704990	5.0682770	1.1530950
H	3.2023540	-2.6323600	-0.9915140
H	5.7518910	-2.0053870	-0.8524270
H	-3.4712240	0.4801100	1.2392810
H	-3.1083430	-2.7050590	-1.0216430
H	-5.6219650	-2.0985220	-1.0402040
H	-0.0256180	-4.6117930	-0.6473900
H	0.1401770	-1.3367800	2.1410490
H	-0.0276140	-6.2230320	1.2534020
H	0.1398440	-2.9332090	4.0288420

H	0.0551050	-5.3824090	3.5940830
S	0.0820750	-2.5604260	-2.5618420

5^a-ΔE₂ (5f)

C	1.3193980	-0.4497500	-0.4869950
P	-0.0000140	-1.6976370	-0.7901970
C	0.7247510	0.7641100	-0.2010580
C	-1.3194060	-0.4497290	-0.4869920
C	-0.7247390	0.7641220	-0.2010560
C	1.4493000	1.9516010	0.0741460
C	0.7444730	3.1656540	0.3603130
C	-1.4492670	1.9516250	0.0741490
C	-0.7444200	3.1656650	0.3603160
C	2.8774170	1.8947030	0.0559200
C	3.5980610	3.0817420	0.3337420
C	1.5075730	4.3001350	0.6255820
C	2.9164590	4.2526680	0.6113550
C	-2.8773850	1.8947500	0.0559270
C	-3.5980090	3.0818010	0.3337520
C	-1.5075010	4.3001580	0.6255880
C	-2.9163870	4.2527150	0.6113650
C	-2.7343740	-0.5387150	-0.5247600
C	-3.5768620	-1.6680130	-0.8124240
C	-3.4774450	0.6316510	-0.2479230
C	-4.9016660	-1.3612130	-0.7489910
S	-5.1964930	0.3105530	-0.3418990
C	-0.0000180	-2.8202620	0.6714540
C	0.0000600	-2.2960810	1.9742430
C	-0.0001070	-4.2063950	0.4806500
C	0.0000490	-3.1554250	3.0731950
C	-0.0001190	-5.0645260	1.5848730
C	-0.0000410	-4.5414690	2.8796810
S	-0.0000280	-2.6231740	-2.5320530
H	4.6846940	3.0732410	0.3268680
H	1.0293690	5.2483600	0.8476320
H	3.4750340	5.1607960	0.8224360
H	-4.6846420	3.0733170	0.3268800
H	-1.0292800	5.2483760	0.8476390
H	-3.4749470	5.1608520	0.8224490
H	-3.1961430	-2.6502190	-1.0687720
H	-5.7436390	-2.0185780	-0.9247900
H	0.0001300	-1.2206750	2.1329750
H	-0.0001620	-4.6034480	-0.5309920
H	0.0001110	-2.7441570	4.0793270
H	-0.0001870	-6.1404090	1.4297380
H	-0.0000490	-5.2094410	3.7373530
C	2.7343650	-0.5387600	-0.5247650
C	3.4774560	0.6315940	-0.2479310
C	3.5768340	-1.6680720	-0.8124280
S	5.1964980	0.3104670	-0.3419100
C	4.9016430	-1.3612930	-0.7490000

H	3.1960980	-2.6502730	-1.0687720
H	5.7436050	-2.0186730	-0.9247990

5^β-ΔE₁-1

C	1.2469890	-0.5947180	-0.4372480
C	0.8418410	0.6987090	-0.1586990
P	-0.2235070	-1.6553340	-0.7344110
C	-0.5885550	0.9228760	-0.1412260
C	-1.3519620	-0.2536100	-0.4380160
C	1.7449360	1.7751130	0.0537080
C	1.2342400	3.0877720	0.3051490
C	-1.1097980	2.1763330	0.0564270
C	-0.2374590	3.2960370	0.3461380
C	3.1479150	1.5128460	-0.0049350
C	4.0403620	2.5896350	0.2028320
C	2.1615970	4.1120660	0.4957740
C	3.5449000	3.8603250	0.4460960
C	-2.5971410	2.4014390	-0.1826010
C	-3.1038420	3.5998700	0.5812520
C	-0.8236710	4.4819900	0.7329070
C	-2.2518120	4.5892290	0.9324270
C	3.5492880	0.1645070	-0.2814890
C	2.6369230	-0.8870650	-0.5093890
C	3.2959710	-2.1337750	-0.7902020
C	4.6530800	-2.0254100	-0.7659420
S	5.1990450	-0.4069600	-0.4068040
C	-2.7307460	-0.1765620	-0.4429280
C	-3.3869350	1.1138020	0.0890880
C	-3.6904050	-1.1186250	-0.8438810
C	-4.8105830	1.0914410	-0.3891060
S	-5.2455960	-0.4311500	-0.9133700
C	-0.3656940	-2.7747400	0.7256910
C	-0.5968250	-4.1431080	0.5454560
C	-0.2515950	-2.2563820	2.0259960
C	-0.7153630	-4.9869130	1.6544010
C	-0.3685750	-3.1008530	3.1307220
C	-0.6016770	-4.4683280	2.9462440
H	5.1136340	2.4230300	0.1646970
H	1.8288300	5.1292960	0.6755960
H	4.2366320	4.6851300	0.5966820
H	-2.7218400	2.6325610	-1.2687650
H	-4.1712590	3.6949590	0.7678660
H	-0.2146120	5.3403260	0.9970410
H	-2.6317870	5.4882740	1.4129810
H	2.7680200	-3.0539820	-1.0133540
H	5.3844860	-2.8032450	-0.9445850
H	-3.4125010	0.9793450	1.1987760
H	-3.5129260	-2.1001870	-1.2627110
H	-0.6794750	-4.5375850	-0.4638090
H	-0.0683840	-1.1955550	2.1780050
H	-0.8945180	-6.0488090	1.5054630

H	-0.2761090	-2.6927650	4.1340720
H	-0.6921710	-5.1253370	3.8077100
S	-0.3431250	-2.6095180	-2.4642330
H	-5.5610130	1.8531950	-0.2268650

5^B-ΔE₁-2

C	1.2554930	-0.5151130	-0.5249840
C	0.7914870	0.7528820	-0.2236470
P	-0.1643880	-1.6529190	-0.7769760
C	-0.6473300	0.9050310	-0.1781110
C	-1.3574710	-0.3115510	-0.4484110
C	1.6439610	1.8506920	0.0714750
C	1.0732190	3.1194790	0.4052420
C	-1.2273790	2.1012640	0.1596640
C	-0.4063880	3.2678690	0.4156480
C	3.0576120	1.6472350	0.0385160
C	3.8994300	2.7408090	0.3453120
C	1.9525960	4.1592250	0.7076940
C	3.3458680	3.9674540	0.6747610
C	-2.7326440	2.1414180	0.3953630
C	-3.2815710	3.5379720	0.2404680
C	-1.0430670	4.4801940	0.5671410
C	-2.4730010	4.6101480	0.3942570
C	3.5205160	0.3340870	-0.3038450
C	2.6574830	-0.7457520	-0.5852460
C	3.3731880	-1.9524980	-0.8998590
C	4.7239700	-1.7868700	-0.8535020
S	5.1948810	-0.1608880	-0.4284780
C	-2.7352670	-0.2772730	-0.5336870
C	-3.4290930	1.0980380	-0.4877380
C	-3.6632900	-1.3162370	-0.7063350
C	-4.8808030	0.8308800	-0.2076770
S	-5.2594120	-0.7682750	-0.4919750
C	-0.1806360	-2.7835610	0.6829120
C	-0.2803390	-4.1675580	0.5005530
C	-0.0952110	-2.2601490	1.9832040
C	-0.2953220	-5.0219280	1.6077190
C	-0.1092660	-3.1148630	3.0861190
C	-0.2096430	-4.4981180	2.8996400
H	4.9792610	2.6192630	0.3271560
H	1.5734010	5.1381680	0.9825890
H	3.9987990	4.8020740	0.9167530
H	-2.9126890	1.8369490	1.4553610
H	-4.3504400	3.6692560	0.0877020
H	-0.4725560	5.3901150	0.7219360
H	-2.8905430	5.6140210	0.3559760
H	2.8878940	-2.8852810	-1.1641180
H	5.4905740	-2.5248990	-1.0523520
H	-3.3673250	1.4748000	-1.5390700
H	-3.4633250	-2.3710270	-0.8357070
H	-0.3449110	-4.5652660	-0.5088180

H	-0.0169700	-1.1867680	2.1365150
H	-0.3722500	-6.0958960	1.4574060
H	-0.0408330	-2.7023340	4.0895730
H	-0.2197290	-5.1631790	3.7596360
S	-0.2999860	-2.6071490	-2.5044470
H	-5.6628830	1.5655840	-0.0733760

