

# Hexahapto-Chromium Complexes of Graphene: A Theoretical Study

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### 1. Complete reference for Gaussian 09

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; and Fox, D. J. Gaussian 09, revision D.01; Gaussian, Inc.: Wallingford, CT, 2013.

## 2. Computational Methods.

All the DFT calculations were carried out with the GAUSSIAN 09 series of programs.<sup>1</sup> Density functional theory B3LYP<sup>2</sup> with a standard 6-31G(d) basis set (SDD basis set for Cr) was used for geometry optimizations. Harmonic frequency calculations were performed for all stationary points to confirm them as a local minima or transition structures and to derive the thermochemical corrections for the enthalpies and free energies. M11-L functional,<sup>3</sup> recently proposed by Truhlar group, is used to calculate the single point energies, which could give more accuracy energetic information.<sup>4</sup> The larger basis set 6-311+G(d) (SDD basis set for Cr) is used in the solvation single point calculations. The energies given in this paper are B3LYP and M11-L calculated Gibbs free energies.

## 3. B3LYP and M11-L absolute calculation energies, enthalpies, and free energies.

Geometry	$E_{(\text{elec-B3LYP})}$	$E_{(\text{elec-M11-L})}$	$H_{(\text{gas phase-M11-L})}$	$G_{(\text{gas phase-M11-L})}$	IF*
<b>1</b>	-232.2438	-232.2427	-232.1366	-232.1694	-
<b>2</b>	-921.8786	-921.9019	-921.6065	-921.6612	-
<b>3</b>	-2068.9051	-2068.9777	-2068.4130	-2068.4981	-
<b>4</b>	-3673.3270	-3673.4745	-3672.5612	-3672.6865	-
<b>5</b>	-5735.1460	-5735.3956	-5734.0538	-5734.2276	-
<b>6</b>	-659.2859	-659.4289	-659.2882	-659.3377	-
<b>7</b>	-1348.8836	-1349.0586	-1348.7396	-1348.8016	-
<b>8</b>	-2495.9158	-2496.1409	-2495.5414	-2495.6429	-
<b>9</b>	-4100.3321	-4100.6343	-4099.6843	-4099.8288	-
<b>10</b>	-6162.1537	-6162.5588	-6161.1800	-6161.3735	-

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<b>11</b>	-551.4860	-551.6380	-551.4224	-551.4690	-
<b>12</b>	-1241.0724	-1241.2638	-1240.8600	-1240.9286	-
<b>13</b>	-2388.1124	-2388.3522	-2387.6784	-2387.7782	-
<b>14</b>	-3992.5253	-3992.8425	-3991.8206	-3991.9607	-
<b>15</b>	-6054.3511	-6054.7674	-6053.3156	-6053.5034	-
<b>16-H</b>	-319.1331	-319.2832	-319.1766	-319.2123	-
<b>16-CH<sub>3</sub></b>	-437.0744	-437.2287	-437.0364	-437.0796	-
<b>16-NH<sub>2</sub></b>	-485.1680	-485.3419	-485.1827	-485.2283	-
<b>16-OMe</b>	-662.6782	-662.8161	-662.6042	-662.6617	-
<b>16-F</b>	-616.8198	-616.9746	-616.8900	-616.9324	-
<b>16-Cl</b>	-1697.9079	-1698.0783	-1697.9966	-1698.0430	-
<b>16-Br</b>	-8031.5453	-8039.9545	-8039.8734	-8039.9238	-
<b>16-CO<sub>2</sub>Me</b>	-1002.7700	-1002.9173	-1002.6670	-1002.7369	-
<b>16-CN</b>	-595.8557	-596.0174	-595.9092	-595.9587	-
<b>17-H</b>	-2388.1124	-2388.3510	-2387.6772	-2387.7770	-
<b>17-CH<sub>3</sub></b>	-2506.0623	-2506.3126	-2505.5514	-2505.6587	-
<b>17-NH<sub>2</sub></b>	-2554.1544	-2554.4229	-2553.6955	-2553.8053	-
<b>17-OMe</b>	-2731.6648	-2731.9045	-2731.1248	-2731.2418	-
<b>17-F</b>	-2685.8048	-2686.0445	-2685.3932	-2685.5001	-
<b>17-Cl</b>	-3766.8793	-3767.1471	-3766.4997	-3766.6051	-
<b>17-Br</b>	-10100.5146	-10109.0204	-10108.3738	-10108.4828	-
<b>17-CO<sub>2</sub>Me</b>	-3071.7421	-3071.9931	-3071.1762	-3071.3067	-

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<b>17-CN</b>	-2664.8321	-2665.0898	-2664.4160	-2664.5248	-
<b>18</b>	-4788.7351	-4789.0748	-4787.9614	-4788.1251	-
<b>18-c</b>	-5215.7375	-5216.2333	-5215.0840	-5215.2659	-
<b>18-d</b>	-5215.7406	-5216.2355	-5215.0866	-5215.2700	-
<b>18-e</b>	-5215.7423	-5216.2372	-5215.0879	-5215.2712	-
<b>18-f</b>	-5215.7433	-5216.2377	-5215.0890	-5215.2723	-
<b>19</b>	-4680.9298	-4681.2844	-4680.0982	-4680.2538	-
<b>19-c</b>	-5000.1230	-5000.6435	-4999.3468	-4999.5183	-
<b>19-d</b>	-5000.1331	-5000.6553	-4999.3610	-4999.5289	-
<b>19-e</b>	-5000.1351				-
<b>19-f</b>	-5000.1338	-5000.6578	-4999.3636	-4999.5314	-
<b>20</b>					-
<b>21</b>	-2954.4864	-2954.7333	-2954.0305	-2954.1475	-
<b>22-ts</b>	-2954.4680	-2954.7131	-2954.0108	-2954.1280	-66.64
<b>23</b>	-2954.4692	-2954.7143	-2954.0112	-2954.1302	-
<b>24-ts</b>	-2954.4680	-2954.7131	-2954.0108	-2954.1280	-66.64
<b>25</b>	-2954.4864	-2954.7333	-2954.0305	-2954.1475	-

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\* IF: The imaginary frequencies for the transition states.

#### 4. B3LYP geometries for all the optimized compounds and transition states.

<b>1</b>				C	1.61861500	3.38157700	-0.00001700
C	0.49813700	-1.30511000	-0.00010200	C	0.30413100	2.83357800	-0.00002600
C	1.37936900	-0.22139500	0.00001800	C	-2.11940600	3.09248400	0.00000700
C	-0.88138700	-1.08377100	0.00006900	C	-0.86413600	3.64803700	-0.00001500
C	0.88130100	1.08386900	0.00007700	H	3.72279500	3.01024000	0.00004000
H	2.45272600	-0.39331300	-0.00016700	H	1.73245600	4.46303200	-0.00003900
C	-1.37946200	0.22125100	-0.00001800	H	-0.74589900	4.72905600	-0.00004200
H	-1.56708000	-1.92726500	-0.00013400	H	-2.99908500	3.73179300	0.00002500
C	-0.49794500	1.30515600	-0.00008400				
H	1.56716000	1.92717700	0.00003700	<b>3</b>			
H	-2.45273000	0.39346200	0.00015100	C	-0.49019000	1.33248800	-0.00115200
H	-0.88545400	2.32076800	0.00004900	C	0.90890900	1.09079300	0.00108700
H	0.88530200	-2.32082600	0.00030800	C	-1.39917500	0.24172600	0.00109800
				C	1.39918700	-0.24173200	-0.00112400
<b>2</b>				C	-0.90887500	-1.09081200	-0.00107700
C	0.15235100	1.41956900	-0.00001400	C	0.49017200	-1.33248500	0.00108500
C	-1.15325600	0.84177100	-0.00000800	C	2.80765700	-0.48509900	0.00052600
C	1.30564100	0.57786000	-0.00000200	C	3.71618900	0.60715100	-0.00026800
C	-1.30564000	-0.57786400	-0.00001100	C	1.82407100	2.18877100	-0.00062200
C	1.15325100	-0.84176900	-0.00000600	C	3.22365700	1.94567300	0.00015500
C	-0.15234700	-1.41956600	0.00000300	C	-1.82405300	-2.18880500	0.00055800
C	-2.60605900	-1.15339500	-0.00001300	C	-3.22365000	-1.94571700	-0.00017600
C	-3.73793800	-0.28916400	0.00000400	C	-2.80764300	0.48509400	-0.00054300
C	-2.30200100	1.68010900	0.00001500	C	-3.71619600	-0.60718900	0.00023600
C	-3.59148100	1.07570000	0.00002400	C	3.29698200	-1.81882900	-0.00021200
H	-4.46846500	1.71870700	0.00005700	C	2.38385600	-2.91450300	0.00022300
H	-4.73139300	-0.73141000	-0.00000600	C	0.98374500	-2.67393600	-0.00052100
C	2.30201100	-1.68011500	-0.00001900	C	-1.33223800	-3.52170200	-0.00018800
C	3.59147400	-1.07570400	0.00000300	C	0.07324100	-3.76443200	0.00022000
C	2.60606500	1.15338800	0.00002200	C	-3.29696400	1.81881900	0.00022300
C	3.73793000	0.28917300	0.00003300	C	-2.38386400	2.91452300	-0.00022900
H	4.46846600	-1.71870400	-0.00000400	C	-0.98375600	2.67392400	0.00056100
H	4.73139600	0.73139300	0.00008500	C	1.33223600	3.52172400	0.00020100
C	-2.72738900	-2.57232100	-0.00000500	C	-0.07326200	3.76447400	-0.00023800
C	-1.61860900	-3.38157100	0.00001000	C	0.57228100	-5.10552000	0.00000300
C	-0.30413700	-2.83358900	0.00001500	C	-0.37682500	-6.18489200	-0.00005200
H	-3.72277900	-3.01026000	-0.00002400	C	-1.72058600	-5.95274900	0.00005100
H	-1.73248100	-4.46302100	0.00002900	C	-4.13569800	-3.04851300	-0.00001400
C	2.11940200	-3.09248100	-0.00002300	C	-5.54494800	-2.76613400	0.00003400
C	0.86413800	-3.64803500	0.00000100	C	-3.62929600	-4.35534400	0.00009800
H	0.74593100	-4.72906000	0.00000700	C	-5.12529600	-0.35815100	-0.00000700
H	2.99906100	-3.73181900	-0.00006000	C	-6.01574500	-1.48631500	-0.00007400
C	2.72738900	2.57233600	0.00001100	C	-2.25239300	-4.61739300	0.00000700

H	0.00237900	-7.20399500	0.00003100	C	-0.71122200	-1.23337600	0.00154300
H	-2.41967900	-6.78554700	-0.00004400	C	-1.42383700	-0.00084600	-0.00155100
H	-4.32551500	-5.19159100	-0.00004000	C	-1.42323600	2.46174100	-0.00111200
H	-6.23819100	-3.60386800	-0.00006000	C	-0.71088400	3.69497700	0.00061900
H	-7.08659200	-1.29748400	-0.00001200	C	1.42050100	2.46337300	0.00106700
C	5.12533200	0.35807900	-0.00000800	C	0.70679800	3.69570900	-0.00070200
C	6.01579200	1.48629300	0.00003900	C	-1.42050300	-2.46340000	-0.00102600
C	-0.57226900	5.10560900	0.00003500	C	-0.70681900	-3.69571900	0.00065000
C	0.37682300	6.18491800	0.00010500	C	1.42323400	-2.46171500	0.00111300
C	4.13570700	3.04851800	-0.00002200	C	0.71088300	-3.69493900	-0.00062200
C	5.54500800	2.76608500	-0.00007800	C	-2.84748200	2.45990500	0.00065700
C	3.62934700	4.35528300	-0.00012100	C	-3.55564700	1.23182000	-0.00067900
C	2.25236700	4.61741900	-0.00001300	C	-2.84380100	-0.00160200	0.00106600
C	1.72061600	5.95272000	-0.00002100	C	-2.84478700	-2.46308700	0.00064300
H	7.08663100	1.29741500	-0.00002900	C	-3.55430300	-1.23589100	-0.00064500
H	6.23825500	3.60381400	0.00001000	C	2.84748500	-2.45989500	-0.00067600
H	4.32555100	5.19153100	0.00002400	C	3.55565300	-1.23181300	0.00073000
H	2.41967100	6.78556400	0.00009900	C	2.84378500	0.00160500	-0.00112000
H	-0.00225200	7.20408900	0.00005200	C	2.84475300	2.46305300	-0.00069200
C	2.87277900	-4.25933400	0.00000600	C	3.55427800	1.23586100	0.00070200
C	1.95727600	-5.32048300	-0.00010600	C	-4.98233000	-1.23597400	0.00032500
C	4.29525700	-4.46627500	-0.00003100	C	-5.68913500	-2.46782300	0.00002500
C	5.58662900	-0.96535300	0.00013800	C	-4.97793200	-3.69799400	-0.00001800
C	4.70790800	-2.05709600	0.00003200	C	-1.42067400	-4.93239600	-0.00031600
C	5.16819200	-3.41876100	0.00009100	C	-0.70720600	-6.16035600	-0.00001500
H	2.33290000	-6.34169600	0.00000700	C	-2.84362200	-4.93106000	-0.00007600
H	4.66696900	-5.48810300	0.00005200	C	1.42603700	-4.93080500	0.00033300
H	6.24039100	-3.59981000	0.00002200	C	0.71394100	-6.15963600	0.00002000
H	6.65890400	-1.15064900	0.00005900	C	-3.55758200	-3.70035000	-0.00030300
C	-5.58659700	0.96535900	-0.00013200	C	-1.42602000	4.93083600	-0.00035100
C	-4.70792700	2.05704800	-0.00001600	C	-0.71391600	6.15963800	-0.00003700
C	-5.16822700	3.41876900	-0.00006000	C	4.98231300	1.23594500	-0.00034700
C	-1.95737600	5.32056000	0.00015600	C	5.68912400	2.46780100	0.00000300
C	-2.87279700	4.25942900	0.00003000	C	1.42065100	4.93237700	0.00030400
C	-4.29537300	4.46631400	0.00007200	C	0.70719600	6.16034600	-0.00002200
H	-2.33297000	6.34179300	0.00006100	C	2.84362200	4.93104600	0.00005000
H	-4.66710500	5.48815000	0.00000100	C	3.55755700	3.70033400	0.00032400
H	-6.24043400	3.59973100	0.00001400	C	4.97791100	3.69799300	0.00000400
H	-6.65888500	1.15059000	-0.00004100	C	-4.98367600	1.23051100	0.00031900
				C	-5.69268000	-0.00314000	0.00005000
4				C	-5.69183500	2.46154200	0.00002600
C	1.42384200	0.00085400	0.00159700	C	-2.84898200	4.92801200	-0.00005400
C	0.71123700	1.23335400	-0.00158200	C	-3.56159700	3.69637300	-0.00031500
C	0.71263100	-1.23258100	-0.00154200	C	-4.98193400	3.69257800	0.00000300
C	-0.71262500	1.23259400	0.00153900	C	2.84898100	-4.92801000	0.00004900

C	3.56158600	-3.69636200	0.00032900	H	3.36782400	8.32484900	0.00015500
C	4.98192900	-3.69255900	0.00000600	H	5.51876700	7.08477600	0.00019800
C	5.69269100	0.00314800	-0.00002800	C	7.13176000	4.90739400	0.00014000
C	4.98366300	-1.23051300	-0.00033300	C	7.81208300	3.73049100	-0.00005800
C	5.69182000	-2.46155200	-0.00000800	H	7.67071800	5.85171700	0.00017500
C	-3.56627200	6.16874100	-0.00019400	H	8.89936200	3.72621200	0.00000600
C	-4.98249100	6.13648900	-0.00027300	C	7.81621500	-3.72202100	-0.00008900
C	-2.83160300	7.37980700	-0.00031200	C	7.13704800	-4.89959100	0.00007600
C	-7.12595900	-0.00381800	0.00021600	H	8.90349900	-3.71629200	-0.00010000
C	-7.80749300	1.23788400	0.00032100	H	7.67698800	-5.84332000	0.00007500
C	-7.80613300	-1.24635200	0.00031400	C	0.68454500	-8.62940900	0.00009200
C	-3.55959600	-6.17264700	-0.00021500	C	-0.67491900	-8.63009500	-0.00011600
C	-4.97590000	-6.14188600	-0.00031100	H	1.23312400	-9.56818800	0.00006300
C	-2.82356200	-7.38280200	-0.00031000	H	-1.22227800	-9.56953400	-0.00011500
C	3.56626400	-6.16874300	0.00019600	C	-7.13181200	-4.90743000	-0.00011900
C	4.98252500	-6.13649600	0.00029300	C	-7.81212900	-3.73052800	0.00007500
C	2.83165200	-7.37977400	0.00030400	C	-7.81619500	3.72204000	0.00011700
C	7.12598200	0.00384400	-0.00019900	C	-7.13703300	4.89963000	-0.00004800
C	7.80752800	-1.23788500	-0.00030600	C	-0.68451100	8.62942600	-0.00011700
C	7.80611000	1.24631700	-0.00029200	C	0.67493600	8.63011900	0.00008500
C	3.55961300	6.17261400	0.00019600	H	-8.89939500	-3.72624000	0.00003500
C	4.97589000	6.14191200	0.00029800	H	-7.67076800	-5.85178900	-0.00016000
C	2.82357000	7.38280100	0.00028800	H	-8.90347500	3.71630800	0.00013300
C	-1.44140700	7.40050100	-0.00010200	H	-7.67694900	5.84337700	-0.00005000
C	-5.69424300	4.94221900	-0.00008300	H	1.22228900	9.56955900	0.00007600
H	-3.37693700	8.32126400	-0.00020800	H	-1.23308200	9.56820100	-0.00010200
H	-5.52638600	7.07876400	-0.00020400				
C	-7.13035800	2.45211300	0.00012500	<b>5</b>			
C	-7.12767800	-2.45978000	0.00010700	C	8.02639900	-7.69800900	-0.00115100
H	-8.89544500	1.23624500	0.00028900	C	6.59659500	-7.48203700	-0.00093100
H	-8.89410500	-1.24628300	0.00023400	C	6.12045200	-6.11916600	-0.00062400
C	-5.68896700	-4.94848400	-0.00011000	C	7.03581700	-5.04017400	-0.00012500
C	-1.43330700	-7.40206000	-0.00009200	C	8.45818700	-5.28749300	-0.00017600
H	-5.51873600	-7.08474700	-0.00024500	C	8.90454000	-6.66279500	-0.00066800
H	-3.36778100	-8.32489000	-0.00019700	C	4.71940600	-5.86962700	-0.00078700
C	1.44142000	-7.40046900	0.00008700	C	6.56104200	-3.69870400	0.00019600
C	5.69425100	-4.94224500	0.00010500	C	5.15750600	-3.44465200	-0.00069000
H	3.37695100	-8.32122700	0.00018800	C	4.23973800	-4.52641900	0.00023300
H	5.52638900	-7.07879900	0.00024900	C	4.67865500	-2.10152300	0.00142700
C	7.13040000	-2.45207600	-0.00011600	C	5.59701800	-1.01788900	-0.00043600
C	7.12763900	2.45976700	-0.00007200	C	7.00395300	-1.27375000	0.00075400
H	8.89547900	-1.23620100	-0.00026000	C	7.47994200	-2.61222400	0.00041100
H	8.89405400	1.24626700	-0.00016200	C	8.89453000	-2.86721100	0.00060000
C	1.43334400	7.40207800	0.00005900	C	9.33983700	-4.22053200	0.00041900
C	5.68894600	4.94846600	0.00010200	H	10.41044500	-4.41391000	0.00055100