5^B-ΔE₂

C	1.2361970	-0.6202980	-0.4886250
C	0.8427660	0.6748250	-0.2072400
P	-0.2695160	-1.6410560	-0.7696590
C	-0.5909410	0.9032730	-0.2004080
C	-1.3645270	-0.1945170	-0.4774690
C	1.7520560	1.7303250	0.0570350
C	1.2553170	3.0424380	0.3443670
C	-1.1138120	2.2101860	0.0832600
C	-0.2139120	3.2818280	0.3598710
C	3.1528530	1.4449230	0.0282910
C	4.0579690	2.5019350	0.2944100
C	2.1926890	4.0400730	0.5979700
C	3.5762560	3.7674240	0.5718770
C	-2.5232800	2.3943330	0.0827680
C	-3.0283650	3.6743650	0.3697960
C	-0.7704970	4.5350170	0.6379110
C	-2.1584080	4.7240110	0.6426490
C	3.5407820	0.1019250	-0.2721650
C	2.6166530	-0.9356330	-0.5352760
C	3.2644470	-2.1875800	-0.8212930
C	4.6215010	-2.0970860	-0.7703860
S	5.1852410	-0.4920500	-0.3765720
C	-2.7901110	-0.0636250	-0.5078020
C	-3.3715100	1.2426210	-0.2197710
C	-3.7498740	-1.0203470	-0.7820080
C	-4.7498500	1.2073680	-0.2869690
S	-5.3370110	-0.3612670	-0.6934670
C	-0.4456240	-2.7277740	0.7080650
C	-0.6796350	-4.0965430	0.5368070
C	-0.3520330	-2.1937880	2.0033190
C	-0.8205110	-4.9274560	1.6528560
C	-0.4922020	-3.0259930	3.1141200
C	-0.7273370	-4.3946340	2.9402660
H	5.1289490	2.3182990	0.2788000
H	1.8759430	5.0535340	0.8200200
H	4.2750030	4.5749140	0.7743080
H	-4.1001910	3.8496650	0.3784300
H	-0.1334650	5.3857660	0.8549510
H	-2.5589840	5.7101890	0.8624740
H	2.7287010	-3.0973970	-1.0672730
H	5.3453750	-2.8822480	-0.9480260
H	-3.5966990	-2.0560010	-1.0532320
H	-0.7505900	-4.5018420	-0.4691080

H	-0.1709690	-1.1316620	2.1471490
H	-1.0030890	-5.9897850	1.5123450
H	-0.4188160	-2.6068620	4.1143330
H	-0.8373350	-5.0412240	3.8072000
S	-0.4288820	-2.5799350	-2.4974920
H	-5.4529910	2.0129540	-0.1243500

6-a

C	-1.2517580	-0.3308010	-0.3020950
C	-0.8306340	0.9741920	-0.1558210
P	0.2429560	-1.3535460	-0.5087140
C	0.6229520	1.2396730	-0.1660810
C	1.3696500	0.1087060	-0.3174390
C	-1.7648510	2.0075510	0.0043500
C	-1.4071100	3.3863420	0.1558200
C	1.0180930	2.6534800	-0.0435310
C	0.0205480	3.7109220	0.1152610
C	2.2957420	3.1673240	-0.0818970
S	2.3198820	4.8845910	0.0739400
C	0.5949520	4.9547730	0.1937240
C	-3.1347370	1.7301710	0.0286140
S	-4.0142370	3.2353280	0.2538830
C	-2.5256100	4.1619060	0.3010860
C	2.8393270	-0.0573290	-0.3139590
C	3.5007540	-0.4672400	-1.4902780
C	3.5618040	0.1502870	0.8635640
C	4.8848860	-0.6496810	-1.4646110
C	4.9539440	-0.0368040	0.8712840
C	5.6218740	-0.4325420	-0.2873730
C	-2.6403170	-0.6662510	-0.3012760
C	-3.0816070	-2.0058540	-0.4685690
C	-3.6049830	0.3925830	-0.1224280
C	-4.4327450	-2.2936980	-0.4576950
C	-4.9901230	0.0366190	-0.1115850
C	-5.3974900	-1.2706740	-0.2726920
C	0.4438170	-2.3529830	1.0238630
C	1.0194520	-3.6270240	0.9514160
C	0.0514130	-1.8376740	2.2696420
C	1.2038940	-4.3791650	2.1152480
C	0.2349510	-2.5923740	3.4290330
C	0.8127190	-3.8643440	3.3534500
S	0.4193580	-2.4050050	-2.1778530
O	-5.8433190	1.0844370	0.0672230
C	-7.2456060	0.8396090	0.0804490
O	-4.9638240	-3.5383740	-0.6188260
C	-4.0736010	-4.6308650	-0.8351000
O	5.6257510	-1.0430950	-2.5427060
C	4.9499450	-1.3151530	-3.7676050
O	5.5710290	0.1931860	2.0699560
C	6.9760720	-0.0028560	2.1604900
H	3.2236470	2.6246550	-0.1877540

H	0.0988590	5.9096560	0.3077160
H	-2.5878530	5.2352820	0.4325700
H	2.9205530	-0.6434030	-2.3862130
H	3.0663870	0.4485110	1.7815690
H	6.6934110	-0.5884050	-0.3197950
H	-2.3413680	-2.7789790	-0.6295270
H	-6.4422520	-1.5556300	-0.2700660
H	1.3108620	-4.0247280	-0.0168080
H	-0.4022300	-0.8521290	2.3353390
H	1.6515740	-5.3677540	2.0512510
H	-0.0757970	-2.1890980	4.3894560
H	0.9546760	-4.4513890	4.2574200
H	-7.5785590	0.4114740	-0.8731250
H	-7.5196460	0.1684840	0.9039110
H	-7.7133620	1.8139340	0.2294260
H	-4.7101730	-5.5097850	-0.9489230
H	-3.4800070	-4.4827760	-1.7452260
H	-3.4034030	-4.7694660	0.0223530
H	5.7263830	-1.6307740	-4.4666450
H	4.2129620	-2.1180240	-3.6456820
H	4.4522400	-0.4166400	-4.1540480
H	7.2490600	-1.0417660	1.9336920
H	7.5184250	0.6737570	1.4870020
H	7.2404270	0.2253570	3.1945640

6-b

C	-1.2076060	-0.3355140	-0.3271200
C	-0.7683470	0.9649630	-0.1928350
P	0.2727660	-1.3792230	-0.5312910
C	0.6881770	1.2112650	-0.2135700
C	1.4198930	0.0695140	-0.3567280
C	-1.6873840	2.0118910	-0.0335770
C	-1.3101830	3.3866520	0.1075790
C	1.1029390	2.6206140	-0.1092210
C	0.1212640	3.6924020	0.0518340
C	2.3865970	3.1171690	-0.1715850
S	2.4351010	4.8356780	-0.0325190
C	0.7129920	4.9292340	0.1115430
C	-3.0607000	1.7531220	0.0009330
S	-3.9183810	3.2711800	0.2234150
C	-2.4172440	4.1778970	0.2561330
C	2.8872040	-0.1145290	-0.3531190
C	3.5422950	-0.5358080	-1.5200360
C	3.6093690	0.0959740	0.8350520
C	4.9320290	-0.7312060	-1.4942220
C	4.9963220	-0.1067830	0.8402530
C	5.6587490	-0.5143830	-0.3210450
C	-2.6007060	-0.6519560	-0.3173670
C	-3.0613680	-1.9862280	-0.4748430
C	-3.5498640	0.4211970	-0.1398360
C	-4.4164710	-2.2550540	-0.4564260

C	-4.9397710	0.0846010	-0.1203390
C	-5.3660690	-1.2177050	-0.2724750
C	0.4697440	-2.3660150	1.0103810
C	1.0887720	-3.6207490	0.9541430
C	0.0351360	-1.8611020	2.2464560
C	1.2757360	-4.3627780	2.1239230
C	0.2202470	-2.6065040	3.4119750
C	0.8424140	-3.8583000	3.3524650
S	0.4338970	-2.4481030	-2.1900080
O	-5.7771650	1.1452060	0.0568330
C	-7.1829250	0.9206430	0.0766330
O	-4.9655920	-3.4927230	-0.6086560
C	-4.0921910	-4.5990700	-0.8242810
O	5.6631130	-1.1365280	-2.5737590
C	4.9819980	-1.4073460	-3.7957230
O	5.7919090	0.0669980	1.9398680
C	5.1859220	0.4572930	3.1653140
H	3.3053700	2.5618300	-0.2922300
H	0.2310650	5.8918090	0.2217750
H	-2.4643320	5.2528370	0.3810590
H	2.9613480	-0.7112320	-2.4157800
H	3.0797490	0.4051150	1.7278870
H	6.7321780	-0.6706740	-0.3084260
H	-2.3329880	-2.7707350	-0.6352210
H	-6.4146870	-1.4879270	-0.2637470
H	1.4112650	-4.0124710	-0.0066210
H	-0.4550120	-0.8924000	2.2991730
H	1.7576700	-5.3357870	2.0720750
H	-0.1267810	-2.2131100	4.3641710
H	0.9843040	-4.4387140	4.2607420
H	-7.5254860	0.4922610	-0.8733640
H	-7.4633190	0.2580620	0.9048210
H	-7.6359210	1.9024400	0.2220100
H	-4.7419980	-5.4690680	-0.9313130
H	-3.5008710	-4.4634320	-1.7377660
H	-3.4202310	-4.7436270	0.0307590
H	5.7541870	-1.7336410	-4.4945570
H	4.2377880	-2.2030130	-3.6699520
H	4.4926460	-0.5060340	-4.1864470
H	4.6990510	1.4374100	3.0771180
H	4.4533940	-0.2868630	3.5037840
H	6.0002930	0.5212000	3.8892890

6-c

C	-1.2618450	-0.3389090	-0.3615700
C	-0.8261380	0.9569070	-0.1819550
P	0.2225760	-1.3754700	-0.5844680
C	0.6297240	1.2055550	-0.1891430
C	1.3638060	0.0726700	-0.3717970
C	-1.7464470	1.9980210	0.0047440
C	-1.3705370	3.3673860	0.1959700

C	1.0441190	2.6082170	-0.0228100
C	0.0619770	3.6739000	0.1704840
C	2.3300670	3.1015220	-0.0397070
S	2.3802680	4.8121860	0.1772580
C	0.6557050	4.9048840	0.2953470
C	-3.1197290	1.7379280	0.0171980
S	-3.9800730	3.2479880	0.2810510
C	-2.4794390	4.1531300	0.3594140
C	2.8340750	-0.0940480	-0.3976100
C	3.4978490	-0.2974230	-1.6063020
C	3.5538810	-0.0742930	0.8182940
C	4.8951440	-0.4629550	-1.6131750
C	4.9376220	-0.2485480	0.7932440
C	5.6190350	-0.4385860	-0.4219780
C	-2.6548540	-0.6557140	-0.3753390
C	-3.1128710	-1.9839510	-0.5832950
C	-3.6064650	0.4110050	-0.1730020
C	-4.4678590	-2.2533640	-0.5908750
C	-4.9962560	0.0736170	-0.1818530
C	-5.4199780	-1.2228900	-0.3831710
C	0.4122800	-2.3894000	0.9421720
C	1.0332500	-3.6420690	0.8655930
C	-0.0312290	-1.9097140	2.1850880
C	1.2136940	-4.4067780	2.0218490
C	0.1476730	-2.6773090	3.3372360
C	0.7720850	-3.9269320	3.2574100
S	0.4035580	-2.4086400	-2.2587840
O	-5.8368310	1.1275440	0.0200960
C	-7.2424580	0.9025440	0.0089820
O	-5.0142910	-3.4851800	-0.7933380
C	-4.1370720	-4.5816190	-1.0416410
O	5.4572680	-0.6429110	-2.8441830
C	6.8625070	-0.8378890	-2.9298070
O	5.7355090	-0.2521160	1.9050260
C	5.1243000	-0.1028750	3.1804490
H	3.2487220	2.5483520	-0.1710410
H	0.1748110	5.8631010	0.4420260
H	-2.5283360	5.2232320	0.5200780
H	2.9547740	-0.3363400	-2.5437130
H	3.0170230	0.0711320	1.7475990
H	6.6940900	-0.5672330	-0.3888250
H	-2.3818000	-2.7616250	-0.7637040
H	-6.4685340	-1.4931930	-0.3970990
H	1.3619090	-4.0138950	-0.1010950
H	-0.5239260	-0.9432860	2.2534250
H	1.6962830	-5.3785370	1.9539100
H	-0.2067760	-2.3032960	4.2945450
H	0.9081040	-4.5252200	4.1549790
H	-7.5689950	0.5062210	-0.9604260
H	-7.5365100	0.2124400	0.8095580
H	-7.6984390	1.8788800	0.1797220

H	-4.7844520	-5.4474860	-1.1893540
H	-3.5356210	-4.4102810	-1.9424130
H	-3.4743770	-4.7584910	-0.1854180
H	7.0792350	-0.9637140	-3.9919650
H	7.4102920	0.0325250	-2.5450440
H	7.1736100	-1.7379320	-2.3834390
H	4.6169180	0.8666400	3.2698220
H	4.4077740	-0.9110190	3.3755420
H	5.9386120	-0.1542760	3.9054840

6-d

C	-1.3055450	-0.3408020	-0.3375540
C	-0.8887700	0.9624130	-0.1676180
P	0.1930440	-1.3577220	-0.5539930
C	0.5637820	1.2318630	-0.1731620
C	1.3135500	0.1071600	-0.3458010
C	-1.8252050	1.9907840	0.0103620
C	-1.4703260	3.3671030	0.1901430
C	0.9563440	2.6427180	-0.0188500
C	-0.0428420	3.6949410	0.1617400
C	2.2339050	3.1571250	-0.0386350
S	2.2563230	4.8703560	0.1598340
C	0.5305060	4.9367000	0.2735630
C	-3.1944080	1.7100480	0.0258850
S	-4.0775260	3.2089230	0.2782000
C	-2.5908320	4.1373590	0.3479480
C	2.7853410	-0.0458820	-0.3549460
C	3.4580050	-0.3384070	-1.5486730
C	3.5026750	0.0656640	0.8465130
C	4.8482480	-0.5002130	-1.5367590
C	4.8898170	-0.1033960	0.8453970
C	5.5789980	-0.3846150	-0.3445040
C	-2.6934560	-0.6788290	-0.3479240
C	-3.1310000	-2.0156540	-0.5445850
C	-3.6611630	0.3744440	-0.1527060
C	-4.4814950	-2.3063410	-0.5470030
C	-5.0454610	0.0152950	-0.1556660
C	-5.4492590	-1.2893030	-0.3454580
C	0.3938860	-2.3663600	0.9738200
C	0.9864650	-3.6322320	0.8938000
C	-0.0158480	-1.8691370	2.2213170
C	1.1707970	-4.3937610	2.0515150
C	0.1676130	-2.6331340	3.3747590
C	0.7625090	-3.8967050	3.2915270
S	0.3834140	-2.3936320	-2.2271180
O	-5.9021330	1.0575290	0.0398600
C	-7.3038220	0.8096380	0.0373500
O	-5.0089640	-3.5484140	-0.7381530
C	-4.1148520	-4.6327180	-0.9787530
O	5.4199800	-0.7717520	-2.7484450
C	6.8232870	-0.9752810	-2.8193590

O	5.5023470	0.0249190	2.0631760
C	6.9072740	-0.1631470	2.1511190
H	3.1621040	2.6172960	-0.1562680
H	0.0336440	5.8883590	0.4092130
H	-2.6557130	5.2077790	0.5006250
H	2.9183580	-0.4490090	-2.4820920
H	2.9981040	0.2758800	1.7836220
H	6.6526970	-0.5122550	-0.3421650
H	-2.3879450	-2.7830890	-0.7193880
H	-6.4934510	-1.5762430	-0.3544860
H	1.2904240	-4.0161220	-0.0762470
H	-0.4836850	-0.8906610	2.2929540
H	1.6311950	-5.3761190	1.9812950
H	-0.1572710	-2.2439500	4.3363690
H	0.9038040	-4.4912910	4.1907010
H	-7.6285340	0.4002690	-0.9272660
H	-7.5828240	0.1213060	0.8448170
H	-7.7749210	1.7797510	0.2025180
H	-4.7485640	-5.5101250	-1.1175700
H	-3.5180240	-4.4596560	-1.8822950
H	-3.4476040	-4.7914980	-0.1225090
H	7.0390000	-1.1829950	-3.8688750
H	7.3753470	-0.0789250	-2.5056790
H	7.1350840	-1.8324130	-2.2075260
H	7.1968700	-1.1742100	1.8349960
H	7.4505890	0.5794550	1.5513240
H	7.1581150	-0.0283610	3.2048330

6-e

C	-1.2007050	-0.3195820	-0.3042740
C	-0.7513570	0.9728710	-0.1492630
P	0.2698550	-1.3738210	-0.5346370
C	0.7083690	1.2068760	-0.1603820
C	1.4290610	0.0610550	-0.3224320
C	-1.6618800	2.0295140	0.0194160
C	-1.2704780	3.3978270	0.1792560
C	1.1364710	2.6102810	-0.0277790
C	0.1642850	3.6893340	0.1402420
C	2.4255710	3.0948190	-0.0643380
S	2.4898070	4.8099760	0.1046370
C	0.7671660	4.9190450	0.2275170
C	-3.0364960	1.7866290	0.0415750
S	-3.8789690	3.3104860	0.2752020
C	-2.3694220	4.2007400	0.3288300
C	2.8947000	-0.1367550	-0.3209910
C	3.5472070	-0.5553050	-1.4991840
C	3.6213890	0.0487950	0.8577120
C	4.9268130	-0.7692780	-1.4738250
C	5.0088560	-0.1694630	0.8648780
C	5.6682590	-0.5743110	-0.2954980
C	-2.5996150	-0.6248220	-0.2996590

C	-3.0777870	-1.9431800	-0.4634660
C	-3.5404470	0.4595940	-0.1160260
C	-4.4367300	-2.2053160	-0.4483350
C	-4.9269940	0.1391820	-0.1057650
C	-5.3767440	-1.1625190	-0.2667670
C	0.4551030	-2.4032670	0.9788210
C	0.8983510	-3.7260550	0.8710150
C	0.1756910	-1.8635760	2.2445440
C	1.0634620	-4.5042330	2.0207290
C	0.3409610	-2.6433150	3.3896690
C	0.7863780	-3.9651650	3.2789450
S	0.4159920	-2.3884800	-2.2272260
O	-5.7566500	1.2071380	0.0741210
C	-7.1643140	1.0056720	0.0917210
O	-4.8009410	-3.5110640	-0.6158830
C	-6.1790360	-3.8542890	-0.6470220
O	5.6586440	-1.1752100	-2.5534660
C	4.9757930	-1.4314330	-3.7779820
O	5.6304700	0.0406850	2.0650660
C	7.0301220	-0.1904090	2.1557220
H	3.3407030	2.5319190	-0.1756180
H	0.2933240	5.8842020	0.3494430
H	-2.4053050	5.2745010	0.4663000
H	2.9632820	-0.7149190	-2.3958250
H	3.1323840	0.3526850	1.7772740
H	6.7358960	-0.7548800	-0.3282700
H	-2.3870110	-2.7635060	-0.6237220
H	-6.4360800	-1.3770260	-0.2545680
H	1.1039190	-4.1390890	-0.1127160
H	-0.1749470	-0.8386920	2.3365870
H	1.4071970	-5.5315210	1.9298870
H	0.1204730	-2.2206190	4.3666030
H	0.9141280	-4.5719390	4.1719890
H	-7.5155040	0.5893730	-0.8609180
H	-7.4584800	0.3453880	0.9174390
H	-7.6012880	1.9941220	0.2415420
H	-6.2091320	-4.9337290	-0.8049180
H	-6.6755630	-3.6140360	0.3026280
H	-6.6991780	-3.3529070	-1.4739690
H	5.7442840	-1.7646020	-4.4776760
H	4.2206700	-2.2170960	-3.6554200
H	4.4985120	-0.5216490	-4.1638110
H	7.2776000	-1.2345440	1.9237970
H	7.5896770	0.4760750	1.4861890
H	7.2991140	0.0259220	3.1911790
6-f			
C	-1.1574120	-0.3259490	-0.3316860
C	-0.6905910	0.9615120	-0.1845760
P	0.2987580	-1.3999900	-0.5589510
C	0.7714970	1.1768440	-0.2027080