H	8.38739400	-8.72359200	-0.00171500	C	-4.71937600	5.86969000	0.00024700
H	9.97526100	-6.85159000	-0.00102200	C	-3.79720400	6.95329700	0.00027300
C	5.68758100	-8.52579800	-0.00135900	C	-0.51920800	5.10234500	0.00169300
C	4.27963400	-8.30721100	-0.00108600	C	-5.11909900	-0.31970400	-0.00152000
C	3.79720200	-6.95326600	-0.00094700	C	-7.03584000	5.04016000	-0.00046500
H	6.05301200	-9.55052200	-0.00118100	C	-6.12044500	6.11918800	-0.00008700
C	2.39891900	-6.70198100	-0.00100000	C	-6.59660200	7.48199600	-0.00005200
C	1.91690400	-5.35570500	0.00046700	C	-5.68747100	8.52583500	0.00039300
C	2.83641800	-4.27307200	-0.00160500	C	-8.02626000	7.69795100	-0.00016900
C	3.27887000	-1.84754100	-0.00202800	C	-8.45814700	5.28749400	-0.00061600
C	2.35751100	-2.93351600	0.00222600	C	-9.33984800	4.22039900	-0.00106000
C	0.95899100	-2.67940800	-0.00279200	C	-8.90446500	6.66265700	-0.00057800
C	0.47886500	-1.33803200	0.00380400	C	-4.27967300	8.30726300	0.00034300
C	0.03923800	-3.76315600	0.00233400	C	-8.89458300	2.86723500	-0.00089200
C	-0.91943000	-1.08374100	-0.00335600	C	9.78328000	-1.77916400	0.00110500
C	-1.36196400	-3.50833500	-0.00219700	C	7.92083100	-0.18846300	0.00072500
C	-1.84116600	-2.17016400	0.00316100	C	6.04021300	1.40825300	-0.00010700
C	2.80008900	-0.50924100	0.00318300	C	4.15952900	3.00080500	-0.00100700
C	1.39832200	-0.25430700	-0.00316600	C	2.28274300	4.59279500	-0.00120300
C	3.71951600	0.57479400	-0.00176200	C	0.40469400	6.18850800	-0.00053100
C	0.91941100	1.08375700	0.00394400	C	-1.47752800	7.78341800	0.00032700
C	3.23959800	1.91563300	0.00264100	C	-3.35083100	9.36143700	0.00064200
C	1.84115100	2.17017700	-0.00250100	C	3.35092600	-9.36136800	-0.00126600
C	0.51920400	-5.10232900	-0.00154600	C	1.47754600	-7.78341000	-0.00074500
C	5.11908600	0.31970500	0.00174200	C	-0.40469900	-6.18849900	0.00055200
C	-1.39834400	0.25431500	0.00385800	C	-2.28273800	-4.59278500	0.00163300
C	-2.80010700	0.50924100	-0.00286800	C	-4.15953500	-3.00080900	0.00165000
C	-0.47887800	1.33805100	-0.00328100	C	-6.04022000	-1.40824800	0.00064000
C	-3.27888900	1.84755800	0.00243200	C	-7.92083400	0.18844300	-0.00057000
C	-0.95899700	2.67942700	0.00327300	C	-9.78332600	1.77905200	-0.00117700
C	-2.35753100	2.93353100	-0.00221400	C	9.33462100	-0.44770100	0.00084700
C	-3.23960200	-1.91561800	-0.00219600	C	7.44335900	1.15191100	0.00073000
C	-3.71951800	-0.57478500	0.00242900	C	5.56216000	2.74386400	0.00092300
C	1.36195000	3.50833900	0.00264600	C	3.68014000	4.33789900	0.00102400
C	-0.03924800	3.76315800	-0.00205500	C	1.80046100	5.93470100	0.00076700
C	-4.67867400	2.10153300	-0.00158500	C	-0.07715200	7.53098100	0.00037200
C	-5.15750900	3.44465000	0.00050800	C	-1.96402900	9.13593800	0.00037200
C	-5.59705100	1.01787600	0.00069400	C	1.96400800	-9.13588200	-0.00091500
C	-6.56109700	3.69865800	-0.00064400	C	0.07715600	-7.53097600	-0.00052700
C	-7.00398800	1.27369300	-0.00083200	C	-1.80044700	-5.93469000	-0.00055000
C	-7.47997200	2.61221600	-0.00067900	C	-3.68014700	-4.33788900	-0.00060400
C	-2.83643300	4.27309000	0.00158800	C	-5.56216600	-2.74387700	-0.00050100
C	-1.91690000	5.35574100	-0.00073000	C	-7.44336200	-1.15191500	-0.00042900
C	-4.23974000	4.52642100	-0.00072100	C	-9.33467400	0.44771100	-0.00075800
C	-2.39887200	6.70202700	0.00060800	H	10.85359300	-1.97354500	0.00090200

H	3.71724800	-10.38564800	-0.00124300	C	-10.22278800	-4.37936300	0.00048000
C	1.01465600	-10.19803400	-0.00090200	C	10.22277500	4.37934300	-0.00002700
C	-0.84737000	-8.61278600	-0.00020600	C	8.32526400	5.97767800	-0.00060000
C	-2.72409400	-7.02162900	0.00055200	C	6.43250000	7.58249100	-0.00095100
C	-4.60524200	-5.42834500	0.00088600	C	4.54041800	9.18811900	-0.00089100
C	-6.48402500	-3.83231900	0.00058600	C	2.65398100	10.79945100	-0.00050600
C	-8.36005500	-2.24042600	-0.00012100	H	11.74906300	2.90134400	0.00042100
C	-10.22791100	-0.66209100	-0.00077700	H	10.92209000	5.21190200	-0.00016400
C	10.22787600	0.66203100	0.00097200	H	9.02841700	6.80786000	-0.00064100
C	8.36005800	2.24039400	0.00054000	H	7.13621600	8.41205000	-0.00092700
C	6.48403400	3.83231600	-0.00005200	H	5.24482700	10.01723700	-0.00090100
C	4.60524000	5.42835000	-0.00044200	H	3.36142700	11.62515800	-0.00060700
C	2.72410100	7.02162200	-0.00037200	H	-10.92209500	-5.21192800	0.00063700
C	0.84740400	8.61279100	0.00004300	H	-9.02842500	-6.80786600	0.00112200
C	-1.01460500	10.19808300	0.00042500	H	-7.13621200	-8.41205100	0.00130200
C	9.77836000	1.97119700	0.00055900	H	-5.24482200	-10.01722700	0.00109700
C	7.88319300	3.57262500	0.00010000	H	-3.36140100	-11.62514700	0.00058700
C	6.00246400	5.17124500	-0.00024700	H	-0.94680600	-12.06409500	-0.00019500
C	4.12366400	6.76490900	-0.00038000	H	0.94683600	12.06412100	-0.00011300
C	2.23959800	8.35967100	-0.00027900	H	-1.38190100	11.22214000	0.00032400
C	0.35039500	9.96814300	0.00001600	H	-3.71724400	10.38569300	0.00049300
C	-0.35038500	-9.96811400	-0.00034300	H	-6.05310800	9.55049300	0.00032500
C	-2.23960800	-8.35966200	0.00028200	H	-8.38747500	8.72349500	-0.00010700
C	-4.12366200	-6.76491100	0.00067500	H	-9.97518300	6.85167100	-0.00065400
C	-6.00245900	-5.17124300	0.00070300	H	-10.41042500	4.41398300	-0.00102900
C	-7.88320200	-3.57261400	0.00035800	H	-10.85363000	1.97352400	-0.00108400
C	-9.77838400	-1.97121100	-0.00021900	H	-11.29816700	-0.46670100	-0.00073400
H	11.29812900	0.46663900	0.00084400	H	-11.74908100	-2.90137600	-0.00008900
H	1.38195300	-11.22208700	-0.00087800				
C	-1.31825000	-11.04221700	-0.00014100	<b>6</b>			
C	-3.18183100	-9.45338500	0.00048500	C	-1.64672700	0.18923600	-1.40522200
C	-5.05510100	-7.85969000	0.00092900	C	-1.62758200	-1.11552000	-0.85947300
C	-6.93067100	-6.26878300	0.00095100	C	-1.62823900	1.30250000	-0.53274300
C	-8.80862800	-4.68061300	0.00055000	C	-1.64440500	-1.31481400	0.54070200
C	-10.68029400	-3.10122300	-0.00002700	H	-1.58759200	-1.97333200	-1.52265100
C	10.68027600	3.10119100	0.00040100	C	-1.64418000	1.12253800	0.87020100
C	8.80862400	4.68059200	-0.00007500	H	-1.58827200	2.30563100	-0.94423800
C	6.93068000	6.26876200	-0.00050600	C	-1.62533500	-0.18968400	1.39772300
C	5.05512500	7.85968700	-0.00065800	H	-1.61814800	-2.31723200	0.95179100
C	3.18185400	9.45339400	-0.00047400	H	-1.61784100	1.97976100	1.53280800
C	1.31828000	11.04224200	-0.00012600	H	-1.58351100	-0.33525400	2.47209800
C	-2.65396200	-10.79943400	0.00039300	H	-1.62244900	0.33444000	-2.47896200
C	-4.54042000	-9.18810300	0.00104000	Cr	0.11837000	-0.00020600	0.00010100
C	-6.43251200	-7.58248000	0.00132100	C	1.19191900	-1.19091200	-0.92254900
C	-8.32527800	-5.97767700	0.00108300	C	1.18920500	1.39501300	-0.57168300

C	1.19505400	-0.20201300	1.49019200	H	3.88188300	-2.81095500	-0.88908700
O	1.84821000	-0.33076100	2.44138800	H	1.97499100	-4.36860500	-0.88300800
O	1.83723700	2.28649800	-0.93688000	H	-0.49588500	-4.76854900	-0.88044900
O	1.84188600	-1.95162800	-1.51152700	H	-2.79354900	-3.89371100	-0.88605300
<b>7</b>				<b>8</b>			
C	0.23154300	-1.41799800	-0.83128600	C	-0.86880200	1.13696000	-0.40430900
C	-1.11110400	-0.90553500	-0.82164200	C	0.54699700	1.31650900	-0.38372500
C	1.34033400	-0.51086500	-0.82098300	C	-1.41434800	-0.18400600	-0.38275200
C	-1.34231900	0.50815200	-0.83267100	C	1.41810400	0.18359900	-0.40621800
C	1.11287000	0.90794600	-0.83114000	C	-0.55097200	-1.32023100	-0.40555900
C	-0.22719500	1.41466200	-0.82228700	C	0.86575900	-1.13237800	-0.38429700
Cr	-0.00080500	0.00051700	1.11102000	Cr	0.00139600	-0.00054800	1.48610500
C	-0.90565600	-1.18209600	2.17029200	C	2.84090000	0.36844900	-0.42323000
C	1.47595400	-0.18882800	2.17118900	C	3.37664500	1.67951900	-0.45004100
C	-0.57514100	1.37582900	2.16836900	C	1.10001800	2.64439400	-0.42709600
O	-0.94492400	2.26227200	2.82790200	C	2.50526800	2.81643500	-0.44811500
O	2.42698500	-0.31182600	2.83295700	C	-1.10224800	-2.64482900	-0.42245200
O	-1.48959700	-1.94373400	2.83089900	C	-2.50750100	-2.81811000	-0.44869400
C	-2.67831700	1.01531800	-0.84980500	C	-2.84087700	-0.36886000	-0.42579700
C	-3.75277900	0.09019900	-0.86971000	C	-3.37587500	-1.67932400	-0.44678000
C	-2.22065700	-1.80996400	-0.85249000	C	3.69371300	-0.76170700	-0.45002000
C	-3.53072800	-1.27072500	-0.87196800	C	3.14159600	-2.08327000	-0.44832800
H	-4.37402700	-1.95626100	-0.88914100	C	1.73922100	-2.27513200	-0.42794500
H	-4.76947500	0.47370900	-0.88536800	C	-0.23474200	-3.76418300	-0.44961500
C	2.22001200	1.81132500	-0.84682100	C	1.18567300	-3.57818300	-0.44821900
C	3.53475400	1.26836700	-0.86736000	C	-3.69261100	0.76190500	-0.44684900
C	2.67838800	-1.01956400	-0.85211600	C	-3.14360300	2.08508700	-0.44867300
C	3.75303100	-0.08953300	-0.87104300	C	-1.74036500	2.27655100	-0.42131700
H	4.37838800	1.95326400	-0.88097300	C	0.23262200	3.76278800	-0.44716600
H	4.76954800	-0.47392700	-0.88661300	C	-1.18791100	3.58026500	-0.44861600
C	-2.86544500	2.42527300	-0.87130200	C	2.05713000	-4.71089100	-0.47940700
C	-1.79849800	3.29325900	-0.87438800	C	1.46862500	-6.02329600	-0.50034600
C	-0.45569400	2.82763200	-0.85414200	C	0.11714400	-6.19948800	-0.49832500
H	-3.88046200	2.81319500	-0.88549700	C	-3.05258100	-4.13938000	-0.47639100
H	-1.97384300	4.36577400	-0.89042500	C	-4.48395200	-4.28449300	-0.49819300
C	1.95601200	3.20431100	-0.86749200	C	-2.18183300	-5.23798900	-0.48625100
C	0.66636900	3.69252200	-0.87209900	C	-4.79424600	-1.85882000	-0.47874900
H	0.49436800	4.76560000	-0.89004600	C	-5.31094300	-3.20133300	-0.50025500
H	2.79654800	3.89297500	-0.88242900	C	-0.78806900	-5.08151600	-0.47675000
C	2.86648800	-2.42363500	-0.87134800	H	2.13237300	-6.88410700	-0.51771100
C	1.79883200	-3.29636300	-0.86763900	H	-0.30363800	-7.20171100	-0.51519000
C	0.46040600	-2.82839700	-0.84702400	H	-2.59968500	-6.24214600	-0.50667800
C	-1.95240200	-3.20556900	-0.87080300	H	-4.89882400	-5.28918700	-0.51556800
C	-0.66720500	-3.69548900	-0.86720000	H	-6.38943800	-3.33682500	-0.51825600

C	4.79412500	1.85890000	-0.47747500	C	-0.24530300	1.41035700	-0.21788600
C	5.30981700	3.20179400	-0.49908900	C	1.34396700	-0.49214500	-0.21868700
C	-2.05963500	4.71279400	-0.47659800	C	1.10013400	0.91380400	-0.19980700
C	-1.46969400	6.02497800	-0.49833200	Cr	-0.00041100	-0.00170400	1.70838900
C	3.05062700	4.13755700	-0.47942800	C	-1.48907900	-0.10221900	2.76884800
C	4.48147200	4.28404800	-0.50090100	C	0.82859600	-1.24344100	2.76726100
C	2.17910600	5.23574500	-0.49056000	C	0.65835100	1.33602500	2.77044900
C	0.78628600	5.08095900	-0.47875000	O	1.08178700	2.19777100	3.42915800
C	-0.11811500	6.19958900	-0.50005200	O	1.36266100	-2.04317500	3.42380900
H	6.38815500	3.33850900	-0.51613800	O	-2.44743500	-0.16769700	3.42701100
H	4.89520900	5.28921900	-0.51848900	C	-0.48756500	2.81669700	-0.22894100
H	2.59751500	6.23980200	-0.51084000	C	-1.82061700	3.29863000	-0.25518300
H	0.30377900	7.20134900	-0.51782500	C	-2.68137400	0.98923800	-0.23803100
H	-2.13248100	6.88651800	-0.51561800	C	-2.91415400	2.38730500	-0.25089200
C	4.00634600	-3.22170100	-0.47938600	C	2.68292200	-0.98558100	-0.22994200
C	3.44402100	-4.50536200	-0.49078300	C	2.91458500	-2.38753800	-0.25784100
C	5.42736700	-2.99790200	-0.50010800	C	0.48441400	-2.81637100	-0.23928400
C	5.62660900	0.73026700	-0.48701300	C	1.82098600	-3.29774500	-0.25381400
C	5.11050100	-0.57316700	-0.47722400	C	0.61075400	3.71825100	-0.25593400
C	5.95193200	-1.74005800	-0.49829800	C	1.94583800	3.22635800	-0.25097300
H	4.10435500	-5.36976300	-0.51038800	C	2.19725800	1.82809000	-0.23679900
H	6.08387600	-3.86423100	-0.51699200	C	3.76683800	-0.07205900	-0.25447200
H	7.02941900	-1.59674100	-0.51479400	C	3.52434500	1.33067200	-0.24952300
H	6.70513200	0.87072200	-0.50701700	C	-0.60995900	-3.71690300	-0.25153400
C	-5.62477000	-0.73015900	-0.49091200	C	-1.94595700	-3.22555700	-0.25517300
C	-5.10939100	0.57370900	-0.47929700	C	-2.19516200	-1.83006900	-0.22992600
C	-5.95172200	1.73943100	-0.50159300	C	-3.76660800	0.07247300	-0.25187300
C	-3.44647400	4.50811100	-0.48683300	C	-3.52508600	-1.32975700	-0.25630400
C	-4.00777600	3.22279400	-0.47707800	C	4.62160500	2.24405800	-0.27595900
C	-5.42859700	2.99796700	-0.49963500	C	5.95296500	1.74884200	-0.29087200
H	-4.10718100	5.37205100	-0.50760300	C	6.19493500	0.34744300	-0.29096600
H	-6.08603100	3.86355500	-0.51736800	C	4.25271100	-2.88002300	-0.27700600
H	-7.02902700	1.59489300	-0.51993000	C	4.49005400	-4.28130700	-0.29556900
H	-6.70346800	-0.87006400	-0.51173800	C	5.34459900	-1.96712600	-0.28482200
C	0.66805300	1.33203400	2.55528200	C	2.06350300	-4.70308200	-0.28064500
C	0.82534900	-1.24221700	2.55483300	C	3.39872900	-5.18990900	-0.29644000
C	-1.48428400	-0.09145300	2.55776400	C	5.10643100	-0.56516800	-0.27419800
O	1.35310700	-2.03694700	3.22108500	C	-2.06338000	4.70534400	-0.27524000
O	1.09527800	2.18494300	3.22149900	C	-3.39797900	5.19162700	-0.29333300
O	-2.43564400	-0.14935700	3.22532800	C	-4.62072600	-2.24233600	-0.27418000
<b>9</b>				C	-5.95291200	-1.74724100	-0.29119100
C	-1.09830600	-0.91717500	-0.21890000	C	-4.25380200	2.88079000	-0.27804800
C	-1.34102200	0.49624700	-0.20039100	C	-4.49063900	4.28143000	-0.29355700
C	0.24117500	-1.40904500	-0.20114500	C	-5.34401000	1.96799300	-0.28533600
				C	-5.10488500	0.56509000	-0.27796900

C	-6.19417200	-0.34779500	-0.29227000	H	2.73706700	-8.55503900	-0.33490300
C	3.04165300	4.13896900	-0.27725900	H	0.28932700	-8.97723200	-0.33254000
C	4.37613100	3.64461900	-0.28374000	C	-3.90667400	-6.45090600	-0.30788500
C	2.79563700	5.53876800	-0.29302500	C	-7.05221400	-2.67494300	-0.30788000
C	-0.96833100	5.61251700	-0.28491500	H	-6.04164100	-6.64678000	-0.32404500
C	0.36819700	5.12341300	-0.27547900	H	-7.63140600	-4.73810600	-0.32395400
C	1.46309400	6.02953100	-0.29323500	C	-5.84232300	4.76954000	-0.31290400
C	0.96810700	-5.61155500	-0.28720600	C	-7.54074800	0.15800800	-0.31071400
C	-0.36750500	-5.12387400	-0.27848700	H	-7.91941900	4.23857600	-0.33195700
C	-1.46210100	-6.02922600	-0.29253300	H	-8.77762000	1.90783600	-0.33026900
C	-4.37603000	-3.64440100	-0.28243500	C	-8.62247800	-0.79732400	-0.32374400
C	-3.04285000	-4.13909400	-0.27371100	C	-8.39144700	-2.13707200	-0.32202600
C	-2.79669200	-5.53808900	-0.29097500	H	-9.64097800	-0.41715200	-0.33456400
C	-1.21200300	7.02543200	-0.30546300	H	-9.22378300	-2.83644700	-0.33202800
C	-0.10234300	7.90671500	-0.31638400	C	-3.62018600	-7.86501700	-0.32249300
C	-2.55092300	7.48417400	-0.31646300	C	-2.34401300	-8.33479800	-0.32464600
C	5.47789500	4.56221100	-0.30475400	H	-4.45842400	-8.55731100	-0.33265600
C	5.20457000	5.95254500	-0.31675800	H	-2.15470800	-9.40534900	-0.33599700
C	6.79455200	4.04329800	-0.31543400	C	5.00226500	-7.06804500	-0.33077100
C	6.69002300	-2.46250000	-0.30487600	C	6.04699100	-6.19809200	-0.32952200
C	7.75679600	-1.53239700	-0.31436700	H	5.18241400	-8.14014400	-0.34254900
C	6.89846300	-3.86411500	-0.31683800	H	7.06882500	-6.56927000	-0.34083700
C	1.21192800	-7.02453600	-0.30860000	C	8.62183500	0.79776000	-0.32330800
C	0.10414700	-7.90531500	-0.31873200	C	8.39055800	2.13786900	-0.32376300
C	2.55263000	-7.48299300	-0.32107400	C	3.62049700	7.86648400	-0.32699800
C	-5.47783300	-4.56183900	-0.30094600	C	2.34475600	8.33629000	-0.32674200
C	-5.20565600	-5.95077900	-0.31099400	C	-5.00150400	7.06816500	-0.32734100
C	-6.79587800	-4.04154500	-0.31102100	C	-6.04642000	6.19782200	-0.32795900
C	-6.68956300	2.46326500	-0.30641300	H	9.22292900	2.83719500	-0.33477500
C	-7.75698700	1.53147800	-0.31698300	H	9.64046100	0.41792600	-0.33446000
C	-6.89850600	3.86299200	-0.31821600	H	4.45895400	8.55848700	-0.33832000
C	-3.63357900	6.60931300	-0.31219400	H	2.15537300	9.40682000	-0.33837800
C	1.20929200	7.44541300	-0.31198400	H	-7.06823200	6.56906300	-0.33958300
H	-2.73558200	8.55615600	-0.33100900	H	-5.18200600	8.14020900	-0.33903100
H	-0.28767700	8.97858700	-0.33088100				
C	3.90700500	6.45199100	-0.31189600	<b>10</b>			
C	7.05161300	2.67530300	-0.30955500	C	7.83058400	-7.89860500	-0.25114300
H	6.04070700	6.64837500	-0.33036300	C	7.59144100	-6.47269000	-0.23585800
H	7.63017600	4.73974400	-0.32904700	C	6.22096600	-6.01916000	-0.21686800
C	7.54044400	-0.15736200	-0.30930800	C	5.15660700	-6.95245600	-0.21632500
C	5.84313100	-4.76934700	-0.31387800	C	5.42735400	-8.37031900	-0.23413700
H	8.77748700	-1.90852900	-0.32847000	C	6.80986300	-8.79365700	-0.25051200
H	7.91941900	-4.23954500	-0.33086600	C	5.94861900	-4.62305200	-0.20017300
C	3.63399100	-6.60901500	-0.31585500	C	3.80786400	-6.50017600	-0.19913500
C	-1.20905800	-7.44394200	-0.31163100	C	3.53159800	-5.10167000	-0.17823300

C	4.59796400	-4.16672400	-0.18032600	C	-1.11128600	5.58169700	-0.16612700
C	2.17939100	-4.64595900	-0.16174600	C	-3.80842000	6.50086100	-0.19419600
C	1.10990100	-5.58190500	-0.16621400	C	-1.39012100	6.98444900	-0.18507400
C	1.38928700	-6.98466500	-0.18951700	C	-2.73612900	7.43747900	-0.19768900
C	2.73565400	-7.43723900	-0.20274000	C	-4.32394000	2.76754800	-0.16175300
C	3.01413700	-8.84646400	-0.22219300	C	-5.38933500	1.82974500	-0.16890600
C	4.37472500	-9.26923500	-0.23649700	C	-4.59885800	4.16723800	-0.17636500
H	4.58614900	-10.33631900	-0.24992300	C	-6.74397100	2.28920600	-0.19345600
H	8.86178700	-8.24290600	-0.26376600	C	-5.94898900	4.62351300	-0.19840800
H	7.01691300	-9.86095400	-0.26240200	C	-7.01749000	3.68264900	-0.20499200
C	8.62020900	-5.54653400	-0.23932600	C	-5.11337500	0.43569500	-0.16244800
C	8.37871500	-4.14238400	-0.22627900	C	0.23504300	5.12617700	-0.15437000
C	7.01774900	-3.68244100	-0.20557400	C	-5.15781100	6.95308400	-0.21153800
H	9.65056500	-5.89528800	-0.25388100	C	-6.22137700	6.02025000	-0.21367400
C	6.74458700	-2.28862200	-0.19237000	C	-7.59239500	6.47345500	-0.23262500
C	5.39023700	-1.82870200	-0.17121700	C	-8.62062900	5.54728000	-0.23800200
C	4.32252700	-2.76681700	-0.15948400	C	-7.83153200	7.89949900	-0.24672600
C	1.90192200	-3.25301500	-0.13228300	C	-5.42820100	8.37139900	-0.22841800
C	2.97761600	-2.31020000	-0.13924300	C	-4.37572400	9.26995000	-0.22946300
C	2.71025700	-0.91828600	-0.11009000	C	-6.81088600	8.79458600	-0.24458300
C	1.35480700	-0.45718600	-0.09691700	C	-8.37905400	4.14255900	-0.22581900
C	3.76923100	0.02096600	-0.13750700	C	-3.01443300	8.84727000	-0.21617100
C	1.07554700	0.93950000	-0.07904500	Cr	-0.00047200	0.00089100	1.80045600
C	3.48986000	1.42270000	-0.13016500	C	0.62533200	1.35772300	2.86366400
C	2.15218700	1.88500800	-0.11733900	C	-1.48903900	-0.13363900	2.86279200
C	0.55683800	-2.80618900	-0.11736700	C	0.86084900	-1.21926800	2.86415300
C	0.27631500	-1.40111100	-0.07837100	O	1.02701700	2.23104900	3.51937000
C	-0.51244400	-3.73345100	-0.12937200	O	1.41518400	-2.00423800	3.52030400
C	-1.07307500	-0.94453500	-0.09705200	O	-2.44700700	-0.22067000	3.51758900
C	-1.86612300	-3.27446000	-0.13526500	C	1.94003400	-9.75316800	-0.22831600
C	-2.15008200	-1.88782700	-0.10872600	C	0.31913900	-7.91825100	-0.19877900
C	5.11579100	-0.43615800	-0.15774900	C	-1.30988500	-6.06613800	-0.17176400
C	-0.23501700	-5.12820800	-0.15856000	C	-2.93537500	-4.21196600	-0.15355200
C	-0.28137900	1.40146800	-0.09764300	C	-4.55734400	-2.35971600	-0.15621300
C	-0.55993100	2.80570500	-0.10857300	C	-6.18417200	-0.50740100	-0.17733900
C	-1.35146900	0.46129300	-0.07953600	C	-7.80911900	1.34958100	-0.20532700
C	-1.90281400	3.25312800	-0.13651900	C	-9.41721200	3.19647900	-0.23496600
C	-2.70873900	0.92092200	-0.11855200	C	9.41799900	-3.19589900	-0.23381200
C	-2.97725000	2.31039900	-0.13132300	C	7.80995700	-1.34953000	-0.20398700
C	1.86648100	3.27316300	-0.13040000	C	6.18592200	0.50704400	-0.17745700
C	0.51199500	3.73322800	-0.13645100	C	4.55915400	2.36035200	-0.15907200
C	-3.48937000	-1.42338600	-0.13799000	C	2.93422900	4.20995300	-0.15827100
C	-3.76818700	-0.02050700	-0.13234500	C	1.30986600	6.06467400	-0.17295200
C	-2.18019100	4.64774800	-0.15530500	C	-0.31946900	7.91793100	-0.19528600
C	-3.53214200	5.10285900	-0.17626800	C	-1.94094900	9.75312800	-0.22180800

C	0.60162100	-9.32722900	-0.21791700	C	9.40305800	3.33783300	-0.22813900
C	-1.02998400	-7.46342500	-0.19192700	C	7.77761200	5.18440800	-0.21685300
C	-2.65357000	-5.61024400	-0.17245200	C	6.15495400	7.03318200	-0.21423700
C	-4.27868700	-3.75333900	-0.16609600	C	4.53588800	8.88486300	-0.22008400
C	-5.90754800	-1.89825800	-0.17704400	C	2.92558400	10.73010000	-0.23220400
C	-7.53356800	-0.04737800	-0.19899200	C	-2.92589400	-10.73176100	-0.23402700
C	-9.16892800	1.81300300	-0.22601000	C	-4.53640000	-8.88653100	-0.21953700
C	9.17015600	-1.81338200	-0.22469400	C	-6.15549100	-7.03423200	-0.21241400
C	7.53486800	0.04728200	-0.19710200	C	-7.77687300	-5.18439600	-0.21555100
C	5.90889300	1.89854500	-0.17455200	C	-9.40150700	-3.33760100	-0.22819900
C	4.27959400	3.75182800	-0.16424300	C	-11.02093000	-1.50048300	-0.24680700
C	2.65279900	5.60875300	-0.17179200	C	10.75769100	2.83206800	-0.24411900
C	1.02975400	7.46244900	-0.18989600	C	9.11498000	4.69133000	-0.23023000
C	-0.60162000	9.32642100	-0.21329600	C	7.47727000	6.55644900	-0.22329800
H	2.15269100	-10.81990500	-0.24217500	C	5.84072500	8.42284200	-0.22443200
H	10.44787500	-3.54570400	-0.24924400	C	4.21112200	10.29377900	-0.23252500
C	10.21690600	-0.84582500	-0.23621400	C	-4.21142100	-10.29551600	-0.23266000
C	8.60120000	0.98972800	-0.21268500	C	-5.84084200	-8.42444800	-0.22243100
C	6.97914800	2.83958300	-0.19470100	C	-7.47675700	-6.55760800	-0.22087500
C	5.35488400	4.69516500	-0.18649900	C	-9.11371300	-4.69154200	-0.22892700
C	3.72596700	6.54727700	-0.19076200	C	-10.75604100	-2.83191200	-0.24444300
C	2.10277800	8.39641700	-0.20402300	H	-2.70868800	-11.79705500	-0.24453300
C	0.49373400	10.23764600	-0.22320100	H	-5.03227400	-11.00841700	-0.24230400
C	-0.49418600	-10.23879700	-0.22763500	H	-6.65952600	-9.14077800	-0.23468800
C	-2.10352700	-8.39773300	-0.20541500	H	-8.29491400	-7.27435700	-0.23442200
C	-3.72628400	-6.54851400	-0.18933300	H	-9.93115200	-5.40928000	-0.24186700
C	-5.35424700	-4.69618100	-0.18474100	H	-11.57002000	-3.55262300	-0.25546000
C	-6.97812900	-2.83970600	-0.19457500	H	5.03203700	11.00660000	-0.24245400
C	-8.59963400	-0.98922700	-0.21406900	H	6.65928900	9.13930500	-0.23652600
C	-10.21540100	0.84609800	-0.23826000	H	8.29493700	7.27377400	-0.23655200
C	-1.81042400	-9.81156000	-0.22203300	H	9.93218500	5.40933900	-0.24309900
C	-3.44320500	-7.94313600	-0.20409900	H	11.57165100	3.55280000	-0.25529700
C	-5.07360200	-6.08828400	-0.19465600	H	12.05042700	1.14629300	-0.25806100
C	-6.69801800	-4.23580400	-0.19751000	H	-12.04867300	-1.14599300	-0.25944700
C	-8.32349000	-2.37752600	-0.21169600	H	-11.24522200	1.19644200	-0.25250600
C	-9.96305900	-0.51487100	-0.23286000	H	-10.44734400	3.54558000	-0.24991900
C	9.96482200	0.51483800	-0.23152300	H	-9.65110500	5.89569900	-0.25227900
C	8.32506300	2.37711800	-0.21133900	H	-8.86274400	8.24377700	-0.25930500
C	6.69850100	4.23527300	-0.19835400	H	-7.01805100	9.86187300	-0.25567600
C	5.07364200	6.08735100	-0.19625200	H	-4.58698700	10.33707600	-0.24253200
C	3.44325700	7.94137400	-0.20446100	H	-2.15287800	10.82000500	-0.23545300
C	1.81022700	9.80994700	-0.21971500	H	0.28064800	11.30441100	-0.23554200
H	-0.28075300	-11.30549200	-0.24039200	H	2.70840400	11.79540400	-0.24208200
H	11.24666900	-1.19633900	-0.25079000				
C	11.02264400	1.50068200	-0.24554100	<b>11</b>			

C	1.64309300	-0.70719300	1.22990100	C	-3.01290400	-2.24429100	-0.84406800
C	1.64309200	0.71165200	1.22732600	C	-2.74328000	-0.85341900	-0.81879700
Cr	0.00014000	0.00000000	-0.00002600	H	-2.24094100	-4.24121700	-0.87316900
C	1.64385000	1.41876800	-0.00257200	H	-4.04939400	-2.57227900	-0.87156700
C	1.64324600	0.70714200	-1.22989600	C	-3.45108900	1.48709600	-0.84176500
C	1.64384800	-1.41876900	0.00257800	C	-3.75502100	0.13838700	-0.84231800
C	1.64324400	-0.71160200	-1.22732100	H	-4.79453200	-0.17986700	-0.86968500
H	1.59641400	-1.25601800	-2.16588900	C	1.99619400	3.18360200	-0.84304900
H	1.59641900	1.24814700	-2.17043400	C	3.01230800	2.24603500	-0.84306900
C	-1.64322600	-1.22954600	-0.70786400	C	2.74272700	0.85520700	-0.81879400
C	-1.64317600	-1.22777700	0.71094400	C	3.45059400	-1.48532900	-0.84371100
C	-1.64407500	0.00176400	1.41861900	C	3.75452800	-0.13661200	-0.84329600
C	-1.64317100	1.22954300	0.70789100	H	4.04875200	2.57419200	-0.87054500
C	-1.64322800	1.22778300	-0.71091800	H	4.79398100	0.18180400	-0.87067200
C	-1.64410600	-0.00176300	-1.41858000	H	4.25293000	-2.21890300	-0.87142600
H	-1.59686100	-2.16974400	-1.24946700	C	1.38690800	-0.31569400	2.54717700
H	-1.59663500	-2.16659700	1.25491700	C	0.96448000	1.04074800	2.54984600
H	-1.59612800	0.00311200	2.50363900	C	-0.42146800	1.35324600	2.55098200
H	-1.59662900	2.16971500	1.24952400	C	-1.38483400	0.30898600	2.55059700
H	-1.59685800	2.16663000	-1.25485900	C	-0.96238300	-1.04743900	2.54645500
H	-1.59656300	-0.00311000	-2.50362400	C	0.42354400	-1.35992100	2.54414300
H	1.59689800	-2.50380900	0.00440900	H	2.44393100	-0.55351000	2.47384700
H	1.59690100	2.50380800	-0.00467900	H	1.69937000	1.83700400	2.47859700
H	1.59666400	1.25598000	2.16594900	H	-0.74373000	2.38783000	2.48090900
H	1.59666700	-1.24810900	2.17049400	H	-2.44197500	0.54714400	2.48008000
<b>12</b>				H	-1.69735500	-1.84336600	2.47248300
C	1.37151600	0.42811600	-0.79063600	H	0.74567700	-2.39414300	2.46851800
C	1.05570100	-0.97341500	-0.79099600	H	-4.25342700	2.22070600	-0.86868300
C	0.31565700	1.40242200	-0.79063600	H	-2.55381200	4.06234100	-0.86812000
C	-0.31612700	-1.40074700	-0.79142800	H	-0.20471600	4.79398500	-0.86915000
C	-1.05625100	0.97506400	-0.79020300	H	2.24033300	4.24298500	-0.87042200
C	-1.37201500	-0.42649600	-0.79063100	<b>13</b>			
Cr	-0.00007500	0.00021300	0.93877000	C	-0.13736900	-1.42323100	-0.39800500
C	-0.63183400	-2.80168600	-0.82067400	C	-1.30144000	-0.59269500	-0.39809300
C	0.43792100	-3.73052100	-0.84527800	C	1.16402000	-0.83033900	-0.39809700
C	2.11116000	-1.94732100	-0.81964400	C	-1.16418600	0.83067700	-0.39756900
C	1.75806200	-3.31929900	-0.84471600	C	1.30127800	0.59302800	-0.39807300
H	2.55334000	-4.06050500	-0.87238100	C	0.13720600	1.42357100	-0.39745000
H	0.20406000	-4.79220300	-0.87340500	Cr	0.00010100	-0.00024600	1.30412800
C	-2.11163900	1.94899700	-0.81759600	C	-2.33607600	1.66663300	-0.41603300
C	-1.75855600	3.32104700	-0.84150200	C	-3.61990100	1.07091000	-0.43667700
C	0.63128000	2.80334200	-0.81860800	C	-2.61141900	-1.18962200	-0.41675300
C	-0.43850700	3.73224100	-0.84206000	C	-3.75775100	-0.35979300	-0.43713800
C	-1.99678700	-3.18186400	-0.84500600	C	2.61125200	1.18996700	-0.41670200