C	1.4775300	0.0212860	-0.3587540
C	-1.5861630	2.0307430	-0.0156030
C	-1.1759650	3.3943390	0.1385090
C	1.2186890	2.5751430	-0.0832130
C	0.2622320	3.6674930	0.0882530
C	2.5135150	3.0425400	-0.1389330
S	2.6016560	4.7581030	0.0188370
C	0.8820150	4.8897380	0.1622320
C	-2.9637830	1.8059890	0.0137780
S	-3.7849390	3.3413400	0.2475080
C	-2.2636100	4.2118880	0.2914200
C	2.9404300	-0.1941060	-0.3586120
C	3.5864780	-0.6115800	-1.5318760
C	3.6667210	-0.0171400	0.8325590
C	4.9717120	-0.8369360	-1.5092060
C	5.0490590	-0.2489350	0.8341950
C	5.7028800	-0.6526130	-0.3332890
C	-2.5603700	-0.6124550	-0.3207960
C	-3.0567220	-1.9248970	-0.4773310
C	-3.4859520	0.4851940	-0.1373020
C	-4.4191430	-2.1687540	-0.4559320
C	-4.8766690	0.1834120	-0.1203990
C	-5.3443810	-1.1127490	-0.2747930
C	0.4770400	-2.4202730	0.9617750
C	1.0479320	-3.6956410	0.8763120
C	0.0754880	-1.9209260	2.2111340
C	1.2204430	-4.4641920	2.0310540
C	0.2461520	-2.6925860	3.3614980
C	0.8208440	-3.9651980	3.2730590
S	0.4388760	-2.4279540	-2.2429740
O	-5.6909770	1.2630410	0.0589890
C	-7.1013700	1.0812890	0.0818070
O	-4.8012140	-3.4699140	-0.6167050
C	-6.1839080	-3.7953820	-0.6410340
O	5.6938700	-1.2423040	-2.5948190
C	5.0052740	-1.4889670	-3.8177440
O	5.8483160	-0.1087560	1.9361740
C	5.2506120	0.2741480	3.1678520
H	3.4195190	2.4676590	-0.2645310
H	0.4222040	5.8618770	0.2825340
H	-2.2848980	5.2865050	0.4251890
H	3.0016390	-0.7622400	-2.4295980
H	3.1435760	0.2889420	1.7302740
H	6.7726910	-0.8321890	-0.3231480
H	-2.3776750	-2.7550510	-0.6374000
H	-6.4064110	-1.3131140	-0.2577380
H	1.3428190	-4.0825440	-0.0951710
H	-0.3778580	-0.9357940	2.2857900
H	1.6631770	-5.4541750	1.9566580
H	-0.0751350	-2.3033900	4.3244350
H	0.9510180	-4.5664600	4.1694710

H	-7.4614000	0.6666230	-0.8682080
H	-7.4020090	0.4281000	0.9108260
H	-7.5239020	2.0763010	0.2294950
H	-6.2284970	-4.8750130	-0.7938860
H	-6.6734230	-3.5443440	0.3094430
H	-6.7005950	-3.2910130	-1.4682790
H	5.7693600	-1.8256210	-4.5205820
H	4.2447150	-2.2697540	-3.6968930
H	4.5341280	-0.5745600	-4.2004150
H	4.7847500	1.2658020	3.0960360
H	4.5023310	-0.4595910	3.4943570
H	6.0660520	0.3088260	3.8926590

6-g

C	-1.2118180	-0.3289490	-0.3642580
C	-0.7504460	0.9533440	-0.1666140
P	0.2503970	-1.3921070	-0.6154580
C	0.7107470	1.1728650	-0.1697710
C	1.4209320	0.0286720	-0.3710250
C	-1.6487660	2.0147470	0.0333940
C	-1.2416610	3.3721130	0.2436740
C	1.1557220	2.5630960	0.0205100
C	0.1973270	3.6470860	0.2278990
C	2.4524420	3.0274260	0.0170980
S	2.5402140	4.7328890	0.2630340
C	0.8176720	4.8623000	0.3757900
C	-3.0261070	1.7874860	0.0383980
S	-3.8520270	3.3126540	0.3184070
C	-2.3323300	4.1822920	0.4135330
C	2.8876150	-0.1654090	-0.4058460
C	3.5459220	-0.3320750	-1.6230440
C	3.6089540	-0.2067480	0.8084190
C	4.9399010	-0.5224830	-1.6391720
C	4.9893490	-0.4046660	0.7737200
C	5.6657000	-0.5583550	-0.4493910
C	-2.6144210	-0.6173380	-0.3782510
C	-3.1065610	-1.9238830	-0.5884700
C	-3.5440050	0.4721130	-0.1671580
C	-4.4686560	-2.1697220	-0.5947870
C	-4.9342980	0.1683500	-0.1806330
C	-5.3978460	-1.1218650	-0.3885830
C	0.4230950	-2.4457210	0.8848890
C	1.0041540	-3.7145450	0.7735730
C	0.0065680	-1.9806690	2.1425670
C	1.1722980	-4.5101730	1.9105990
C	0.1732820	-2.7789200	3.2754030
C	0.7584590	-4.0447600	3.1610970
S	0.4133140	-2.3759640	-2.3186280
O	-5.7531090	1.2398840	0.0261250
C	-7.1632630	1.0560250	0.0179670
O	-4.8464390	-3.4647470	-0.8080060

C	-6.2278560	-3.7890130	-0.8747460
O	5.4972000	-0.6633000	-2.8775810
C	6.8977890	-0.8843940	-2.9734790
O	5.7883620	-0.4661010	1.8831580
C	5.1810540	-0.3546300	3.1642310
H	3.3590020	2.4559530	-0.1195750
H	0.3577110	5.8284210	0.5370700
H	-2.3568710	5.2510670	0.5875450
H	3.0006830	-0.3243350	-2.5599530
H	3.0754810	-0.0897100	1.7436680
H	6.7382850	-0.7076520	-0.4235470
H	-2.4238580	-2.7462570	-0.7715890
H	-6.4597300	-1.3238560	-0.3940460
H	1.3102280	-4.0746560	-0.2048620
H	-0.4558190	-1.0014670	2.2372340
H	1.6221830	-5.4952330	1.8156850
H	-0.1601710	-2.4161090	4.2445460
H	0.8844590	-4.6672530	4.0435670
H	-7.5062670	0.6762330	-0.9527440
H	-7.4771970	0.3723620	0.8169800
H	-7.5900000	2.0444620	0.1949270
H	-6.2682050	-4.8619710	-1.0700730
H	-6.7384550	-3.5751200	0.0737930
H	-6.7270140	-3.2531080	-1.6928860
H	7.1107820	-0.9721480	-4.0402300
H	7.4644470	-0.0419060	-2.5552310
H	7.1902360	-1.8120040	-2.4641760
H	4.6909220	0.6196490	3.2907970
H	4.4504260	-1.1567340	3.3296250
H	5.9949640	-0.4477780	3.8855710

6-h

C	-1.2539610	-0.3299950	-0.3395030
C	-0.8105770	0.9607340	-0.1576780
P	0.2222510	-1.3761980	-0.5799660
C	0.6479020	1.2002770	-0.1619480
C	1.3732630	0.0621970	-0.3470550
C	-1.7245950	2.0111080	0.0299450
C	-1.3375540	3.3768360	0.2214650
C	1.0719510	2.6004310	0.0066780
C	0.0969050	3.6728450	0.1976270
C	2.3607190	3.0861810	-0.0071570
S	2.4216000	4.7965090	0.2092980
C	0.6976320	4.9003020	0.3228930
C	-3.0983750	1.7636420	0.0411200
S	-3.9463510	3.2798560	0.3037940
C	-2.4395900	4.1730790	0.3836650
C	2.8417050	-0.1196680	-0.3617760
C	3.5067460	-0.4041540	-1.5616090
C	3.5626600	-0.0438300	0.8402750
C	4.8934510	-0.5938140	-1.5548240

C	4.9460520	-0.2407060	0.8338760
C	5.6279830	-0.5141850	-0.3619740
C	-2.6520040	-0.6392700	-0.3474050
C	-3.1250560	-1.9553430	-0.5417330
C	-3.5972530	0.4384300	-0.1467930
C	-4.4831900	-2.2216050	-0.5413060
C	-4.9827660	0.1137000	-0.1521470
C	-5.4274690	-1.1856150	-0.3438150
C	0.4050050	-2.4170050	0.9274870
C	0.8760490	-3.7295580	0.8114120
C	0.0960340	-1.8983910	2.1951290
C	1.0396320	-4.5178790	1.9544140
C	0.2595370	-2.6882870	3.3336960
C	0.7329280	-3.9996130	3.2145770
S	0.3879780	-2.3716870	-2.2777350
O	-5.8171940	1.1751480	0.0449750
C	-7.2241640	0.9690440	0.0465450
O	-4.8424070	-3.5246320	-0.7391500
C	-6.2190280	-3.8695130	-0.7975420
O	5.4580430	-0.8549000	-2.7722220
C	6.8558870	-1.0906330	-2.8483670
O	5.5627800	-0.1464220	2.0528550
C	6.9631080	-0.3677700	2.1351120
H	3.2767100	2.5270180	-0.1299080
H	0.2220520	5.8613370	0.4683890
H	-2.4793850	5.2434610	0.5444690
H	2.9635120	-0.4879380	-2.4956990
H	3.0633150	0.1590730	1.7817360
H	6.6988620	-0.6636600	-0.3636690
H	-2.4304800	-2.7694540	-0.7166920
H	-6.4862150	-1.4035030	-0.3433550
H	1.1030780	-4.1271000	-0.1740520
H	-0.2768960	-0.8820230	2.2937270
H	1.4042970	-5.5373450	1.8567440
H	0.0149430	-2.2819590	4.3118830
H	0.8586560	-4.6146380	4.1022850
H	-7.5662150	0.5722950	-0.9177280
H	-7.5231200	0.2900850	0.8552680
H	-7.6656780	1.9526400	0.2140670
H	-6.2445980	-4.9449370	-0.9816290
H	-6.7294820	-3.6532030	0.1505500
H	-6.7288610	-3.3493950	-1.6193460
H	7.0658150	-1.2848260	-3.9016570
H	7.4296790	-0.2134950	-2.5195620
H	7.1475080	-1.9657070	-2.2521690
H	7.2293900	-1.3788850	1.7992880
H	7.5224190	0.3736770	1.5486640
H	7.2181530	-0.2587510	3.1908140