C	3.75758400	0.36014000	-0.43755900	C	4.62317800	-3.29782000	-0.47045100
C	2.33591400	-1.66629700	-0.41702600	C	3.35661500	-3.90041000	-0.46191900
C	3.61973100	-1.07056000	-0.43760800	C	3.17709100	-5.32875000	-0.47948000
C	-2.19067900	3.07433200	-0.43605600	C	-0.54468600	-5.65258600	-0.47027300
C	-0.88264400	3.67031800	-0.43593500	C	0.74113000	-5.09221300	-0.46181100
C	0.27513100	2.85643400	-0.41592000	C	1.93686400	-5.89388500	-0.47943500
C	2.73713000	2.59958200	-0.43691200	H	-0.64902800	-6.73545600	-0.48828700
C	1.56702500	3.43430900	-0.43634900	H	1.82979900	-6.97588600	-0.49571100
C	2.19051300	-3.07398200	-0.43752000	H	4.06390200	-5.95781900	-0.49580800
C	0.88247400	-3.66996900	-0.43742500	H	5.50881600	-3.92960400	-0.48851000
C	-0.27529400	-2.85609800	-0.41696200	C	1.41245700	-0.14594900	2.93550000
C	-2.73729700	-2.59923400	-0.43746500	C	0.83173500	1.14903100	2.93657300
C	-1.56719200	-3.43395800	-0.43738700	C	-0.58009600	1.29374900	2.93694400
C	1.69963400	4.85741900	-0.46028400	C	-1.41118300	0.14334000	2.93668900
C	3.02646500	5.41611000	-0.47787000	C	-0.83046000	-1.15163900	2.93555600
C	4.13598800	4.62463200	-0.47825600	C	0.58136800	-1.29635200	2.93473000
C	5.05642900	0.95677800	-0.46171200	H	2.49054800	-0.25594500	2.87026600
C	6.20362700	0.08711000	-0.47948600	H	1.46659600	2.02736200	2.87218100
C	5.16777600	2.35493400	-0.46985500	H	-1.02335400	2.28267100	2.87248600
C	4.78072500	-1.90413600	-0.46200500	H	-2.48932700	0.25341300	2.87244700
C	6.07292800	-1.26950400	-0.47961500	H	-1.46535900	-2.02988000	2.87033700
C	4.03960500	3.18824700	-0.46111000	H	1.02456500	-2.28517500	2.86837700
H	5.12655700	5.07291800	-0.49458900	H	-6.95654000	1.90369100	-0.49437900
H	6.15772000	2.80603600	-0.48792700	H	-5.50898900	3.92997300	-0.48632100
H	7.19183500	0.54052000	-0.49587000	H	-4.06407700	5.95818700	-0.49310300
H	6.95636400	-1.90332400	-0.49603100	H	-1.82997800	6.97625300	-0.49295700
C	-4.78089400	1.90449400	-0.46062600	H	0.64884800	6.73582300	-0.48595800
C	-6.07310100	1.26986700	-0.47830000	H	3.12793900	6.49864200	-0.49380600
C	-1.69980800	-4.85706300	-0.46180200				
C	-3.02663900	-5.41574600	-0.47938100	<b>14</b>			
C	-5.05660400	-0.95642100	-0.46132900	C	3.57940100	7.88660700	-0.32505300
C	-6.20380000	-0.08675000	-0.47863700	C	4.77005100	7.22898600	-0.32463100
C	-5.16794700	-2.35457700	-0.46996400	C	2.32228600	7.17844900	-0.30771700
C	-4.03977400	-3.18788600	-0.46168400	C	4.84007400	5.78789900	-0.30708800
C	-4.13616000	-4.62427000	-0.47932600	C	3.60376000	5.05407800	-0.28553700
H	-7.19201300	-0.54014800	-0.49505700	C	2.35941700	5.74134200	-0.28566300
H	-6.15789300	-2.80567000	-0.48805800	C	3.63630800	3.63240600	-0.26621800
H	-5.12673400	-5.07254500	-0.49566800	C	4.88049800	2.94234400	-0.27653800
H	-3.12811500	-6.49827400	-0.49568000	C	6.10939600	3.68300500	-0.29960900
C	-0.74130400	5.09256800	-0.45985100	C	6.04906300	5.09765700	-0.31213200
C	0.54451400	5.65294600	-0.46830600	C	1.09424400	7.83407300	-0.31358800
C	-1.93703400	5.89424700	-0.47703600	C	-0.13534000	7.13185100	-0.30075200
C	-4.62335200	3.29817800	-0.46859500	C	-0.10800100	5.69735100	-0.27668200
C	-3.35678400	3.90076700	-0.46001400	C	1.13868000	5.01179600	-0.26730400
C	-3.17726700	5.32910800	-0.47710700	C	2.41500900	2.89482400	-0.24165400

C	1.16469300	3.58540200	-0.23942800	C	3.77131600	-3.49177500	-0.26762400
C	-0.05425900	2.86297600	-0.21953700	C	2.57541900	-5.64754000	-0.28562900
C	-0.02706300	1.43128400	-0.19152800	C	1.39062300	-7.78675700	-0.31247800
C	-1.29955600	3.53862200	-0.23961300	C	-1.39060200	7.78691400	-0.31341100
C	-1.25321700	0.69224600	-0.19768000	C	-2.57537200	5.64768300	-0.28554500
C	-2.52304100	2.80120600	-0.24185500	C	-3.77124000	3.49189900	-0.26640000
C	-2.50662100	1.38442000	-0.21737400	C	-4.96410400	1.33248700	-0.26640000
C	2.45257100	1.47843200	-0.21668400	C	-6.15230900	-0.82764000	-0.28537000
C	1.22616300	0.73911700	-0.19685000	C	-7.33233900	-2.96948200	-0.31287900
C	3.68763100	0.78430400	-0.24219000	C	7.37862000	1.57816300	-0.30656400
C	1.25323400	-0.69213200	-0.19240000	C	6.17935900	-0.59362200	-0.28532400
C	3.71478400	-0.64383400	-0.24001400	C	4.98867200	-2.75502100	-0.27661100
C	2.50670100	-1.38433400	-0.22059300	C	3.79305100	-4.91365300	-0.28549000
C	-1.32796700	4.96503000	-0.26725100	C	2.59313300	-7.08504100	-0.30711800
C	4.91021300	1.51982700	-0.26625300	C	-2.59310900	7.08519100	-0.30745300
C	-1.22611100	-0.73899300	-0.19149800	C	-3.79299700	4.91378400	-0.28541600
C	-2.45258300	-1.47835900	-0.21977100	C	-4.98859300	2.75510800	-0.27651900
C	0.02708400	-1.43118900	-0.19682400	C	-6.17931800	0.59370000	-0.28530800
C	-2.41502900	-2.89472200	-0.23966400	C	-7.37859700	-1.57808400	-0.30700300
C	0.05428900	-2.86281500	-0.21656200	C	-3.87625200	7.74498200	-0.32458500
C	-1.16467100	-3.58523500	-0.24159900	C	-5.05612200	5.60007600	-0.30687900
C	-3.71471400	0.64390500	-0.24200000	C	-6.24445700	3.44868400	-0.29961400
C	-3.68762500	-0.78424100	-0.24007000	C	-7.43292200	1.29724100	-0.30658800
C	2.52313000	-2.80109300	-0.23988600	C	-8.62033900	-0.84361600	-0.32404000
C	1.29960200	-3.53844900	-0.24179900	C	8.62036800	0.84370400	-0.32364800
C	-3.63631400	-3.63229500	-0.26742000	C	7.43296500	-1.29715000	-0.30696100
C	-3.60373400	-5.05395900	-0.28565700	C	6.24453800	-3.44859900	-0.30034500
C	-4.88049400	-2.94226100	-0.27661500	C	5.05616700	-5.59996200	-0.30728300
C	-4.84003800	-5.78779300	-0.30758800	C	3.87627200	-7.74485300	-0.32425500
C	-6.10940100	-3.68293800	-0.30039000	C	8.64610200	-0.51625700	-0.32394300
C	-6.04902500	-5.09756800	-0.31322900	C	7.43959900	-2.68927300	-0.31279200
C	-1.13866800	-5.01163900	-0.26632500	C	6.23810500	-4.86435600	-0.31297600
C	0.10803600	-5.69717600	-0.27678500	C	5.04117700	-7.04251700	-0.32446100
C	-2.35939000	-5.74120500	-0.28579400	C	-5.04114500	7.04263600	-0.32416400
C	0.13536700	-7.13166200	-0.30015600	C	-6.23805700	4.86446300	-0.31198300
C	-2.32223900	-7.17829900	-0.30746100	C	-7.43955500	2.68937600	-0.31180500
C	-1.09420400	-7.83391000	-0.31271400	C	-8.64606700	0.51634700	-0.32368200
C	1.32802300	-4.96487000	-0.26625900	C	-0.78090300	1.18509200	3.15205300
C	-4.91019200	-1.51976600	-0.26738600	C	-1.41759600	-0.08411100	3.15313700
C	-4.76999100	-7.22887100	-0.32506800	C	-0.63691900	-1.26982700	3.15314100
C	-3.57934300	-7.88646500	-0.32485600	C	0.78038100	-1.18673700	3.15106600
Cr	0.00003900	0.00003100	1.52911500	C	1.41702000	0.08238900	3.15379700
C	7.33236300	2.96956400	-0.31181200	C	0.63633600	1.26817300	3.15480300
C	6.15234500	0.82771600	-0.28536400	H	-1.37681100	2.09031200	3.08675000
C	4.96415600	-1.33242000	-0.26759800	H	-2.49957800	-0.14744300	3.08944500

H	-1.12341800	-2.23836900	3.08919000	C	-9.86887600	-2.78134000	-0.22965100
H	1.37630500	-2.09188500	3.08500900	H	-10.95628400	-2.81360900	-0.24498400
H	2.49903400	0.14577100	3.09066000	H	-9.59917800	-7.37628700	-0.26611200
H	1.12281900	2.23681300	3.09225000	H	-10.88931200	-5.28927900	-0.26131300
H	5.99505600	-7.56424500	-0.33866600	C	-6.89937000	-7.58485100	-0.24083600
H	3.89277900	-8.83191500	-0.33857300	C	-5.47379200	-7.58011000	-0.22696600
H	7.19012000	-5.39073800	-0.32980600	C	-4.79505000	-6.31384300	-0.20274700
H	8.39216900	-3.21466000	-0.32961700	H	-7.41428600	-8.54307100	-0.25791400
H	9.59566700	-1.04568300	-0.33825700	C	-3.37525500	-6.27524800	-0.18953300
H	9.54910900	1.40887700	-0.33811700	C	-2.69760100	-5.01539700	-0.16237400
H	8.26407300	3.53103500	-0.32916300	C	-3.44573000	-3.80788800	-0.15349400
H	6.98015100	5.66015500	-0.32956600	C	-3.52609400	-1.33692600	-0.12682100
H	5.70320500	7.78688400	-0.33924800	C	-2.77199100	-2.55696400	-0.12181300
H	3.55479700	8.97358000	-0.33970800	C	-1.35742500	-2.52364400	-0.10499100
H	1.07448500	8.92172400	-0.33082400	C	-0.67738900	-1.25934900	-0.07584100
H	-1.41166000	8.87454100	-0.33055100	C	-0.60533700	-3.72225900	-0.12211800
H	-3.89277900	8.83204400	-0.33897700	C	0.75198700	-1.21632000	-0.08566800
H	-5.99503700	7.56434600	-0.33838100	C	0.82831300	-3.67899200	-0.12716700
H	-7.19008400	5.39082600	-0.32897600	C	1.50679400	-2.43712600	-0.09832500
H	-8.39211600	3.21478200	-0.32878500	C	-2.86399400	-0.08629800	-0.09794900
H	-9.59563100	1.04578300	-0.33797700	C	-1.42931500	-0.04305500	-0.08572200
H	-9.54908600	-1.40878100	-0.33857500	C	-3.60018500	1.12216100	-0.12605800
H	-8.26406000	-3.53094400	-0.33012600	C	-0.75181500	1.21631000	-0.07645700
H	-6.98010500	-5.66008900	-0.33054200	C	-2.92080600	2.38538500	-0.12047600
H	-5.70313700	-7.78678600	-0.33971400	C	-1.50667600	2.43721400	-0.10442400
H	-3.55472600	-8.97343500	-0.33946500	C	-1.27768900	-4.97397700	-0.15381500
H	-1.07442700	-8.92155300	-0.33004900	C	-5.02051500	1.08025800	-0.14532900
H	1.41166300	-8.87438000	-0.32970000	C	1.42938700	0.04309300	-0.07662000
				C	2.86414600	0.08637200	-0.10411500
				C	0.67762300	1.25949000	-0.08484100
				C	3.52631200	1.33703000	-0.12168100
				C	1.35744500	2.52366600	-0.09880500
				C	2.77206700	2.55694800	-0.12697500
				C	2.92088800	-2.38523800	-0.12595600
				C	3.60041100	-1.12209900	-0.12098200
				C	-0.82822600	3.67914500	-0.12164700
				C	0.60543600	3.72223600	-0.12729600
				C	4.94653000	1.38053100	-0.15077600
				C	5.61938400	2.63985500	-0.16840400
				C	5.69232100	0.17155900	-0.15716600
				C	7.04409300	2.68050900	-0.19082600
				C	7.12225000	0.21459900	-0.18087100
				C	7.79142100	1.46741400	-0.19457800
				C	3.44589600	3.80792000	-0.14962700
				C	2.69767900	5.01535600	-0.16437600
<b>15</b>							
C	-9.08857900	-6.41645600	-0.25082900				
C	-7.64240600	-6.41719200	-0.23449700				
C	-6.96883700	-5.14012000	-0.21233600				
C	-7.71288800	-3.93621000	-0.20970000				
C	-9.15652600	-3.96791400	-0.22892300				
C	-9.80241700	-5.26166200	-0.24801100				
C	-5.54620900	-5.10311000	-0.19500900				
C	-7.04400000	-2.68044500	-0.18980700				
C	-5.61921900	-2.63980800	-0.17010600				
C	-4.87299700	-3.84686900	-0.17020100				
C	-4.94638800	-1.38050600	-0.14715200				
C	-5.69209100	-0.17149100	-0.15929100				
C	-7.12205600	-0.21453200	-0.17909600				
C	-7.79128800	-1.46732600	-0.19363700				
C	-9.22741500	-1.50838300	-0.21424100				

C	4.87314500	3.84688400	-0.17166500	C	7.19268100	-2.25157000	-0.18505600
C	3.37533800	6.27523500	-0.18748200	C	9.30161200	-0.95033100	-0.21198800
C	5.54634600	5.10317100	-0.19370900	H	-11.03106900	-0.33221700	-0.23610500
C	4.79515500	6.31386500	-0.20155400	H	-5.22772400	-9.71920500	-0.25562500
C	1.27778300	4.97406200	-0.14987700	C	-2.52541300	-9.93737700	-0.24216900
C	5.02065700	-1.08014400	-0.14911400	C	-0.44745500	-8.64756900	-0.21402500
C	7.71302500	3.93632700	-0.20996900	C	1.64633600	-7.35465800	-0.19159400
C	6.96868900	5.14010600	-0.21181300	C	3.74690100	-6.06054200	-0.18058700
C	7.64240200	6.41717300	-0.23369000	C	5.84346500	-4.75996500	-0.18466200
C	6.89939300	7.58482100	-0.23893700	C	7.93591400	-3.46484100	-0.20051600
C	9.08853200	6.41646900	-0.25028500	C	10.01848400	-2.18245500	-0.22334100
C	9.15656100	3.96799400	-0.22956600	C	-10.01832400	2.18252900	-0.22160500
C	9.86898300	2.78144200	-0.23139800	C	-7.93576500	3.46492500	-0.20016500
C	9.80243800	5.26173700	-0.24848600	C	-5.84332700	4.76005200	-0.18578300
C	5.47386100	7.58011900	-0.22525900	C	-3.74681200	6.06066700	-0.18237200
C	9.22754400	1.50848700	-0.21573800	C	-1.64623100	7.35471600	-0.19266000
Cr	-0.00008200	-0.00000100	1.62907800	C	0.44755300	8.64761600	-0.21356100
C	-9.94383300	-0.29942400	-0.22022200	C	2.52553100	9.93740300	-0.24030800
C	-7.86544600	0.99571800	-0.19043300	C	-9.37865300	3.40978900	-0.21792500
C	-5.76791100	2.29677300	-0.16575200	C	-7.26536000	4.71139700	-0.20083700
C	-3.66863800	3.59353000	-0.14991800	C	-5.16639800	6.01380600	-0.19253800
C	-1.57468200	4.88803100	-0.15203000	C	-3.07038500	7.30956400	-0.19631600
C	0.52361500	6.18632700	-0.17273700	C	-0.96713000	8.60500500	-0.21198900
C	2.62497800	7.48113200	-0.20217100	C	1.14174500	9.91369500	-0.23561700
C	4.71257900	8.76137000	-0.23524700	C	-1.14162400	-9.91366300	-0.23634500
C	-4.71248000	-8.76133300	-0.23769700	C	0.96723500	-8.60494600	-0.21166400
C	-2.62487900	-7.48112300	-0.20334400	C	3.07049200	-7.30947000	-0.19539900
C	-0.52352700	-6.18630600	-0.17123900	C	5.16650400	-6.01370800	-0.19158400
C	1.57475500	-4.88799500	-0.14838000	C	7.26550600	-4.71130500	-0.20042300
C	3.66880700	-3.59343900	-0.14626500	C	9.37881400	-3.40970800	-0.21855000
C	5.76809000	-2.29668300	-0.16418200	H	-11.10570600	2.14920400	-0.23618200
C	7.86561800	-0.99564400	-0.19141900	H	-3.04114300	-10.89517300	-0.25934500
C	9.94396000	0.29952000	-0.22249700	C	-0.34397900	-11.11986400	-0.25327000
C	-9.30144200	0.95041700	-0.21047400	C	1.73646300	-9.82686200	-0.23138300
C	-7.19252900	2.25165600	-0.18390800	C	3.82778300	-8.53033700	-0.21644200
C	-5.09570900	3.54659400	-0.16401800	C	5.92021600	-7.23682900	-0.21202600
C	-2.99455800	4.84390800	-0.15757200	C	8.01482500	-5.94557700	-0.21850400
C	-0.89486100	6.14363100	-0.16935400	C	10.10133700	-4.66235600	-0.23308700
C	1.20071300	7.44053200	-0.19476600	C	-10.10119600	4.66241900	-0.23274800
C	3.30735600	8.74541700	-0.22593000	C	-8.01469800	5.94565700	-0.21934700
C	-3.30724900	-8.74540700	-0.22761900	C	-5.92011200	7.23691900	-0.21368300
C	-1.20061800	-7.44048800	-0.19609800	C	-3.82767400	8.53043500	-0.21807900
C	0.89494700	-6.14354800	-0.17125400	C	-1.73634700	9.82693600	-0.23217600
C	2.99463500	-4.84375400	-0.16004400	C	0.34412100	11.11990800	-0.25287100
C	5.09584300	-3.54648500	-0.16580200	C	1.01298900	-11.07892400	-0.25079000

C	3.11918800	-9.76720200	-0.23231400
C	5.23144000	-8.46172400	-0.22241600
C	7.34344000	-7.15579700	-0.22293500
C	9.45827700	-5.85796000	-0.23294800
C	-9.45814500	5.85802900	-0.23365600
C	-7.34331900	7.15588100	-0.22492300
C	-5.23131200	8.46179900	-0.22490800
C	-3.11906300	9.76728900	-0.23427700
C	-1.01284600	11.07898600	-0.25145900
H	-11.18779900	4.62460300	-0.24474800
H	-10.02552100	6.78547500	-0.24616800
H	-7.91483700	8.08152200	-0.23983400
H	-5.80313400	9.38706000	-0.24113500
H	-3.69139000	10.69241300	-0.25005700
H	-1.58876500	12.00114900	-0.26554300
H	10.02564200	-6.78541600	-0.24520200
H	7.91494000	-8.08144900	-0.23784400
H	5.80325300	-9.38698800	-0.23868300
H	3.69152500	-10.69232000	-0.24808300
H	1.58892600	-12.00107900	-0.26459400
H	-0.86350300	-12.07490400	-0.26877400
H	0.86366600	12.07494000	-0.26826600
H	3.04127900	10.89518700	-0.25764200
H	5.22783300	9.71923500	-0.25337100
H	7.41431300	8.54304800	-0.25614600
H	9.59909200	7.37632300	-0.26542100
H	10.88933000	5.28939800	-0.26200900
H	10.95638700	2.81371900	-0.24667300
H	11.03119800	0.33233500	-0.23823800
H	11.10586800	-2.14913200	-0.23778900
H	11.18794000	-4.62455500	-0.24521200
C	0.10811100	-1.41561600	3.26210800
C	1.27874100	-0.61327500	3.26366500
C	1.16935000	0.80137500	3.26484200
C	-0.11061700	1.41424600	3.26312500
C	-1.28116300	0.61192900	3.26228900
C	-1.17178000	-0.80280800	3.26253800
H	0.19220700	-2.49609800	3.19905900
H	2.25648600	-1.08107100	3.20263900
H	2.06372200	1.41374600	3.20455700
H	-0.19464500	2.49476700	3.20079700
H	-2.25877600	1.07982800	3.20011200
H	-2.06606500	-1.41515800	3.20069200

**16-H**

Cr	-0.00003900	-0.00002000	0.94494900
C	1.35033200	0.47725800	-0.55111400
C	0.26185300	1.40784800	-0.55118400
C	-1.08842600	0.93074400	-0.55083100
C	-1.35026600	-0.47725300	-0.55120400
C	-0.26182300	-1.40780200	-0.55121700
C	1.08845900	-0.93073100	-0.55080500
H	2.37277600	0.83870300	-0.47361400
H	0.46002400	2.47402600	-0.47358600
H	-1.91264800	1.63547500	-0.47301700
H	-2.37272700	-0.83868200	-0.47375100
H	-0.45997200	-2.47399700	-0.47368800
H	1.91270400	-1.63542800	-0.47298600

**16-CH<sub>3</sub>**

Cr	-0.00091100	-0.00041300	1.06848300
C	0.44668500	1.36997900	-0.42389300
C	-0.95299000	1.06035400	-0.44209400
C	-1.40963800	-0.29834800	-0.42473400
C	-0.44137200	-1.35551800	-0.44272600
C	0.96359700	-1.07129700	-0.42419100
C	1.39541200	0.29544600	-0.44001100
H	-1.67973100	1.86861800	-0.39007400
H	-0.77762000	-2.38921600	-0.39168000
H	2.45866500	0.52057300	-0.38563500
C	0.91584700	2.81111000	-0.33472400
H	1.00504600	3.17488500	0.69833400
H	1.89833000	2.93164500	-0.80352300
H	0.22015700	3.48126000	-0.85129700
C	-2.89218400	-0.61256300	-0.33460400
H	-3.25169600	-0.70970400	0.69919600
H	-3.48801900	0.17448100	-0.80912400
H	-3.12421100	-1.55394400	-0.84427600
C	1.97741400	-2.19791500	-0.33463000
H	2.25463900	-2.45067800	0.69824200
H	1.58741600	-3.11180600	-0.79525300
H	2.90225900	-1.93369200	-0.85884500

**16-NH<sub>2</sub>**

Cr	0.00039700	0.00076800	1.06437600
C	-0.14030200	1.41606600	-0.42330200
C	-1.30928000	0.59159100	-0.46728700
C	-1.15622900	-0.83079100	-0.42391700
C	0.14137900	-1.43223000	-0.45831400
C	1.29644600	-0.58767100	-0.42258700

C	1.16766800	0.83714000	-0.46694400
H	-2.29920600	1.03836800	-0.40254000
H	0.24934200	-2.51129000	-0.37576300
H	2.04931200	1.47108600	-0.40004400
N	-0.27134800	2.82747700	-0.21977100
H	-1.17511400	3.16094300	-0.54199600
H	0.44822800	3.33908200	-0.72284600
N	-2.30835400	-1.65563900	-0.21832600
H	-2.17658200	-2.57711500	-0.62513000
H	-3.13522900	-1.24243800	-0.63969500
N	2.58298400	-1.18276700	-0.21972400
H	3.32640300	-0.54838900	-0.49653000
H	2.68225000	-2.03679300	-0.76161000

#### 16-OMe

Cr	-0.00100400	-0.00078800	1.40562000
C	-1.34853500	-0.44963000	-0.07332400
C	-0.28922300	-1.41116400	-0.10209600
C	1.06297300	-0.94413000	-0.07185500
C	1.36599800	0.45400200	-0.10077400
C	0.28546000	1.39153300	-0.07208400
C	-1.07691200	0.95487800	-0.10237600
H	-0.50625600	-2.47039300	-0.00931500
H	2.39173700	0.79566800	-0.00675400
H	-1.88566900	1.67247900	-0.00935700
O	-2.65643400	-0.88482600	0.10302500
O	2.09389900	-1.85922400	0.10385400
O	0.56228900	2.74172600	0.10494200
C	-3.34453200	-1.11955100	-1.12185600
H	-4.35142900	-1.45262100	-0.85784000
H	-3.41081300	-0.20282700	-1.72426400
H	-2.84760400	-1.89931900	-1.71577100
C	2.64661100	-2.32953100	-1.12180800
H	3.44087900	-3.03284800	-0.85918100
H	1.88965500	-2.84558100	-1.72881400
H	3.07133700	-1.50446400	-1.71050500
C	0.70074000	3.45572000	-1.11981900
H	0.91562000	4.49425000	-0.85569500
H	1.52709000	3.05549500	-1.72372900
H	-0.22394900	3.41491000	-1.71225700

#### 16-F

Cr	0.00008800	-0.00018600	1.06718000
C	-0.42340500	1.32873200	-0.43230800
C	-1.41379500	0.30901500	-0.45907700

C	-0.93901000	-1.03086800	-0.43232700
C	0.43934700	-1.37889800	-0.45953000
C	1.36227600	-0.29772400	-0.43216700
C	0.97439600	1.06987500	-0.45926400
H	-2.47178300	0.54011900	-0.42537200
H	0.76797100	-2.41077700	-0.42587700
H	1.70376900	1.87036300	-0.42569100
F	-0.83492100	2.62085300	-0.30717100
F	2.68712900	-0.58715900	-0.30674100
F	-1.85231000	-2.03325400	-0.30690300

#### 16-Cl

Cr	0.00000000	-0.00010900	1.09799000
C	-1.38314200	-0.25695500	-0.38786400
C	-0.48182300	-1.36201900	-0.40417700
C	0.91380200	-1.06949700	-0.38779700
C	1.41997700	0.26369300	-0.40422300
C	0.46904300	1.32620800	-0.38802000
C	-0.93846700	1.09804300	-0.40405400
H	-0.84246600	-2.38183700	-0.34525400
H	2.48327200	0.46131000	-0.34537000
H	-1.64131800	1.92017100	-0.34512800
Cl	2.05919500	-2.40856200	-0.21656600
Cl	-3.11562400	-0.57860000	-0.21696900
Cl	1.05667400	2.98752300	-0.21700700

#### 16-Br

Cr	0.00016600	-0.00023900	1.12904300
C	1.28773500	-0.56547300	-0.34807700
C	1.16422900	0.85517500	-0.36498700
C	-0.15439700	1.39781400	-0.34796100
C	-1.32276100	0.58052000	-0.36485700
C	-1.13323300	-0.83276800	-0.34781000
C	0.15869500	-1.43645100	-0.36460000
H	2.03537800	1.49484900	-0.29995100
H	-2.31232300	1.01464500	-0.29991700
H	0.27718900	-2.51083700	-0.29943300
Br	-0.36463100	3.29960600	-0.12673700
Br	3.04055900	-1.33395500	-0.12739000
Br	-2.67609500	-1.96524600	-0.12781500

#### 16-CO<sub>2</sub>Me

Cr	-0.00020500	0.00008300	1.16785200
C	1.15152500	-0.85895100	-0.35788500
C	1.31058800	0.56485700	-0.32245700

C	0.16801500	1.42655600	-0.35819000	N	-0.70488900	3.96073600	-0.22813500
C	-1.14460900	0.85251300	-0.32262300				
C	-1.31962500	-0.56788500	-0.35815400	<b>17-H</b>			
C	-0.16615700	-1.41747000	-0.32275100	C	-0.50247500	-1.33843100	-0.39804100
H	2.30854500	0.97586100	-0.23324800	C	-1.41083700	-0.23398900	-0.39770600
H	-1.99952100	1.51128700	-0.23346000	C	0.90827400	-1.10413800	-0.39794300
H	-0.30948400	-2.48718700	-0.23337400	C	-0.90849300	1.10480800	-0.39748300
C	-2.65114900	-1.21038600	-0.22188400	C	1.41066700	0.23461800	-0.39765400
C	2.37363200	-1.69074500	-0.22126300	C	0.50228900	1.33914400	-0.39757200
C	0.27750400	2.90097600	-0.22219900	Cr	0.00004600	-0.00005000	1.30513300
O	-2.83390000	-2.40995600	-0.12084600	C	-1.82286600	2.21660700	-0.41608900
O	2.09788100	-3.01753600	-0.22937500	C	-3.21724600	1.97498500	-0.43751500
O	-0.66994900	3.65909000	-0.12134700	C	-2.83084200	-0.46997100	-0.41606400
O	-3.66201100	-0.30795700	-0.22890500	C	-3.72226200	0.62927500	-0.43693400
O	3.50370900	-1.24906900	-0.11903100	C	2.83064400	0.47069300	-0.41602900
O	1.56451200	3.32520900	-0.22909700	C	3.72208300	-0.62860200	-0.43711300
C	-4.97932800	-0.86350400	-0.10877500	C	1.82266800	-2.21598800	-0.41684300
H	-5.08884300	-1.39818700	0.83912200	C	3.21705200	-1.97425300	-0.43801500
H	-5.65942900	-0.01208100	-0.14909100	C	-1.31644300	3.53809400	-0.43685500
H	-5.18075800	-1.55623700	-0.93019900	C	0.10146100	3.77366400	-0.43611900
C	1.74177100	4.74385000	-0.10914000	C	1.00799900	2.68677700	-0.41530800
H	1.33357200	5.10606500	0.83878000	C	3.31871400	1.79903200	-0.43589300
H	2.81912700	4.90742600	-0.14968800	C	2.40557400	2.90920600	-0.43571600
H	1.24223800	5.26439100	-0.93053900	C	1.31625000	-3.53742400	-0.43784100
C	3.23811300	-3.88006700	-0.11013600	C	-0.10163600	-3.77298300	-0.43717500
H	2.84130600	-4.89495600	-0.15095700	C	-1.00816000	-2.68614500	-0.41615700
H	3.93823700	-3.70722900	-0.93182500	C	-3.31890700	-1.79836800	-0.43624100
H	3.75630300	-3.70786600	0.83759100	C	-2.40576900	-2.90847600	-0.43639300
				C	2.90361500	4.24894600	-0.45949600
<b>16-CN</b>				C	4.32999700	4.44367600	-0.47724400
Cr	-0.00021300	0.00006100	1.09543000	C	5.19561600	3.39105900	-0.47826600
C	-1.09798400	-0.92432500	-0.42919600	C	5.13124200	-0.38993900	-0.46255500
C	0.25120700	-1.41134200	-0.39455900	C	6.01307900	-1.52788900	-0.48140300
C	1.34951300	-0.48881300	-0.42885000	C	5.60218700	0.93121600	-0.47074600
C	1.09675500	0.92307000	-0.39448400	C	4.12162100	-3.08099800	-0.46315400
C	-0.25136500	1.41305700	-0.42917400	C	5.53425700	-2.80391700	-0.48161800
C	-1.34766000	0.48812500	-0.39512100	C	4.72932200	2.02913100	-0.46111200
H	0.44065500	-2.47616800	-0.31482700	H	6.26864000	3.56667100	-0.49486500
H	1.92416300	1.61958500	-0.31467200	H	6.67532400	1.10972500	-0.48934300
H	-2.36459700	0.85642600	-0.31572500	H	7.08511100	-1.34656700	-0.49841700
C	-2.18996600	-1.84356900	-0.31851200	H	6.22253700	-3.64558500	-0.49893700
C	2.69162500	-0.97484100	-0.31811400	C	-4.12173900	3.08174200	-0.46251100
C	-0.50146900	2.81834100	-0.31837000	C	-5.53440200	2.80473000	-0.48117400
N	-3.07766000	-2.59078300	-0.22765100	C	-2.90387600	-4.24823700	-0.46047100
N	3.78268500	-1.36988600	-0.22804600	C	-4.33025200	-4.44289200	-0.47813400

C	-5.13146700	0.39081400	-0.46250000	C	1.41633200	-0.19639600	-0.52680200
C	-6.01319100	1.52872900	-0.48127800	C	0.53743200	-1.32473400	-0.52561600
C	-5.60240000	-0.93041000	-0.47091900	C	0.87857200	1.12839700	-0.52756600
C	-4.72954200	-2.02826100	-0.46148200	C	-0.87888700	-1.12801000	-0.52669800
C	-5.19592600	-3.39024600	-0.47885200	C	-0.53816900	1.32504400	-0.52706500
H	-7.08526400	1.34758700	-0.49845000	C	-1.41686700	0.19693600	-0.52816000
H	-6.67555200	-1.10882500	-0.48957500	Cr	-0.00019300	0.00166100	1.18223100
H	-6.26896700	-3.56567700	-0.49533600	C	-1.76370200	-2.26307800	-0.57145000
H	-4.70947000	-5.46192400	-0.49410600	C	-1.22287000	-3.57087500	-0.60094600
C	0.60765700	5.11029400	-0.45961200	C	1.07826400	-2.65829200	-0.57068800
C	1.99491700	5.31733500	-0.46745600	C	0.20082000	-3.76886600	-0.59989300
C	-0.33861400	6.19519200	-0.47724300	C	-1.07881700	2.65858500	-0.57219900
C	-3.60727700	4.38657600	-0.47057600	C	-0.20153500	3.76893200	-0.61490300
C	-2.22765600	4.63931600	-0.46127000	C	1.76308100	2.26341700	-0.57314000
C	-1.68299200	5.97184300	-0.47824400	C	1.22227400	3.57089800	-0.61621500
C	3.60711900	-4.38584800	-0.47152100	C	-3.16364600	-2.05857800	-0.61917600
C	2.22757400	-4.63860800	-0.46236000	C	-3.70418600	-0.72667500	-0.62103300
C	1.68284000	-5.97119100	-0.47953200	C	-2.84206700	0.39523700	-0.57495300
C	-1.99512500	-5.31662800	-0.46869600	C	-2.48183000	2.84419600	-0.60368700
C	-0.60794200	-5.10962400	-0.46089800	C	-3.36524400	1.71034400	-0.60565900
C	0.33841300	-6.19454800	-0.47867500	C	3.16345000	2.05896900	-0.60672700
H	-2.37715800	-6.33525600	-0.48648700	C	3.70389700	0.72714100	-0.60743700
H	-0.04616100	-7.21156500	-0.49471000	C	2.84159400	-0.39495900	-0.57395200
H	2.37569600	-6.80911200	-0.49635600	C	2.48094500	-2.84380100	-0.61612500
H	4.29806500	-5.22613100	-0.49033800	C	3.36452200	-1.70980000	-0.61863600
C	1.32549400	-0.51239600	2.93586600	C	-4.78100700	1.90295900	-0.65262100
C	1.10430600	0.88948000	2.93784600	C	-5.28327200	3.25188500	-0.67847100
C	-0.22041600	1.39915800	2.93951100	C	-4.44582600	4.32693900	-0.67523200
C	-1.32393300	0.50652000	2.93911900	C	-0.74275600	5.09112600	-0.65849100
C	-1.10283500	-0.89547900	2.93524100	C	0.17450600	6.20033200	-0.69415300
C	0.22198900	-1.40501700	2.93387700	C	-2.13493000	5.26185500	-0.66668800
H	2.33692700	-0.90143800	2.87006300	C	2.10391000	4.69503700	-0.66221700
H	1.94667800	1.57131600	2.87338900	C	1.52423600	6.01260100	-0.69618900
H	-0.38983800	2.46972200	2.87705000	C	-3.01492100	4.17002100	-0.64648800
H	-2.33545000	0.89578000	2.87595100	H	-4.85148700	5.33549300	-0.70172300
H	-1.94522600	-1.57704700	2.86859200	H	-2.54332500	6.26984000	-0.69880700
H	0.39127500	-2.47527100	2.86620800	H	-0.23664800	7.20664400	-0.72371000
H	-6.22274200	3.64634700	-0.49842700	H	2.19475100	6.86814500	-0.72730000
H	-4.29813400	5.22693300	-0.48938800	C	-2.10453300	-4.69522400	-0.64692500
H	-2.37569000	6.80992200	-0.49504500	C	-1.52494800	-6.01294300	-0.67275800
H	0.04576200	7.21230800	-0.49307800	C	4.78002000	-1.90229800	-0.66747200
H	2.37685500	6.33600600	-0.48514900	C	5.28206100	-3.25119000	-0.70333900
H	4.70929300	5.46268600	-0.49299900	C	0.74203300	-5.09127000	-0.64404800
				C	-0.17519100	-6.20066200	-0.67116300
				C	2.13395200	-5.26156300	-0.66741900