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C	-1.3338270	-0.3061020	-0.2891060
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C	-0.7080110	0.9000810	-0.0741630
P	-0.0220700	-1.6052480	-0.4162740
C	0.7212790	0.9058400	0.0065770
C	1.3436860	-0.3689550	-0.2170650
C	-1.3944460	2.1122100	0.0817260
C	-0.7348800	3.3779170	0.2936920
C	1.3795260	2.0584840	0.2582050
C	0.7426060	3.3588950	0.3257180
C	2.8661060	2.0278470	0.4297920
S	3.3582320	3.8102040	0.1301050
C	1.6777450	4.3526830	0.2781980
C	-2.7816230	2.1262270	0.0200070
S	-3.3240980	3.7836670	0.2430920
C	-1.6749070	4.3718750	0.4002850
C	2.7028860	-0.4252970	-0.4066370
C	3.4235850	-1.6240620	-0.7078160
C	3.4814470	0.9283810	-0.4656010
C	4.7924610	-1.6267010	-0.7366900
C	4.9703430	0.7439970	-0.2592910
C	5.5824920	-0.4480700	-0.4391340
C	-2.7674590	-0.3378780	-0.3733500
C	-3.4702880	-1.5445720	-0.6176400
C	-3.4987440	0.9013900	-0.2080140
C	-4.8518720	-1.5410000	-0.6931550
C	-4.9220290	0.8430760	-0.2883760
C	-5.5878320	-0.3445880	-0.5223280
C	-0.1031860	-2.5702550	1.1572450
C	-0.0444070	-3.9683950	1.1337590
C	-0.2131920	-1.9038660	2.3883620
C	-0.0930450	-4.6945390	2.3280210
C	-0.2617960	-2.6304020	3.5788590
C	-0.2015240	-4.0280190	3.5506340
S	0.0060590	-2.7600930	-2.0272400
O	-5.5483590	2.0432560	-0.1180750
C	-6.9679600	2.1008750	-0.1946470
O	-5.6182900	-2.6433200	-0.9346000
C	-4.9607810	-3.8891280	-1.1508780
O	5.5626110	-2.7104090	-0.9999030
C	4.9168120	-3.9462520	-1.3108380
O	5.5928360	1.9096660	0.0272720
C	7.0132700	1.9148350	0.1640140
H	3.1217050	1.8214970	1.4821550
H	1.4897840	5.4209450	0.2588720
H	-1.5204740	5.4309170	0.5682110
H	2.8520590	-2.5284910	-0.8764130
H	3.3615720	1.2691490	-1.5148420
H	6.6556450	-0.5769440	-0.3686020
H	-2.8986680	-2.4510110	-0.7717590
H	-6.6672890	-0.3988650	-0.5890580
H	0.0345950	-4.4784300	0.1773510
H	-0.2641950	-0.8186150	2.4199820

H	-0.0487740	-5.7805780	2.2998640
H	-0.3497790	-2.1063340	4.5272500
H	-0.2414970	-4.5929480	4.4787150
H	-7.3228610	1.7784690	-1.1814890
H	-7.4302530	1.4827090	0.5851160
H	-7.2290530	3.1482420	-0.0349990
H	-5.7561820	-4.6119330	-1.3401330
H	-4.2921000	-3.8382770	-2.0187200
H	-4.3893110	-4.1936390	-0.2650880
H	5.7214450	-4.6518750	-1.5218070
H	4.3240010	-4.3015230	-0.4597310
H	4.2716390	-3.8383060	-2.1901650
H	7.3257680	1.2534240	0.9810390
H	7.4920370	1.6021180	-0.7715930
H	7.2831740	2.9458280	0.3949140

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C	1.3491300	0.2973400	-0.3649400
C	0.7325500	-0.9224590	-0.2075910
P	0.0264900	1.5727770	-0.5908850
C	-0.6974050	-0.9575470	-0.2564270
C	-1.3273620	0.3218290	-0.4147830
C	1.4280990	-2.1255920	-0.0248540
C	0.7773110	-3.4017980	0.1495150
C	-1.3468010	-2.1391240	-0.1713530
C	-0.7007160	-3.4011190	0.1285530
C	-2.8304900	-2.1762220	-0.3628660
S	-3.3140400	-3.7919020	0.4525370
C	-1.6299740	-4.3461340	0.4584490
C	2.8160680	-2.1149710	0.0104450
S	3.3708570	-3.7630400	0.2703550
C	1.7251800	-4.3792580	0.3202350
C	-2.6937790	0.4147330	-0.3137380
C	-3.4286320	1.6310970	-0.4739620
C	-3.4691840	-0.8637110	0.1451190
C	-4.7978990	1.6228460	-0.5044460
C	-4.9542670	-0.7697820	-0.1323220
C	-5.5746340	0.4055790	-0.3815860
C	2.7845200	0.3526290	-0.3598790
C	3.4805110	1.5728740	-0.5500590
C	3.5250310	-0.8757410	-0.1583730
C	4.8639250	1.5931370	-0.5387530
C	4.9493090	-0.7925640	-0.1456170
C	5.6079600	0.4080120	-0.3286600
C	0.0055900	2.5726110	0.9628920
C	-0.0352350	3.9704320	0.9068730
C	0.0276610	1.9318590	2.2122230
C	-0.0554830	4.7215100	2.0866300
C	0.0074800	2.6829030	3.3882580
C	-0.0343830	4.0801720	3.3272970
S	0.0689250	2.6926940	-2.2249680

O	5.5845240	-1.9831650	0.0563190
C	7.0068400	-2.0153010	0.0726880
O	5.6249350	2.7098930	-0.7247340
C	4.9609610	3.9457040	-0.9754220
O	-5.5781880	2.7138370	-0.6988920
C	-4.9462930	3.9813730	-0.8842710
O	-5.5664500	-1.9692690	-0.0139600
C	-6.9821830	-2.0399240	-0.1804890
H	-3.0658910	-2.3031700	-1.4326030
H	-1.4360880	-5.3661500	0.7729430
H	1.5786170	-5.4427840	0.4654450
H	-2.8688300	2.5375390	-0.6700120
H	-3.3676670	-0.8698050	1.2500260
H	-6.6463350	0.4888220	-0.5148440
H	2.9042070	2.4711010	-0.7319280
H	6.6883810	0.4808930	-0.3266260
H	-0.0466200	4.4600490	-0.0634840
H	0.0647120	0.8469120	2.2687980
H	-0.0850110	5.8071430	2.0332940
H	0.0274400	2.1783560	4.3509960
H	-0.0481970	4.6643710	4.2441460
H	7.4197090	-1.6784410	-0.8863870
H	7.4057300	-1.3956170	0.8855610
H	7.2756860	-3.0592660	0.2415050
H	5.7540600	4.6828450	-1.1116450
H	4.3481360	3.8886000	-1.8832230
H	4.3307400	4.2355480	-0.1252190
H	-5.7590590	4.6975940	-1.0117560
H	-4.3468760	4.2493210	-0.0061170
H	-4.3110560	3.9742680	-1.7774600
H	-7.4913780	-1.4356770	0.5798750
H	-7.2714640	-1.6990770	-1.1817850
H	-7.2411490	-3.0917900	-0.0555680

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C	-1.3434800	-0.3149480	-0.3445990
C	-0.7187550	0.8940730	-0.1629960
P	-0.0000040	-1.5855510	-0.5252440
C	0.7187840	0.8940600	-0.1629930
C	1.3434870	-0.3149740	-0.3445850
C	-1.3960110	2.1049650	0.0184660
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C	0.7391520	3.3770690	0.2139330
C	2.7878550	2.1076240	0.0182970
S	3.3347610	3.7604620	0.2721840
C	1.6830760	4.3589740	0.3648740
C	-2.7878030	2.1076750	0.0182970
S	-3.3346800	3.7605230	0.2721880
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C	2.7741460	-0.3587790	-0.3681080

C	3.5039700	0.8802660	-0.1757390
C	3.4802320	-1.5710180	-0.5797410
C	4.9313300	0.8127590	-0.1962310
C	4.8624500	-1.5735810	-0.5988230
C	5.5972430	-0.3786940	-0.3997480
C	-2.7741390	-0.3587270	-0.3681220
C	-3.4802470	-1.5709510	-0.5797660
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C	-4.8624640	-1.5734900	-0.5988420
C	-4.9313020	0.8128480	-0.1962340
C	-5.5972360	-0.3785920	-0.3997560
C	-0.0000260	-2.5535130	1.0459360
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C	-0.0003890	-4.6887000	2.1946290
C	0.0001850	-2.6327670	3.4707130
C	-0.0001260	-4.0314180	3.4267770
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H	-5.7839180	-4.6476960	-1.2018500
H	-4.3507340	-3.8714960	-1.9408250
H	-4.3759000	-4.2236130	-0.1836130
H	7.3735940	1.7310180	-0.9871000
H	7.2386130	3.1043040	0.1512250
H	7.4022840	1.4389900	0.7833620
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H	5.7838440	-4.6477880	-1.2019110