17-CH<sub>3</sub>



C	3.01382800	-4.16935600	-0.66095900	C	2.28967300	-1.84765400	2.89723700
C	4.44459100	-4.32617700	-0.69987200	H	2.05619600	-2.80607400	2.42373400
H	0.23594400	-7.20706600	-0.69785500	H	3.16686800	-1.42667700	2.39656300
H	2.54233800	-6.26951500	-0.70065500	H	2.56872700	-2.05193300	3.94032400
H	4.85006500	-5.33466400	-0.73113500				
H	6.35903900	-3.39772400	-0.73710600	17-NH <sub>2</sub>			
C	-5.11835500	-0.52522300	-0.67037700	C	-1.00866500	1.01437100	-0.58053600
C	-5.62446500	0.78284200	-0.67861400	C	0.37345700	1.38151500	-0.58016800
C	-5.96963500	-1.68560200	-0.70983300	C	-1.38255100	-0.36825800	-0.58218300
C	-3.49001100	-4.47920900	-0.67313400	C	1.38395200	0.36649500	-0.57983800
C	-4.03824500	-3.18815000	-0.66680900	C	-0.37358200	-1.38140800	-0.57989600
C	-5.45739000	-2.94843300	-0.70807900	C	1.01086200	-1.01379300	-0.57993000
C	3.48977300	4.47935100	-0.67382900	Cr	-0.00125500	0.00014800	1.09003600
C	4.03828400	3.18868100	-0.65326400	C	2.77479300	0.73513100	-0.59016700
C	5.45760600	2.94908600	-0.68503700	C	3.13479700	2.10495400	-0.60599500
C	5.62397400	-0.78213400	-0.67935100	C	0.74805600	2.77053800	-0.59044100
C	5.11832200	0.52580200	-0.65643400	C	2.11954500	3.12460600	-0.60605100
C	5.96982200	1.68621700	-0.68672100	C	-0.74972700	-2.77018900	-0.59085700
H	6.70104800	-0.93199800	-0.71529800	C	-2.11957400	-3.12505900	-0.61071400
H	7.04594900	1.53310100	-0.71730200	C	-2.77292900	-0.73820700	-0.59191400
H	6.12310800	3.80857800	-0.71423400	C	-3.13388500	-2.10636200	-0.61116700
H	4.15803900	5.33729900	-0.70805500	C	3.76702700	-0.27366800	-0.60933100
C	0.22311700	1.41295500	2.85122300	C	3.39186500	-1.66140800	-0.60895500
C	-1.09397200	0.88244600	2.84269000	C	2.02644300	-2.03285800	-0.59000000
C	-1.33456800	-0.51747900	2.84690700	C	0.25658700	-3.76691200	-0.60563800
C	-0.21650600	-1.39331600	2.83722700	C	1.64734100	-3.39756000	-0.60515100
C	1.11576400	-0.90184600	2.84405300	C	-3.76527300	0.27244900	-0.60711100
C	1.31490800	0.50449200	2.83920500	C	-3.38975100	1.66147900	-0.60645800
H	-1.93918800	1.56440600	2.79320800	C	-2.02332400	2.03452400	-0.59099800
H	-0.38486300	-2.46583200	2.78166500	C	-0.25634900	3.76721200	-0.60957400
H	2.32828900	0.89495400	2.78821500	C	-1.64581400	3.39821500	-0.60955600
H	-2.19547400	-6.86859100	-0.70064500	C	2.65883100	-4.40735300	-0.62284800
H	-4.15826800	-5.33714300	-0.70791100	C	2.24227000	-5.78555400	-0.63480700
H	-6.12273100	-3.80789500	-0.74142700	C	0.92488700	-6.13541500	-0.63525800
H	-7.04562800	-1.53243600	-0.74444500	C	-2.48754900	-4.50593700	-0.63057700
H	-6.70155100	0.93271700	-0.71412800	C	-3.88981600	-4.83466900	-0.64556100
H	-6.36038100	3.39849700	-0.70746200	C	-1.48250000	-5.48387600	-0.63318600
C	0.45741000	2.90221500	2.90933700	C	-4.51641500	-2.46824400	-0.63110500
H	-0.35438200	3.45636900	2.42819500	C	-4.85128900	-3.86899600	-0.64578000
H	0.51614200	3.23967800	3.95351400	C	-0.12059100	-5.14551400	-0.62370800
H	1.39512700	3.18072500	2.41889100	H	0.63869200	-7.18468600	-0.64904500
C	-2.74220100	-1.05706900	2.90237900	H	-1.76606700	-6.53445500	-0.64869400
H	-3.07303000	-1.15584600	3.94563500	H	-4.17093400	-5.88530500	-0.66096400
H	-3.44688700	-0.39185600	2.39407600	H	-5.90317500	-4.14536800	-0.66146300
H	-2.81369500	-2.04550600	2.43837000	C	4.51734800	2.46761600	-0.62479400

C	4.85192400	3.86795900	-0.63784800	H	-2.91710500	-1.67252200	3.14831100
C	-2.65772500	4.40735200	-0.62947000	N	2.71882000	-0.76122400	2.78688700
C	-2.24121500	5.78603700	-0.64409300	H	3.35613700	-0.07233500	3.16415900
C	2.48834100	4.50545000	-0.62493700	H	2.90490700	-1.68622400	3.15133100
C	3.89021100	4.83385000	-0.63791300	N	-0.70191900	2.73861900	2.78686100
C	1.48238300	5.48385800	-0.63381800	H	-1.62066000	2.94577700	3.15570400
C	0.12151400	5.14538800	-0.62988100	H	0.00308800	3.36086600	3.15947700
C	-0.92413500	6.13576600	-0.64439300				
H	4.17149200	5.88442200	-0.65250500	<b>17-OMe</b>			
H	1.76655100	6.53426300	-0.65003000	C	-0.63216600	1.28311300	-0.71317400
H	-0.63774400	7.18498900	-0.66008700	C	0.79464200	1.18841900	-0.71198200
H	-3.01051600	6.55482500	-0.65947300	C	-1.42724100	0.09287000	-0.71174800
C	4.39653800	-2.67774000	-0.62872300	C	1.42797500	-0.09537500	-0.71373500
C	4.00921500	-4.02547900	-0.63162400	C	-0.79602500	-1.18992200	-0.71242500
C	5.77710500	-2.26745300	-0.64357900	C	0.63251500	-1.28324600	-0.71125500
C	5.49137000	1.45740100	-0.63363300	Cr	0.00052100	0.00048000	0.96941800
C	5.14692600	0.09803700	-0.62954400	C	2.86386200	-0.19041000	-0.74088800
C	6.13269700	-0.95197200	-0.64407400	C	3.64276100	0.99150900	-0.76899500
C	-5.48999700	-1.45897200	-0.63444900	C	1.59441700	2.38512000	-0.74377300
C	-5.14555700	-0.09857400	-0.62516900	C	3.00690000	2.28180900	-0.77023200
C	-6.13084400	0.95126500	-0.63722900	C	-1.59616900	-2.38576900	-0.73899300
C	-4.00722400	4.02604200	-0.63293300	C	-3.00703500	-2.28404300	-0.77031400
C	-4.39510400	2.67742600	-0.62447700	C	-2.86364800	0.18723400	-0.74473200
C	-5.77517100	2.26706500	-0.63694000	C	-3.64237600	-0.99459400	-0.77469200
H	-4.77520200	4.79696200	-0.64853200	C	3.48121400	-1.46306300	-0.77208800
H	-6.54061600	3.03969000	-0.65082000	C	2.68207900	-2.65779700	-0.77343600
H	-7.18132100	0.66965300	-0.65146300	C	1.26919000	-2.57428100	-0.74242000
H	-6.54179700	-1.73785200	-0.65044100	C	-0.96197500	-3.65132900	-0.76516800
C	-1.02209000	-0.99576900	2.79565500	C	0.47344100	-3.74581700	-0.76765300
C	0.34804000	-1.37024600	2.76313200	C	-3.48033000	1.46218200	-0.77141400
C	1.37046400	-0.38425900	2.79758600	C	-2.68072900	2.65780500	-0.76776000
C	1.00959300	0.98962500	2.76159800	C	-1.26760900	2.57418800	-0.73934200
C	-0.35535700	1.38229800	2.79758500	C	0.96032000	3.65053900	-0.77207200
C	-1.36463400	0.38288500	2.75951900	C	-0.47411500	3.74508900	-0.76898900
H	0.61677100	-2.42244100	2.71248800	C	1.10901900	-5.02589100	-0.80112600
H	1.78643400	1.74843500	2.70930500	C	0.27410600	-6.19869000	-0.82154600
H	-2.41022000	0.67602400	2.70636700	C	-1.08583400	-6.10857600	-0.81936100
H	5.90375400	4.14447200	-0.65244900	C	-3.79754700	-3.47442600	-0.80232000
H	6.54300200	1.73690100	-0.64992500	C	-5.23093500	-3.33768100	-0.82840100
H	7.18313100	-0.67017600	-0.65995200	C	-3.15798500	-4.72190400	-0.81008900
H	6.54243300	-3.04020900	-0.65895400	C	-5.06836800	-0.89559600	-0.80964400
H	4.77673900	-4.79685500	-0.64701300	C	-5.83360200	-2.11545400	-0.83205000
H	3.01145900	-6.55444600	-0.64824900	C	-1.75961500	-4.83645800	-0.79665700
N	-2.02362700	-1.97411800	2.78247000	H	-1.69252700	-7.01089900	-0.83983800
H	-1.74651500	-2.87153300	3.15796200	H	-3.76220200	-5.62648400	-0.83367700

H	-5.83278800	-4.24321000	-0.84978800	H	0.75706900	-7.17282600	-0.84391800
H	-6.91830600	-2.04111800	-0.85667700	O	-2.48021300	-1.24751500	2.72270900
C	5.06797700	0.89338400	-0.80314200	O	0.15854800	2.77550600	2.72093200
C	5.83284500	2.11277200	-0.82695000	O	2.32187200	-1.52066200	2.72897100
C	-1.10994100	5.02482200	-0.80165100	C	-3.67263300	-0.48330600	2.85901300
C	-0.27483900	6.19774100	-0.82521200	H	-3.84581800	0.15608200	1.98690900
C	3.79775300	3.47216200	-0.80377500	H	-4.48158600	-1.21169200	2.93349900
C	5.23091900	3.33556200	-0.82697700	H	-3.64653900	0.12968000	3.76950500
C	3.15679700	4.72079700	-0.81536100	C	2.25537800	-2.93548900	2.86722500
C	1.75906500	4.83597300	-0.80540900	H	1.78594800	-3.40640000	1.99707300
C	1.08499700	6.10858800	-0.82694000	H	3.29048500	-3.27267500	2.94043000
H	5.83298300	4.24090800	-0.84978900	H	1.71278500	-3.21734200	3.77910900
H	3.76166400	5.62499500	-0.84047900	C	1.41677400	3.42575400	2.86002000
H	1.69152800	7.01101600	-0.84987700	H	2.06118600	3.25218200	1.99181700
H	-0.75810600	7.17176200	-0.84630300	H	1.19079400	4.49093300	2.92899900
C	3.30943100	-3.94224500	-0.80755300	H	1.93013300	3.09958800	3.77405000
C	2.51083400	-5.09511400	-0.81507400				
C	4.74856900	-3.99491300	-0.83287500	<b>17-F</b>			
C	5.66799100	-0.37482700	-0.81755500	C	1.28513000	0.62645100	-0.57093900
C	4.90736500	-1.55234300	-0.80712600	C	1.18649600	-0.79859500	-0.56996900
C	5.50572500	-2.86188100	-0.83292700	C	0.09789500	1.42608700	-0.57095800
C	-5.66747200	0.37242700	-0.81982900	C	-0.09968200	-1.42693300	-0.56993500
C	-4.90661800	1.55175800	-0.80661300	C	-1.18561600	0.79898400	-0.57018300
C	-5.50504800	2.86104100	-0.82952700	C	-1.28447600	-0.62902100	-0.57040900
C	-2.51007800	5.09478700	-0.81244500	Cr	0.00001800	0.00064600	1.13532700
C	-3.30848000	3.94110200	-0.80089100	C	-0.19921000	-2.86300900	-0.58062600
C	-4.74703700	3.99369900	-0.82670000	C	0.98077900	-3.64467400	-0.59498300
H	-2.99113400	6.07042500	-0.83674600	C	2.38046800	-1.60270200	-0.58063600
H	-5.22487800	4.97032300	-0.84872100	C	2.27183400	-3.01393000	-0.59488400
H	-6.59009300	2.92974700	-0.85397900	C	-2.37956100	1.60322600	-0.58065800
H	-6.75291800	0.44435900	-0.84630300	C	-2.27181300	3.01369800	-0.59710600
C	-1.28842700	-0.58378000	2.67310500	C	0.19730500	2.86213600	-0.58141800
C	-0.13320500	-1.41151600	2.64584100	C	-0.98152900	3.64405900	-0.59747200
C	1.15136700	-0.82019800	2.67595300	C	-1.47458000	-3.47494700	-0.59747800
C	1.29046100	0.59385900	2.64520900	C	-2.66567500	-2.67274600	-0.59755800
C	0.13637100	1.41131500	2.67253400	C	-2.57787500	-1.26091300	-0.58087100
C	-1.15783900	0.82449000	2.64414700	C	-3.64649000	0.97220000	-0.59518000
H	-0.27308700	-2.48433600	2.61319900	C	-3.74576200	-0.46125800	-0.59537900
H	2.29004100	1.00785900	2.61212100	C	1.47375700	3.47368100	-0.59669700
H	-2.01723900	1.48171900	2.60918100	C	2.66557500	2.67099300	-0.59711400
H	6.91753600	2.03828700	-0.84957000	C	2.57858900	1.25829300	-0.58205000
H	6.75341600	-0.44601000	-0.84340600	C	3.64704600	-0.97279600	-0.59774000
H	6.59080800	-2.93030600	-0.85675600	C	3.74626600	0.45979300	-0.59855900
H	5.22652500	-4.97147900	-0.85693700	C	-5.02800500	-1.09236200	-0.61267500
H	2.99132600	-6.07110000	-0.84028100	C	-6.19838900	-0.25434300	-0.62398400

C	-6.10423300	1.10533900	-0.62350500	C	0.80700800	1.18516500	2.74806100
C	-3.45972900	3.80844800	-0.61423700	H	-2.50659700	0.19059200	2.69607800
C	-3.31923700	5.24119900	-0.62714100	H	1.09059100	-2.26280300	2.69868900
C	-4.70883000	3.17164300	-0.61886000	H	1.41684400	2.07928900	2.69307200
C	-0.87833400	5.06955000	-0.61513500	H	2.01623200	-6.92417100	-0.63365600
C	-2.09488200	5.83935200	-0.62758400	H	-0.46776900	-6.74975200	-0.63211900
C	-4.82955000	1.77405700	-0.61183200	H	-2.95199500	-6.58066800	-0.64056300
H	-7.00433600	1.71525500	-0.63409400	H	-4.98852800	-5.20895000	-0.64089000
H	-5.61129800	3.77925000	-0.63077500	H	-6.07882200	-2.97056600	-0.63307300
H	-4.22277500	5.84600200	-0.63786900	H	-7.17397400	-0.73435600	-0.63492000
H	-2.01665700	6.92380600	-0.63866100	F	-1.19126000	2.47788300	2.70891600
C	0.87780300	-5.07012100	-0.61194600	F	-1.54789200	-2.26722300	2.71494000
C	2.09431100	-5.83968800	-0.62302200	F	2.73982300	-0.20400400	2.71153300
C	5.02847900	1.09112200	-0.61707500				
C	6.19908500	0.25314700	-0.63011800	<b>17-CI</b>			
C	3.45956000	-3.80882500	-0.61164600	C	1.27365200	-0.64741200	-0.67116000
C	3.31890600	-5.24140200	-0.62282400	C	0.07600400	-1.42698700	-0.67114200
C	4.70931800	-3.17174500	-0.61938000	C	1.19725200	0.78033900	-0.67198100
C	4.83002100	-1.77487900	-0.61530700	C	-1.19880900	-0.77933900	-0.67074900
C	6.10492700	-1.10626100	-0.62922800	C	-0.07675200	1.42753700	-0.67104400
H	4.22237900	-5.84633000	-0.63332100	C	-1.27515100	0.64752500	-0.67042700
H	5.61150600	-3.77976000	-0.63149100	Cr	0.00057000	-0.00022800	1.08543900
H	7.00492300	-1.71630200	-0.64035900	C	-2.40460200	-1.56367400	-0.72240800
H	7.17459000	0.73327200	-0.64190700	C	-2.31852700	-2.97613800	-0.75764300
C	-3.95177300	-3.29613900	-0.61574000	C	0.15304500	-2.86331000	-0.72269900
C	-5.10118400	-2.49323400	-0.62055700	C	-1.03870200	-3.62634000	-0.75785400
C	-4.01022000	-4.73455500	-0.62928400	C	-0.15313500	2.86395700	-0.72260000
C	-0.39287900	-5.66438600	-0.61982200	C	1.03752300	3.62662800	-0.77300100
C	-1.56896700	-4.90106200	-0.61539300	C	2.40266100	1.56516900	-0.72369800
C	-2.87999800	-5.49579000	-0.62909300	C	2.31697300	2.97655400	-0.77342000
C	0.39170900	5.66347500	-0.62068700	C	-3.66059500	-0.91392800	-0.77151700
C	1.56836300	4.89970600	-0.61394900	C	-3.73719000	0.51906900	-0.77132700
C	2.87932100	5.49420500	-0.62648700	C	-2.55768500	1.29894100	-0.72192600
C	5.10154600	2.49127900	-0.62266900	C	-1.41954900	3.49557000	-0.75730600
C	3.95151200	3.29455800	-0.61504400	C	-2.62260500	2.71257900	-0.75686700
C	4.00977400	4.73282500	-0.62706700	C	3.65948200	0.91468900	-0.75868800
H	6.07895900	2.96906400	-0.63553200	C	3.73612700	-0.51868900	-0.75828600
H	4.98803200	5.20735700	-0.63859600	C	2.55591100	-1.29941300	-0.72301200
H	2.95145900	6.57909100	-0.63757800	C	1.41833900	-3.49471700	-0.77224800
H	0.46709000	6.74880600	-0.63301900	C	2.62106400	-2.71195100	-0.77217600
C	-0.60454000	1.25900600	2.74743400	C	-3.89805400	3.35603800	-0.81078300
C	-1.42727400	0.10970100	2.75003400	C	-3.93436800	4.79440800	-0.84508300
C	-0.78555100	-1.14968900	2.75007000	C	-2.79230300	5.53777200	-0.84550900
C	0.62112300	-1.28752000	2.75160400	C	0.95692500	5.05237100	-0.82831700
C	1.39088800	-0.10210700	2.74859900	C	2.18432600	5.80290700	-0.87259800

C	-0.30349500	5.66620500	-0.83996900	H	2.51076400	0.11649200	2.65764200
C	3.51621200	3.75179700	-0.82906000	H	-4.31385700	-5.77540000	-0.87867700
C	3.39907400	5.18564200	-0.87291100	H	-5.66780400	-3.68805300	-0.87863400
C	-1.49166000	4.92226400	-0.81166200	H	-7.02732900	-1.60524000	-0.90573700
H	-2.84652500	6.62321800	-0.87799400	H	-7.15839400	0.84768400	-0.90553400
H	-0.36159000	6.75190100	-0.88003900	H	-6.02861100	3.06361000	-0.87789800
H	2.12236500	6.88779800	-0.90901300	H	-4.90498000	5.28333900	-0.87725600
H	4.31208700	5.77493000	-0.90947600	Cl	-3.15964800	-0.14916400	2.76774700
C	-3.51804900	-3.75187100	-0.81186300	Cl	1.45518700	2.81144800	2.76340500
C	-3.40083200	-5.18588600	-0.84629700	Cl	1.71145400	-2.66534500	2.76162200
C	3.89620800	-3.35496900	-0.82695700				
C	3.93256900	-4.79318200	-0.87024600	<b>17-Br</b>			
C	-0.95835200	-5.05258500	-0.81203600	C	-0.77737900	1.19943200	-0.96115000
C	-2.18593900	-5.80317700	-0.84638700	C	0.64989400	1.27309200	-0.96162400
C	0.30244400	-5.66563400	-0.83958700	C	-1.42741600	-0.07369300	-0.96202400
C	1.49014800	-4.92094300	-0.82730500	C	1.42726100	0.07359900	-0.96199000
C	2.79060800	-5.53644900	-0.87048000	C	-0.65020700	-1.27284200	-0.96165200
H	-2.12411900	-6.88820100	-0.87890900	C	0.77734800	-1.19923000	-0.96167700
H	0.36053000	-6.75133700	-0.87948600	Cr	0.00009900	-0.00005100	0.80308000
H	2.84464900	-6.62179300	-0.90651400	C	2.86364100	0.14696200	-1.02204600
H	4.90313900	-5.28193700	-0.90609400	C	3.49789200	1.41180600	-1.06130900
C	-5.00834800	1.16992600	-0.82611200	C	1.30375000	2.55403000	-1.02112100
C	-5.05941800	2.57087000	-0.83814200	C	2.71740600	2.61616300	-1.06035600
C	-6.19157600	0.35159800	-0.86955300	C	-1.30475600	-2.55339200	-1.02173400
C	-4.75653600	-3.09496100	-0.83899400	C	-2.71706600	-2.61543800	-1.08028000
C	-4.85505300	-1.69655800	-0.82659200	C	-2.86372500	-0.14769200	-1.02238400
C	-6.11883500	-1.00901000	-0.86975400	C	-3.49738200	-1.41132800	-1.08142100
C	4.75509600	3.09568300	-0.84099200	C	3.62364200	-1.04504600	-1.08078900
C	4.85447500	1.69734600	-0.81296500	C	2.97103400	-2.32285000	-1.07965100
C	6.11838100	1.00967700	-0.84671600	C	1.55986500	-2.40582700	-1.02091200
C	5.05805500	-2.57053400	-0.83900200	C	-0.52645500	-3.73504700	-1.05877100
C	5.00784400	-1.16954700	-0.81191200	C	0.90687700	-3.66131700	-1.05865500
C	6.19116700	-0.35106900	-0.84621200	C	-3.62445300	1.04543200	-1.06057700
H	6.02725100	-3.06328500	-0.87856400	C	-2.97174900	2.32356500	-1.05926900
H	7.15817500	-0.84705800	-0.87823800	C	-1.55917800	2.40661700	-1.02001300
H	7.02705200	1.60585200	-0.87903000	C	0.52614400	3.73459700	-1.07744100
H	5.66635400	3.68876900	-0.88092700	C	-0.90683200	3.66085800	-1.07725700
C	0.64675900	1.24690800	2.70520800	C	1.68692800	-4.85770200	-1.11930500
C	-0.76929100	1.20173800	2.70066800	C	0.99697400	-6.12018200	-1.15556200
C	-1.40062100	-0.06654900	2.70711800	C	-0.36385900	-6.19021400	-1.15562000
C	-0.65353600	-1.27046000	2.69823100	C	-3.36248600	-3.88886400	-1.14371500
C	0.76057100	-1.18302500	2.70513700	C	-4.80043300	-3.92231400	-1.19646400
C	1.42941000	0.06587200	2.69758900	C	-2.58057300	-5.05230100	-1.15414400
H	-1.35390900	2.11294200	2.66312200	C	-4.92330500	-1.48007500	-1.14668000
H	-1.15025200	-2.23234500	2.65892500	C	-5.54136500	-2.77884900	-1.19798100

C	-1.17975500	-5.00520900	-1.11950400	H	6.88188000	-2.13589400	-1.23997600
H	-0.86187400	-7.15605500	-1.19079900	H	5.76443100	-4.32359000	-1.23758200
H	-3.07522600	-6.02026000	-1.19984300	H	3.67631800	-5.67319500	-1.19947200
H	-5.29092600	-4.89175600	-1.23899200	H	1.59141700	-7.02989500	-1.19070600
H	-6.62654900	-2.83040200	-1.24146100	Br	2.94588600	-1.52994600	2.52096200
C	4.92439800	1.48095600	-1.12528800	Br	-2.79826300	-1.78573700	2.52049000
C	5.54267800	2.77994800	-1.16412000	Br	-0.14687800	3.31531400	2.52039600
C	-1.68692500	4.85655500	-1.13988300				
C	-0.99703300	6.11871700	-1.18938200				
C	3.36339700	3.88992900	-1.12252000	<b>17-CO<sub>2</sub>Me</b>			
C	4.80166000	3.92348300	-1.16277800	C	1.37957500	-0.37388800	-0.90102000
C	2.58039800	5.05248300	-1.15441700	C	0.36431200	-1.38169300	-0.90008800
C	1.17948500	5.00402100	-1.14051300	C	1.01498900	1.00698000	-0.90026100
C	0.36368300	6.18872400	-1.18964900	C	-1.01401200	-1.00715200	-0.90214500
H	5.29239000	4.89301700	-1.19980900	C	-0.36543500	1.38217800	-0.90165300
H	3.07492700	6.02047800	-1.20067900	C	-1.37910200	0.37589400	-0.90071100
H	0.86176400	7.15429100	-1.23127700	Cr	-0.00083700	0.00021500	0.86859200
H	-1.59150700	7.02816300	-1.23077300	C	-2.03402300	-2.02024300	-0.95791200
C	3.74358000	-3.52343800	-1.14316600	C	-1.66344200	-3.38503800	-0.99787100
C	3.08517300	-4.76094400	-1.15383200	C	0.73148200	-2.77169800	-0.95734000
C	5.17731700	-3.40942900	-1.19558200	C	-0.27950000	-3.76126400	-0.99796800
C	5.66568300	0.29141800	-1.15963200	C	-0.73287900	2.77194000	-0.95790200
C	5.04909800	-0.96741600	-1.14610100	C	0.27813600	3.76114100	-1.01277400
C	5.79711400	-2.19601800	-1.19704400	C	2.03525300	2.01997900	-0.95836600
C	-5.66581000	-0.29114300	-1.15966400	C	1.66297600	3.38491300	-1.01351100
C	-5.05053500	0.96815400	-1.12453900	C	-3.39617600	-1.63933500	-1.01221400
C	-5.79883100	2.19692300	-1.16249400	C	-3.76269400	-0.25198000	-1.01258800
C	-3.08539300	4.76114700	-1.15322200	C	-2.76656600	0.75289400	-0.95828400
C	-3.74495200	3.52437200	-1.12109000	C	-2.10024400	3.13349800	-0.99744600
C	-5.17901800	3.41042900	-1.16081200	C	-3.11813800	2.12309700	-0.99768700
H	-3.67644300	5.67345000	-1.19907400	C	3.39771000	1.63933100	-0.99842400
H	-5.76640300	4.32464600	-1.19702600	C	3.76374800	0.25270900	-0.99699600
H	-6.88379700	2.13694000	-1.19986600	C	2.76693300	-0.75061900	-0.95688700
H	-6.75134100	-0.34712500	-1.20664700	C	2.09979000	-3.13191600	-1.01134100
C	-1.18395400	-0.75620900	2.42243500	C	3.11806900	-2.12068500	-1.01032800
C	0.06347000	-1.42671300	2.41461400	C	-4.49778700	2.49365600	-1.06081300
C	1.24633600	-0.64805500	2.42255000	C	-4.82611800	3.89415000	-1.10007800
C	1.20344900	0.76754100	2.41397900	C	-3.85877400	4.85380900	-1.09970300
C	-0.06248800	1.40250600	2.42282300	C	-0.09131800	5.13992000	-1.08014700
C	-1.26682400	0.65759700	2.41537600	C	0.95698000	6.12409600	-1.13849900
H	0.11194000	-2.50776800	2.37868400	C	-1.44984400	5.48474900	-1.09535400
H	2.11581700	1.34968400	2.37701500	C	2.67967100	4.38763400	-1.08356300
H	-2.22715700	1.15676400	2.38060000	C	2.27288200	5.76713600	-1.14134600
H	6.62804600	2.83167400	-1.20205100	C	-2.46087700	4.51523000	-1.06021800
H	6.75121100	0.34731300	-1.20669300	H	-4.13202100	5.90552000	-1.13577400
				H	-1.72738800	6.53560200	-1.14244500

H	0.67504700	7.17310000	-1.18666200	H	-5.87574700	4.17527700	-1.13754400
H	3.04641500	6.52962800	-1.19314300	C	2.24384600	-1.85317700	2.49996000
C	-2.67980800	-4.38830100	-1.06080300	C	0.48173300	2.86801800	2.50488200
C	-2.27405900	-5.76812900	-1.10157700	C	-2.72511800	-1.01822500	2.50071400
C	4.49694700	-2.49018100	-1.07718500	O	3.40627900	-1.49863500	2.43359700
C	4.82508300	-3.89006700	-1.13546000	O	1.78944800	3.19423400	2.62396800
C	0.08939300	-5.14125900	-1.06229800	O	-2.99864800	-2.20221400	2.43201600
C	-0.95929600	-6.12595800	-1.10237500	O	1.87187400	-3.14883000	2.61877800
C	1.44792800	-5.48468200	-1.09674500	O	-0.40759700	3.69660400	2.44249100
C	2.45977700	-4.51362100	-1.08141100	O	-3.66130100	-0.04861800	2.62244900
C	3.85793200	-4.85116200	-1.13866100	C	2.95041400	-4.09235300	2.69015500
H	-0.67799700	-7.17553000	-1.14041700	H	2.47511700	-5.06899000	2.78769600
H	1.72559800	-6.53546100	-1.14867700	H	3.56207300	-4.05199500	1.78607800
H	4.13166600	-5.90228900	-1.19026600	H	3.58169400	-3.88384600	3.55870800
H	5.87453900	-4.17030300	-1.18343600	C	-5.01809700	-0.50976700	2.69261300
C	-5.13946700	0.12713600	-1.08173100	H	-5.62511300	0.39070100	2.79209900
C	-5.47456300	1.48888500	-1.09556400	H	-5.28973000	-1.05707700	1.78724800
C	-6.13085400	-0.91490900	-1.13911900	H	-5.15399300	-1.16250500	3.55972700
C	-4.02494300	-3.99758100	-1.09535100	C	2.06729700	4.60002000	2.69591100
C	-4.40556400	-2.64864400	-1.07904800	H	1.57045400	5.04223900	3.56428000
C	-5.78202700	-2.23298200	-1.13690800	H	3.15065300	4.67662100	2.79425600
C	4.02655100	3.99699100	-1.09829600	H	1.72720900	5.10964200	1.79164700
C	4.40840800	2.64877400	-1.06267600				
C	5.78549600	2.23298100	-1.10200500	<b>17-CN</b>			
C	5.47493800	-1.48611600	-1.09296200	C	-0.38833200	1.37469800	-0.62848400
C	5.14081000	-0.12580800	-1.05916100	C	0.99770300	1.02292600	-0.62806700
C	6.13297000	0.91546500	-1.10004900	C	-1.38449100	0.35178400	-0.62811700
H	6.52375500	-1.77121200	-1.14010200	C	1.38549300	-0.35128100	-0.62703400
H	7.18035400	0.62610800	-1.13615400	C	-0.99617600	-1.02446500	-0.62771400
H	6.55381900	3.00130200	-1.14065600	C	0.38780400	-1.37576900	-0.62720500
H	4.79780900	4.76271200	-1.15066900	Cr	-0.00027600	0.00045000	1.18003600
C	0.26588900	1.39719400	2.50794300	C	2.77897600	-0.70584800	-0.66427600
C	-1.07633200	0.92587200	2.48286800	C	3.75909800	0.31567100	-0.69012800
C	-1.34360500	-0.46994800	2.50677800	C	2.00025600	2.05364300	-0.66624900
C	-0.26374900	-1.39660300	2.48035300	C	3.36980400	1.69516800	-0.69159100
C	1.07855200	-0.93027800	2.50546500	C	-1.99998100	-2.05395000	-0.66599300
C	1.34124000	0.46811100	2.48048100	C	-3.36874200	-1.69567500	-0.70267200
H	-1.88465400	1.64338400	2.43981400	C	-2.77839800	0.70460900	-0.66570400
H	-0.48052200	-2.45553300	2.43590100	C	-3.75796100	-0.31633800	-0.70198600
H	2.36639600	0.81054200	2.43552100	C	3.15310200	-2.07037500	-0.69859000
H	-3.04834500	-6.53047800	-1.13813100	C	2.15313000	-3.09718900	-0.69867800
H	-4.79631500	-4.76322600	-1.14314300	C	0.77913100	-2.75931500	-0.66441700
H	-6.54951100	-3.00162700	-1.18512300	C	-1.60541300	-3.41348000	-0.69151000
H	-7.17801600	-0.62632200	-1.19020300	C	-0.21604600	-3.76615500	-0.69024100
H	-6.52341400	1.77380800	-1.14683100	C	-3.15275700	2.06987600	-0.68986800

C	-2.15267400	3.09681300	-0.68999200	H	-6.55252000	1.66155800	-0.77306300
C	-0.77793000	2.75873000	-0.66616900	C	-1.37529900	-0.38215600	2.78789700
C	1.60591200	3.41238600	-0.70306300	C	-0.35648600	-1.38191200	2.75565600
C	0.21670300	3.76498900	-0.70237900	C	1.01781500	-0.99654900	2.78976900
C	0.17655800	-5.14029500	-0.72816800	C	1.37428800	0.38548600	2.75601300
C	-0.85562600	-6.14271300	-0.75313900	C	0.35342600	1.38308700	2.78781700
C	-2.17662400	-5.80740600	-0.75474500	C	-1.02168900	1.00065500	2.75335600
C	-4.36231600	-2.72161700	-0.74262600	H	-0.62556900	-2.43024700	2.70138900
C	-5.74606700	-2.32976900	-0.77342500	H	2.41676300	0.67658800	2.70220400
C	-3.95785500	-4.06397300	-0.75213800	H	-1.79491400	1.75782300	2.69713900
C	-5.14135000	0.03882100	-0.74041500	H	7.17048500	0.74690900	-0.77398900
C	-6.11607500	-1.01861700	-0.77217700	H	6.55268800	-1.66445800	-0.77118000
C	-2.60580200	-4.43406800	-0.73117200	H	5.94530600	-4.07559700	-0.78546800
H	-2.93765200	-6.58335600	-0.77728900	H	4.23173300	-5.83521300	-0.78572100
H	-4.71699400	-4.84265700	-0.77902100	H	1.83747500	-6.50624000	-0.77167800
H	-6.50131000	-3.11119200	-0.79604100	H	-0.55673400	-7.18770600	-0.77442900
H	-7.16843000	-0.74734300	-0.79377100	C	-2.75337900	-0.76694200	2.78231300
C	5.14321000	-0.04040200	-0.72788900	C	0.70898700	2.76900200	2.78241100
C	6.11793700	1.01797100	-0.75285300	C	2.04004300	-1.99772100	2.78402400
C	-0.17496500	5.13845200	-0.74064500	N	-3.87417000	-1.07995800	2.81109700
C	0.85629400	6.14083900	-0.77234100	N	2.87143000	-2.81198200	2.81156700
C	4.36353400	2.72223500	-0.73125400	N	0.99774400	3.89628800	2.81120600
C	5.74778500	2.32961800	-0.75463700				
C	3.95778500	4.06399500	-0.75234400	<b>18-a</b>			
C	2.60518000	4.43278200	-0.74291000	C	-6.85117600	0.71755600	-0.40674900
C	2.17679200	5.80563900	-0.77363500	C	-5.62069700	1.42925500	-0.34137800
H	6.50329500	3.11095400	-0.77715600	C	-6.85075700	-0.72025100	-0.39350700
H	4.71611900	4.84346400	-0.77914300	C	-4.37673600	0.71425100	-0.31527600
H	2.93791700	6.58132500	-0.79616200	C	-5.62008600	-1.43294800	-0.34743400
H	0.55720800	7.18564500	-0.79384000	C	-4.37781100	-0.71641700	-0.30148500
C	2.53720600	-4.47278500	-0.73645000	Cr	-5.70873200	0.00529300	1.53815100
C	1.54150300	-5.45975300	-0.74631500	C	-3.14336300	1.42880000	-0.28155000
C	3.94040600	-4.78820100	-0.76516200	C	-3.15206100	2.85959300	-0.30284200
C	5.49871200	-1.39638800	-0.74589700	C	-5.61961100	2.86861700	-0.37510700
C	4.53845100	-2.41788300	-0.73617100	C	-4.39082100	3.56795400	-0.34518000
C	4.89091700	-3.81219600	-0.76498800	C	-5.61926500	-2.87159600	-0.36466000
C	-5.49826600	1.39459700	-0.74774900	C	-6.85138900	-3.56885900	-0.43262000
C	-4.53916100	2.41691500	-0.72704300	C	-8.09027700	-1.43651100	-0.47357400
C	-4.89119100	3.81205000	-0.74888000	C	-8.08107300	-2.85526900	-0.48473600
C	-1.53975100	5.45934000	-0.74785300	C	-1.92268300	0.71632700	-0.25910900
C	-2.53631600	4.47349500	-0.72714100	C	-1.92297200	-0.71829000	-0.25445300
C	-3.94033000	4.78843500	-0.74888600	C	-3.14302000	-1.43105700	-0.28303400
H	-1.83462200	6.50614200	-0.77307100	C	-4.39002400	-3.57082900	-0.33875600
H	-4.23195300	5.83550100	-0.76907200	C	-3.15171900	-2.86168800	-0.29490200
H	-5.94564300	4.07572500	-0.76909500	C	-9.31041800	-0.71833700	-0.54411400