6f-b

C	-1.3971470	-0.3419350	-0.3491720
C	-0.7751390	0.8667690	-0.1580310
P	-0.0520040	-1.6067230	-0.5591590
C	0.6630440	0.8691410	-0.1602080
C	1.2889840	-0.3356850	-0.3525410
C	-1.4556990	2.0742730	0.0345260
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C	0.6752970	3.3510940	0.2373120
C	2.7271060	2.0927350	0.0303070
S	3.2676620	3.7449700	0.2954780
C	1.6147610	4.3367680	0.3943430
C	-2.8475580	2.0734260	0.0361640
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C	2.7230490	-0.3773000	-0.3687230
C	3.4497630	0.8673970	-0.1692160
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C	4.8216130	-1.5819870	-0.5779200
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C	-2.8276330	-0.3889130	-0.3717490
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C	-4.9125860	-1.6077960	-0.6103100
C	-4.9879980	0.7747520	-0.1864440
C	-5.6506860	-0.4167220	-0.3997490
C	-0.0473510	-2.6130530	0.9866400
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C	6.9135460	2.0664520	0.0029630
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H	7.0647930	-3.9257030	-1.0109460

6f-c

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C	0.7194200	0.8419190	-0.1566840
C	1.3426090	-0.3625050	-0.3585420
C	-1.3966970	2.0526740	0.0468880
C	-0.7388430	3.3203520	0.2627430
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C	0.7388730	3.3203470	0.2627400
C	2.7868460	2.0582680	0.0476750
S	3.3318770	3.7067490	0.3280610
C	1.6805610	4.3021600	0.4297830
C	-2.7868250	2.0582880	0.0476820
S	-3.3318440	3.7067730	0.3280750
C	-1.6805230	4.3021720	0.4297880
C	2.7765030	-0.4076030	-0.3734800
C	3.5065670	0.8330760	-0.1616190
C	3.4869300	-1.6073800	-0.5855200
C	4.9268980	0.7670780	-0.1755790
C	4.8717390	-1.6165540	-0.5900770
C	5.6057770	-0.4255600	-0.3828350
C	-2.7765000	-0.4075810	-0.3734810
C	-3.4869360	-1.6073520	-0.5855270
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C	-4.8717450	-1.6165170	-0.5900800
C	-4.9268870	0.7671130	-0.1755700
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C	0.0001460	-2.0763870	2.1966410
C	-0.0002070	-4.8611620	1.9614520
C	0.0001260	-2.8732270	3.3417810
C	-0.0000500	-4.2678120	3.2255810
S	-0.0000120	-2.6528250	-2.2806840
O	-5.5529490	1.9624060	0.0306500

C	-6.9735540	2.0203200	0.0268600
O	-5.4658580	-2.8280400	-0.8033140
C	-6.8830560	-2.9126350	-0.8477810
O	5.5529690	1.9623670	0.0306330
C	6.9735740	2.0202730	0.0268370
O	5.4658430	-2.8280820	-0.8033070
C	6.8830410	-2.9126890	-0.8477620
H	1.5254590	5.3594370	0.6080570
H	-1.5254130	5.3594480	0.6080620
H	2.9529980	-2.5335550	-0.7678540
H	6.6865460	-0.4414650	-0.3871920
H	-2.9530110	-2.5335290	-0.7678690
H	-6.6865430	-0.4414180	-0.3871810
H	-0.0002990	-4.5174470	-0.1765290
H	0.0002810	-0.9937860	2.2954160
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H	0.0002490	-2.4065440	4.3236090
H	-0.0000640	-4.8875150	4.1189200
H	-7.3796080	1.7036090	-0.9421990
H	-7.3968020	1.4011210	0.8280280
H	-7.2257130	3.0671280	0.2034130
H	-7.1087060	-3.9632500	-1.0384500
H	-7.3340520	-2.6134200	0.1078120
H	-7.2967370	-2.3003590	-1.6600460
H	7.3796220	1.7035550	-0.9422220
H	7.2257410	3.0670800	0.2033840
H	7.3968220	1.4010750	0.8280050
H	7.2967340	-2.3004220	-1.6600270
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H	7.1086830	-3.9633080	-1.0384230

5. NMR spectra

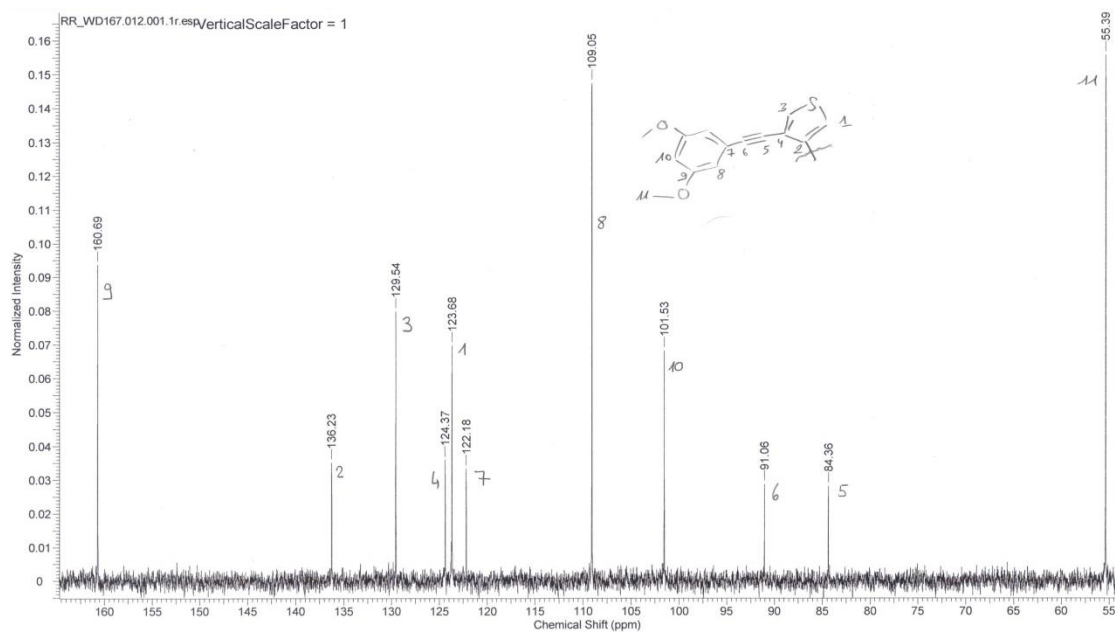
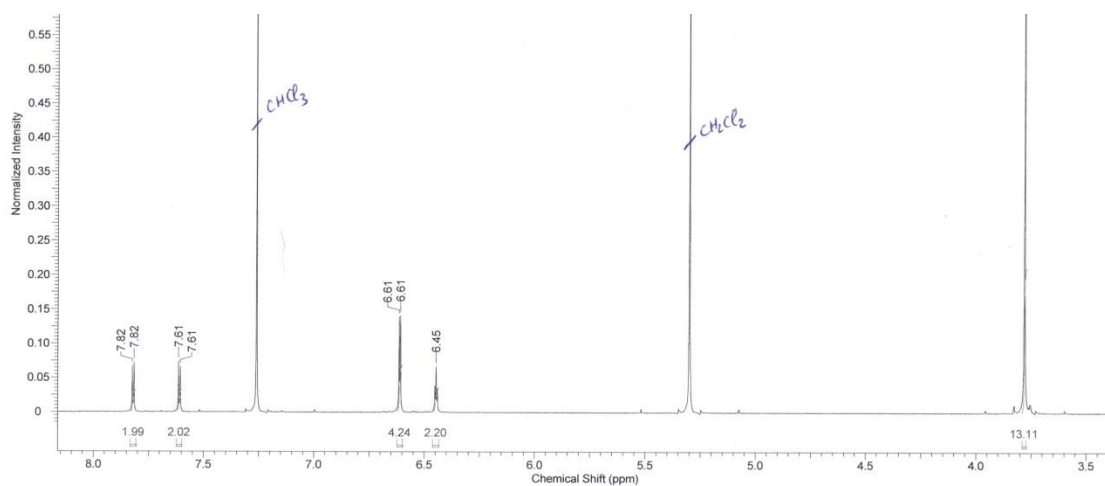
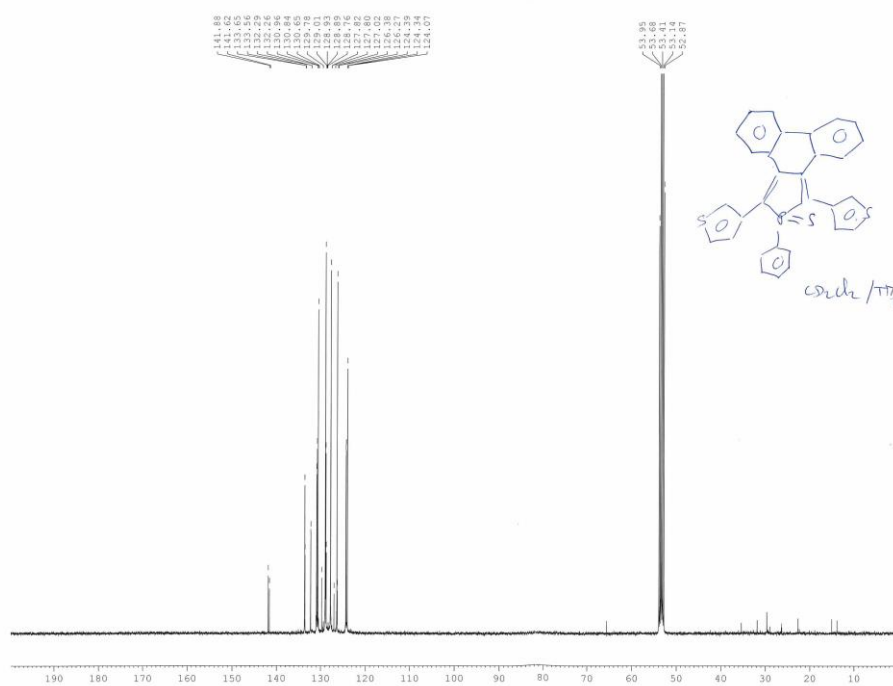
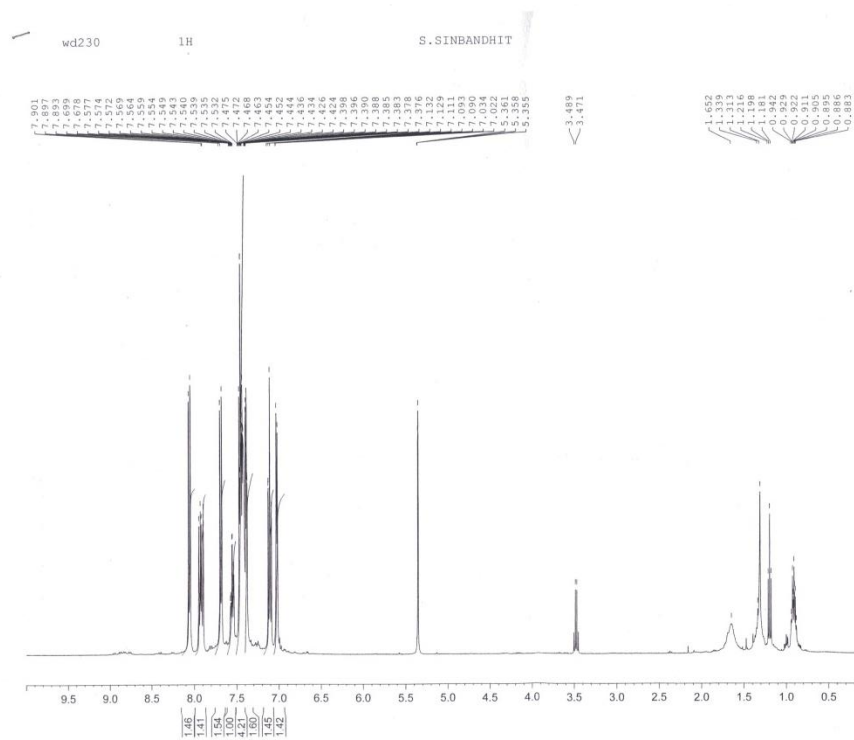


Figure S8: ¹H NMR (400 MHz, CD₂Cl₂) and ¹³C NMR spectra of **2**



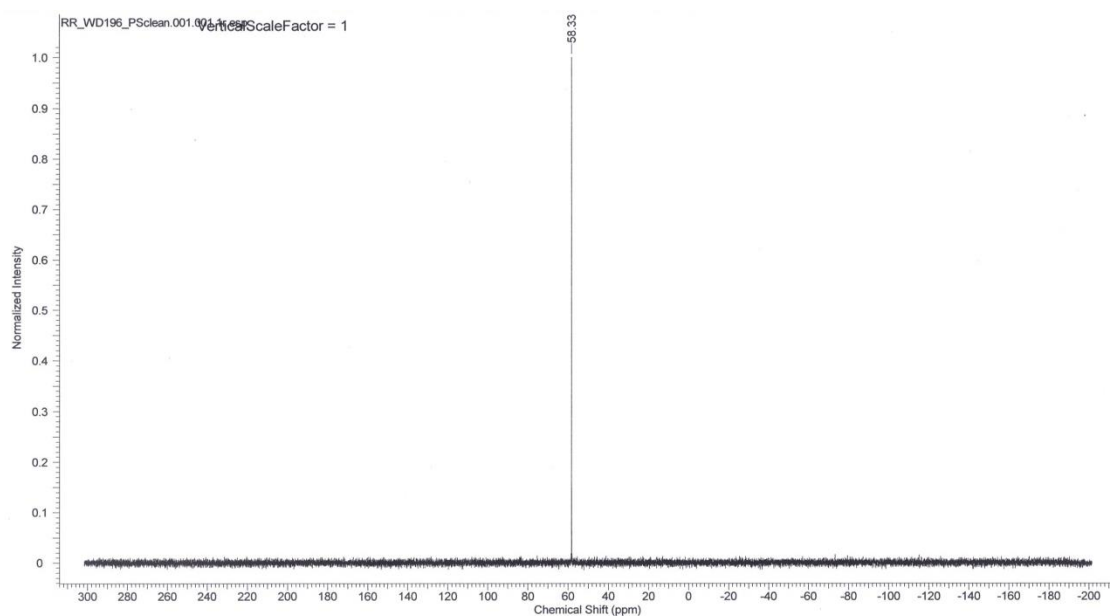
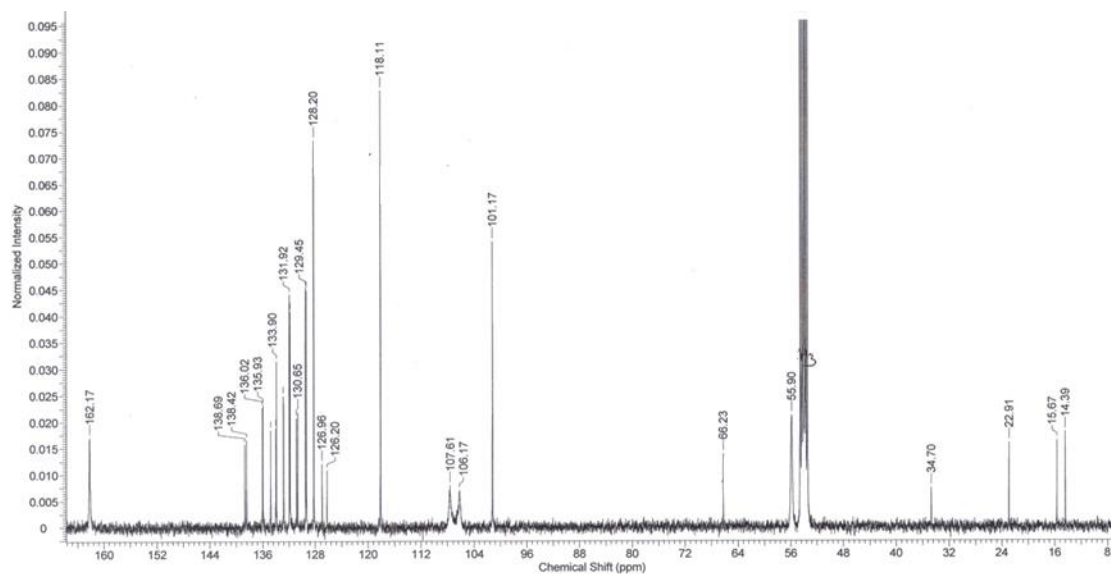


Figure S10: ^1H NMR (400 MHz, CD_2Cl_2), ^{31}C NMR and ^{31}P NMR spectra of **4**

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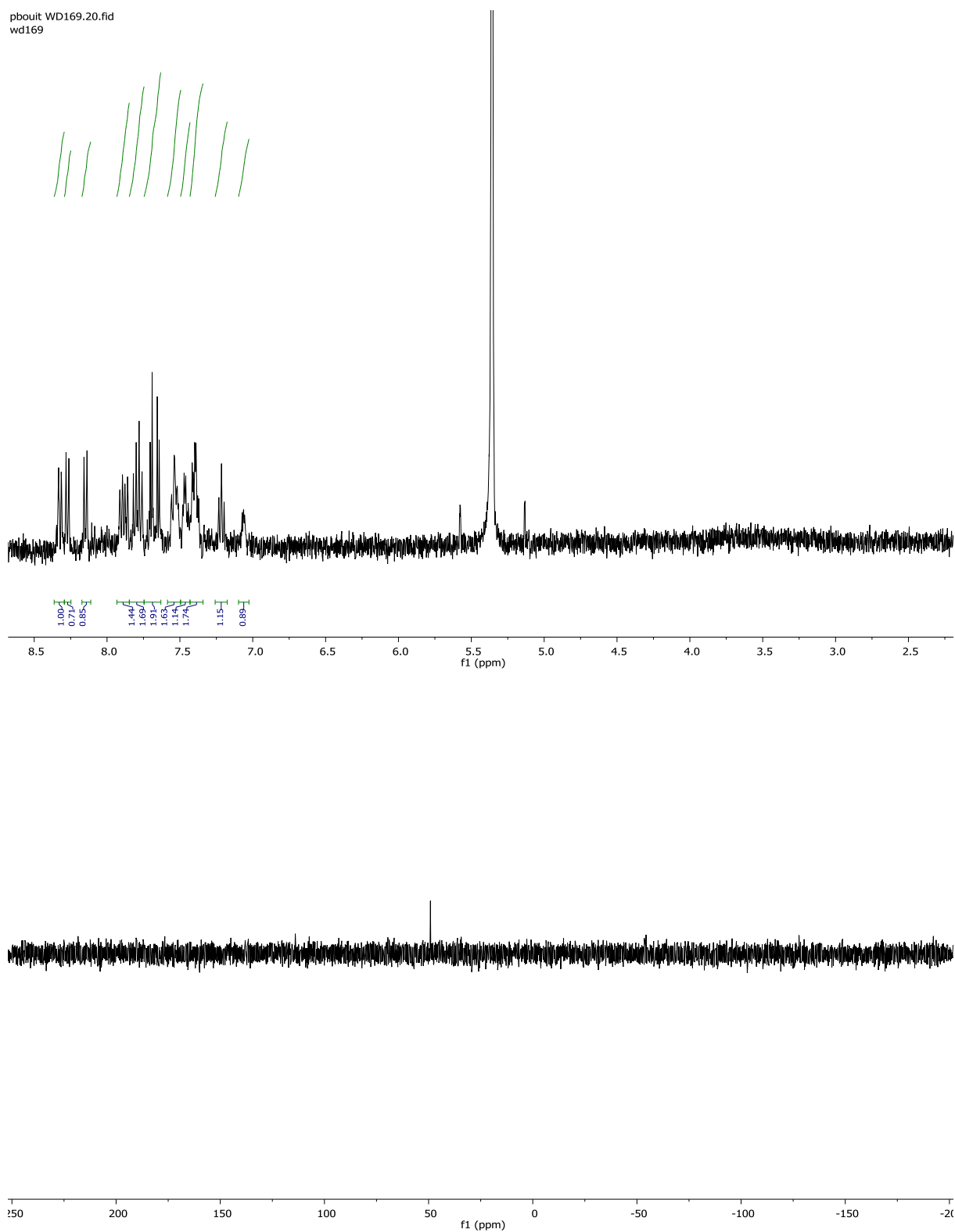
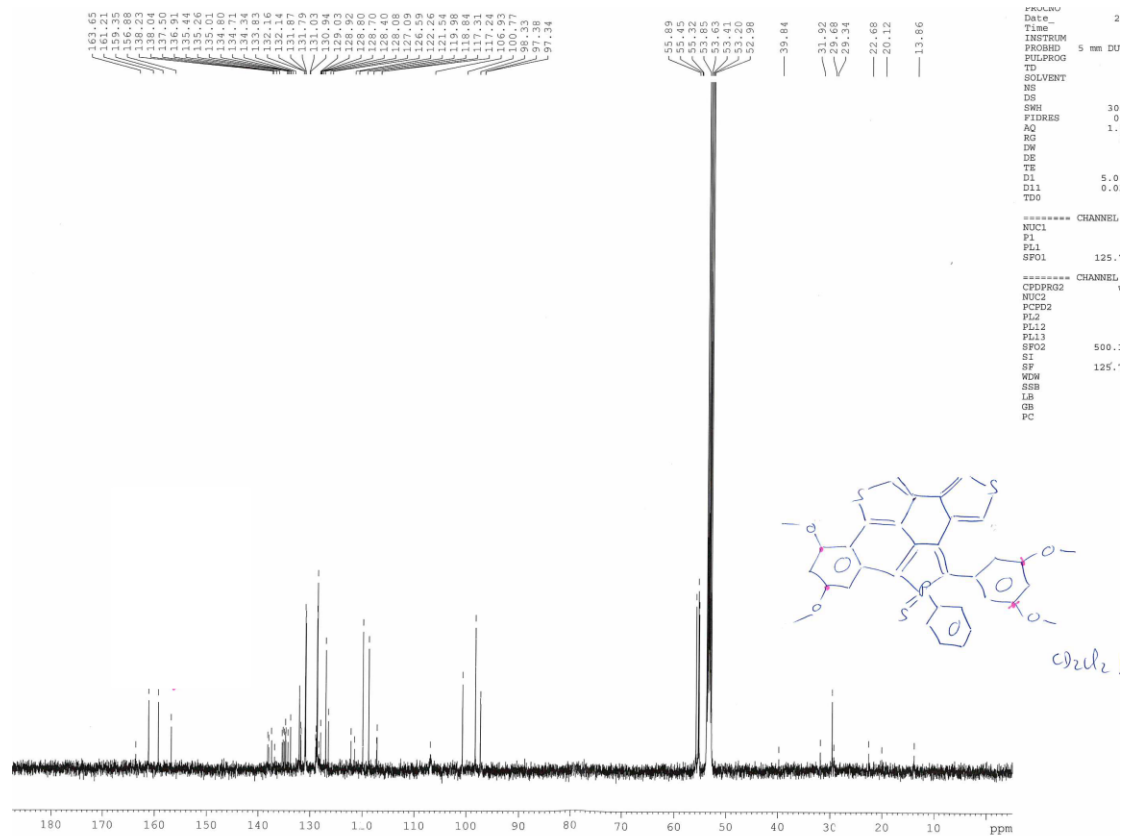
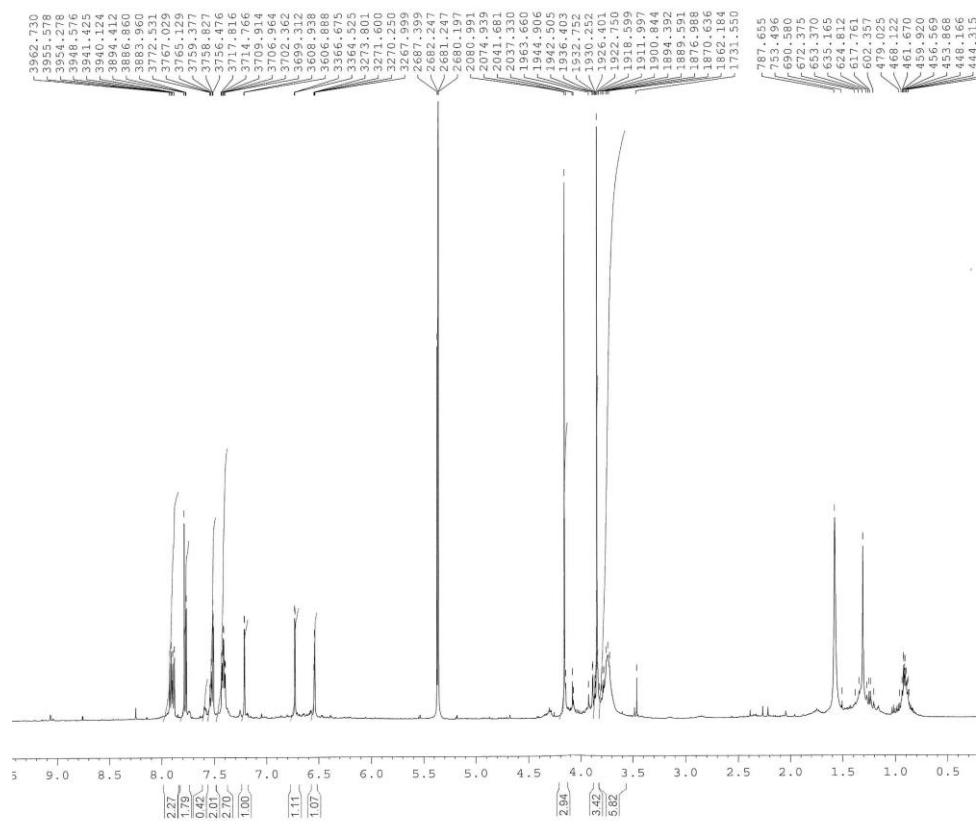


Figure S11: ^1H NMR (400 MHz, CD_2Cl_2) and ^{31}P NMR spectra of **5**



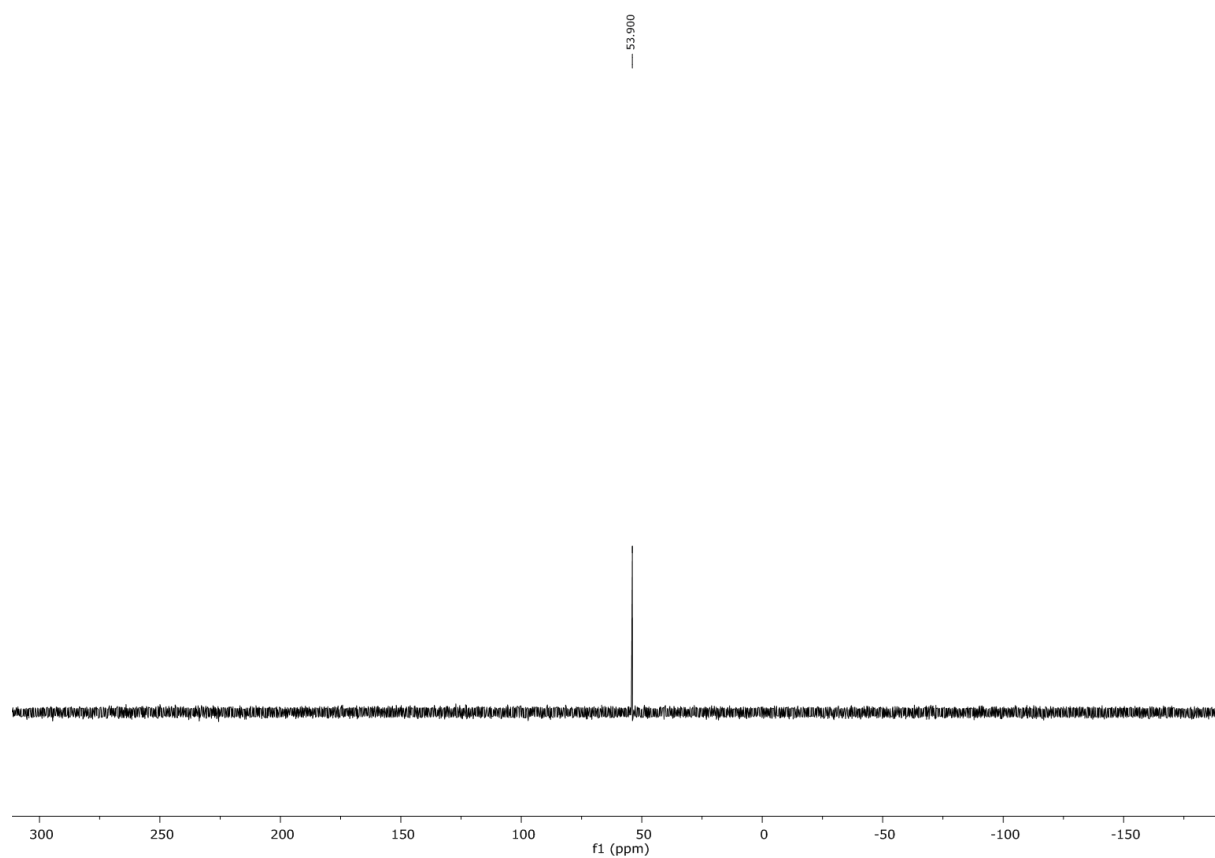


Figure S12: ^1H NMR (400 MHz, CD_2Cl_2) and ^{31}P NMR spectra of **6**