C	-9.31081000	0.71480200	-0.54665100	H	-11.46133600	-3.38500500	-0.67161200
C	-8.09068500	1.43328400	-0.47366500	C	-5.10432200	1.34875600	2.63126100
C	-6.85190300	3.56549700	-0.43949900	C	-4.94258200	-1.24338100	2.64351600
C	-8.08164700	2.85221100	-0.49201000	C	-7.24907600	-0.08424700	2.52387800
C	-1.92706700	-3.56804500	-0.27117200	O	-4.45063700	-2.04529400	3.32811400
C	-1.92755400	-5.01400200	-0.28262100	O	-4.71725600	2.21188800	3.30889500
C	-3.16604500	-5.69253500	-0.32616800	O	-8.23978800	-0.14121200	3.13232200
C	-6.84666500	-5.01052200	-0.45107900	C	0.53483500	3.56558700	-0.20973000
C	-8.11933200	-5.69115000	-0.51582600	C	1.76359700	2.85808300	-0.17488400
C	-5.64021600	-5.69006100	-0.40997100	C	0.53472700	5.01242900	-0.21624500
C	-9.32840700	-3.56402800	-0.55759800	C	-0.69890600	5.69196100	-0.25731300
C	-9.29188600	-5.00715600	-0.56655000	C	1.76387200	1.42582900	-0.17248500
C	-4.38919800	-5.01212600	-0.35715400	C	1.76420500	-1.42677000	-0.17255600
H	-3.16629500	-6.77998300	-0.33698200	C	2.99401200	-0.71545200	-0.14164700
H	-5.64034100	-6.77765700	-0.42179700	C	1.76423100	-2.85901400	-0.17540900
H	-8.11733600	-6.77819800	-0.52463000	C	2.99384700	0.71481800	-0.14075100
H	-10.23683100	-5.54245800	-0.61596300	C	0.53570600	-3.56682400	-0.20848000
C	-1.92782300	3.56614100	-0.27560400	C	-0.69765700	-5.69350700	-0.25263000
C	-1.92848900	5.01207500	-0.28887800	C	0.53586000	-5.01359100	-0.21466400
C	-9.32917000	3.56053300	-0.56365500	H	-0.69884100	6.77940400	-0.26357400
C	-9.29275600	5.00367800	-0.57494000	H	-0.69727000	-6.78096600	-0.25844900
C	-4.39006600	5.00931300	-0.36709700	C	2.99638200	3.56563200	-0.14391600
C	-3.16716500	5.69000900	-0.33603400	C	4.22285600	2.85784700	-0.11031600
C	-5.64111500	5.68686400	-0.42211300	C	2.99718900	5.01059800	-0.14640900
C	-6.84745700	5.00730000	-0.46157300	C	4.22250000	1.42453100	-0.11007100
C	-8.12015900	5.68776800	-0.52703500	C	1.76810100	5.69145300	-0.18333200
H	-3.16783700	6.77744600	-0.34757900	C	4.22286700	-1.42486300	-0.11086700
H	-5.64139000	6.77445200	-0.43492700	C	5.45112300	-0.71410100	-0.07946400
H	-8.11815800	6.77479600	-0.53727700	C	4.22358600	-2.85818100	-0.11308600
H	-10.23772400	5.53887700	-0.62490200	C	2.99730500	-3.56625000	-0.14567300
C	-0.69152800	-1.42867800	-0.23160600	C	5.45093100	0.71405500	-0.07813200
C	-0.69341000	-2.85956500	-0.23572000	C	1.76947100	-5.69235400	-0.18396900
C	0.53575400	-0.71711000	-0.20126200	C	2.99845600	-5.01118000	-0.14901700
C	-0.69390800	2.85800200	-0.23879800	H	1.76880800	6.77894700	-0.18625400
C	-0.69183500	1.42705600	-0.23136900	H	1.77043400	-6.77986000	-0.18706900
C	0.53570100	0.71586500	-0.20193100	C	5.45649900	3.56472600	-0.07831000
C	-10.51835000	-2.84505900	-0.61902900	C	6.68352500	2.85572000	-0.04593700
C	-10.54368500	-1.43349000	-0.61657900	C	5.45702300	5.00721400	-0.07868800
C	-11.76054100	-0.68700100	-0.68506300	C	6.68293700	1.42434200	-0.04666100
C	-10.51914500	2.84136200	-0.62254200	C	4.23692300	5.68903600	-0.11277600
C	-10.54409000	1.42964000	-0.61836300	C	6.68333300	-1.42409600	-0.04838000
C	-11.76083400	0.68278300	-0.68543100	C	7.90963500	-0.71408400	-0.01681000
H	-11.46222200	3.38103100	-0.67595900	C	6.68432900	-2.85548000	-0.05012100
H	-12.70019200	1.22742200	-0.73776200	C	7.90943200	0.71462000	-0.01544500
H	-12.69974100	-1.23202100	-0.73640500	C	5.45747700	-3.56478000	-0.08237300

C	4.23840300	-5.68938500	-0.11770200	C	4.31786500	0.71649100	-0.44018900
C	5.45839400	-5.00726700	-0.08446900	Cr	5.79406200	0.01600900	1.33494800
H	4.23816400	6.77661300	-0.11350300	C	3.09582100	-1.43598200	-0.35245800
H	4.23989700	-6.77697300	-0.11930200	C	3.09416600	-2.86463300	-0.38865700
C	7.91848400	3.56165300	-0.01362600	C	5.55575400	-2.87259200	-0.55697500
C	9.14218600	2.85132500	0.01756300	C	4.32641800	-3.57321500	-0.48012700
C	7.91380200	5.00508500	-0.01291800	C	5.55657400	2.86799600	-0.57324400
C	6.70911100	5.68546600	-0.04481100	C	6.78288500	3.56423000	-0.70746500
C	9.14284100	1.42647800	0.01638000	C	8.01749500	1.43151200	-0.81684000
C	9.14326100	-1.42565700	0.01391500	C	8.00763000	2.85089400	-0.83201600
C	10.37363300	-0.71270400	0.04565200	C	1.87228000	-0.71940700	-0.30613200
C	9.14302800	-2.85050200	0.01247500	C	1.86921600	0.71696800	-0.28930800
C	10.37342600	0.71382700	0.04703700	C	3.09702500	1.43365400	-0.35447700
C	7.91951500	-3.56113300	-0.01931300	C	4.32937600	3.56865500	-0.48796600
C	6.71070200	-5.68525200	-0.05279600	C	3.09502900	2.86228300	-0.39196700
C	7.91524500	-5.00456800	-0.02090700	C	9.23163600	0.71252700	-0.96271000
H	6.70995100	6.77323800	-0.04427900	C	9.23030000	-0.72023300	-0.95833100
H	6.71182300	-6.77303200	-0.05374600	C	8.01636300	-1.43816900	-0.81474900
C	10.39352400	3.55985900	0.05037000	C	6.78089300	-3.57055900	-0.69461100
C	11.58393300	2.84286900	0.08004100	C	8.00599800	-2.85656100	-0.81818100
C	10.35946400	5.00258600	0.05113300	C	1.86659600	3.57194900	-0.34712000
C	9.18648900	5.68690700	0.02124000	C	1.86662100	5.01656600	-0.38073000
C	11.60854600	1.43007900	0.07910300	C	3.10661000	5.69209200	-0.46022700
C	11.60897800	-1.42866300	0.07623000	C	6.77730200	5.00693100	-0.73227100
C	12.82624300	-0.68488600	0.10786000	C	8.04515000	5.68676300	-0.86558800
C	11.58478100	-2.84145200	0.07436700	C	5.57520900	5.68707200	-0.63568500
C	12.82603300	0.68659900	0.10926700	C	9.24936200	3.55876100	-0.97374700
C	10.39458000	-3.55873500	0.04359500	C	9.21276800	5.00219500	-0.97917700
C	9.18815500	-5.68608600	0.01118200	C	4.32661500	5.01080000	-0.52355100
C	10.36094500	-5.00146900	0.04165500	H	3.10775400	6.77924400	-0.48422100
H	9.18415600	6.77408800	0.02253400	H	5.57532300	6.77452100	-0.65297300
H	11.30602100	5.53695800	0.07676100	H	8.04323000	6.77373400	-0.87400500
H	12.52826000	3.38270700	0.10510900	H	10.15371300	5.53717000	-1.08029100
H	13.76632200	1.23186600	0.13400700	C	1.86318700	-3.57234000	-0.34765700
H	13.76669400	-1.22992000	0.13144300	C	1.86308700	-5.01707700	-0.38232300
H	12.52927400	-3.38105900	0.09812400	C	9.24683600	-3.56588900	-0.96192700
H	11.30767400	-5.53561100	0.06573400	C	9.20988700	-5.00921900	-0.96281600
H	9.18613300	-6.77327300	0.01052800	C	4.32343400	-5.01541700	-0.51238600
				C	3.10210200	-5.69491800	-0.45494700
				C	5.57188200	-5.69310300	-0.61864200
				C	6.77444200	-5.01284800	-0.71425000
				C	8.04228300	-5.69324300	-0.84520400
				H	3.10126000	-6.78203800	-0.47821500
				H	5.57144000	-6.78049600	-0.63532400
				H	8.04027000	-6.78024300	-0.85108200
<b>18-c</b>							
C	6.78473200	-0.72058400	-0.65525500				
C	5.55879300	-1.43562200	-0.53904900				
C	6.78535700	0.71645900	-0.68177300				
C	4.32264500	-0.71855300	-0.42279900				
C	5.56196500	1.42854000	-0.52866700				

H	10.15072300	-5.54466100	-1.06258400	C	-3.06293200	3.56926400	-0.27578300
C	0.62965900	1.43479800	-0.26840700	C	-5.52082400	-0.71237600	-0.26919500
C	0.63115500	2.87273400	-0.28717700	C	-1.83338400	5.69568000	-0.29825600
C	-0.60327500	0.71926800	-0.24958100	C	-3.06252200	5.01490600	-0.28107600
C	0.62914800	-2.87302600	-0.29724600	H	-1.83961200	-6.78113100	-0.32168800
C	0.62812400	-1.43218800	-0.25347800	H	-1.83499900	6.78305300	-0.30777300
C	-0.60686800	-0.71995000	-0.27579900	C	-5.52730600	-3.56361100	-0.27158300
C	10.43353900	2.83959400	-1.10364200	C	-6.75338800	-2.85358000	-0.26374100
C	10.45833200	1.42722200	-1.10409600	C	-5.52811400	-5.00645700	-0.27435600
C	11.66883300	0.68006100	-1.24211400	C	-6.75202900	-1.42178100	-0.26293400
C	10.43105800	-2.84763700	-1.09653500	C	-4.30799800	-5.68952700	-0.28583100
C	10.45706100	-1.43591900	-1.10095900	C	-6.75087900	1.42699000	-0.26077000
C	11.66785800	-0.68992800	-1.24149000	C	-7.97846800	0.71715000	-0.25379700
H	11.36925500	-3.38819700	-1.20162300	C	-6.75094400	2.85870100	-0.25920300
H	12.60242400	-1.23516400	-1.34647600	C	-7.97914700	-0.71093600	-0.25458700
H	12.60390200	1.22408700	-1.34864600	C	-5.52458900	3.56779100	-0.26533700
H	11.37209300	3.37910000	-1.21043600	C	-4.30325300	5.69242000	-0.27389600
C	4.93984100	-1.08650000	2.53654200	C	-5.52417300	5.01029100	-0.26484700
C	5.55295100	1.46068700	2.44868000	H	-4.31061000	-6.77700900	-0.28922100
C	7.37204700	-0.32257300	2.19598600	H	-4.30509200	6.77991900	-0.27513900
O	5.44060300	2.39216900	3.13286400	C	-7.98957800	-3.55876400	-0.25677100
O	4.41095700	-1.79928100	3.28575000	C	-9.21285100	-2.84756200	-0.24777800
O	8.38439900	-0.53915600	2.72802500	C	-7.98575700	-5.00202700	-0.25774500
C	-0.59893700	-3.57067400	-0.29458800	C	-6.78089300	-5.68354800	-0.26708300
C	-1.83480400	-2.86096000	-0.28305200	C	-9.21280300	-1.42231400	-0.24699900
C	-0.60105700	-5.01712200	-0.31844400	C	-9.21167700	1.42950300	-0.24431800
C	0.63231000	-5.69592100	-0.35594000	C	-10.44255700	0.71725000	-0.23622900
C	-1.84235400	-1.43329800	-0.26771500	C	-9.21057000	2.85471200	-0.24287100
C	-1.84122600	1.43520800	-0.27079400	C	-10.44317200	-0.70906000	-0.23740400
C	-3.06130700	0.71970400	-0.27198500	C	-7.98678400	3.56496500	-0.25043400
C	-1.83208600	2.86182900	-0.27313800	C	-6.77617600	5.68853500	-0.25615500
C	-3.06309300	-0.71692000	-0.27797200	C	-7.98176500	5.00802900	-0.24850200
C	-0.59635100	3.57231100	-0.28828100	H	-6.78276900	-6.77125100	-0.26764900
C	0.63693700	5.69741700	-0.34870900	H	-6.77710700	6.77623700	-0.25435300
C	-0.59691500	5.01856700	-0.30887200	C	-10.46491300	-3.55532100	-0.23924200
H	0.63196300	-6.78312400	-0.37285900	C	-11.65531700	-2.83742300	-0.22999000
H	0.63741500	6.78455200	-0.36672400	C	-10.43199000	-4.99790000	-0.24014700
C	-3.06574100	-3.56710500	-0.28224800	C	-9.25908000	-5.68312000	-0.24901000
C	-4.29288500	-2.85726300	-0.27618400	C	-11.67914900	-1.42476200	-0.22873700
C	-3.06657600	-5.01288500	-0.29141300	C	-11.67804200	1.43396400	-0.22604000
C	-4.29263700	-1.42506900	-0.27324100	C	-12.89600000	0.69085300	-0.21735600
C	-1.83792700	-5.69378400	-0.31096600	C	-11.65310100	2.84655800	-0.22459800
C	-4.29147500	1.42859600	-0.27342000	C	-12.89652900	-0.68072200	-0.21867300
C	-5.51991600	0.71666500	-0.26783300	C	-10.46209500	3.56352000	-0.23261000
C	-4.29026400	2.86034500	-0.27039400	C	-9.25443300	5.69024700	-0.23818700

C	-10.42795600	5.00600800	-0.23061800
H	-9.25752800	-6.77025000	-0.24892400
H	-11.37916300	-5.53165600	-0.23292700
H	-12.60020300	-3.37674300	-0.22286600
H	-13.83740500	-1.22540600	-0.21144400
H	-13.83644800	1.23626000	-0.20906700
H	-12.59755000	3.38662300	-0.21623500
H	-11.37466900	5.54055800	-0.22211700
H	-9.25194000	6.77736900	-0.23579500
Cr	0.60142100	-0.02132500	1.62361200
C	1.60444400	1.06407800	2.72207700
C	-0.86174700	0.34681300	2.65821900
C	0.94362200	-1.46963300	2.70489000
O	-1.80351400	0.58259300	3.30017300
O	2.22116800	1.76785900	3.40968300
O	1.12353000	-2.40181200	3.37355800

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C	-6.98537100	0.71821500	-0.57940600
C	-5.75490900	1.43019200	-0.50861100
C	-6.98519100	-0.71927000	-0.57081800
C	-4.51234600	0.71476000	-0.47628800
C	-5.75455300	-1.43251600	-0.51933800
C	-4.51331100	-0.71627500	-0.46646200
Cr	-5.85112400	-0.00000100	1.35963200
C	-3.27891400	1.43101100	-0.43737600
C	-3.28651000	2.86043200	-0.46022000
C	-5.75357000	2.87009200	-0.53954000
C	-4.52590700	3.56961200	-0.50639600
C	-5.75367400	-2.87179900	-0.54013600
C	-6.98619300	-3.56875600	-0.61417200
C	-8.22435000	-1.43558400	-0.65625700
C	-8.21529800	-2.85455900	-0.66996700
C	-2.05807100	0.71936200	-0.41028700
C	-2.05808600	-0.72153900	-0.40383200
C	-3.27884300	-1.43295900	-0.44247000
C	-4.52604100	-3.57154800	-0.50955000
C	-3.28666600	-2.86203700	-0.45769900
C	-9.44371700	-0.71719500	-0.72957500
C	-9.44397700	0.71624100	-0.72867700
C	-8.22452200	1.43450800	-0.65030200
C	-6.98607300	3.56724600	-0.60727800
C	-8.21542200	2.85371500	-0.66474800
C	-2.06244100	-3.57014200	-0.43126100
C	-2.06200500	-5.01665300	-0.45038200

C	-3.30094400	-5.69373100	-0.49957600
C	-6.98154400	-5.00987700	-0.63490600
C	-8.25384300	-5.69027900	-0.70506600
C	-5.77492300	-5.69010400	-0.59072300
C	-9.46235600	-3.56290100	-0.74783200
C	-9.42612500	-5.00580300	-0.75872200
C	-4.52456600	-5.01255600	-0.53183900
H	-3.30208100	-6.78103100	-0.51413000
H	-5.77543400	-6.77758700	-0.60429700
H	-8.25213800	-6.77725000	-0.71505700
H	-10.37093800	-5.54090700	-0.81178600
C	-2.06209100	3.56829200	-0.43272600
C	-2.06144800	5.01485500	-0.45359700
C	-9.46262400	3.56213600	-0.73833700
C	-9.42631000	5.00511900	-0.74593900
C	-4.52423900	5.01093200	-0.52955500
C	-3.30057300	5.69197600	-0.50100200
C	-5.77470500	5.68860600	-0.58562600
C	-6.98142900	5.00868500	-0.62725100
C	-8.25380800	5.68933800	-0.69392300
H	-3.30172400	6.77932500	-0.51523300
H	-5.77507500	6.77614700	-0.59771700
H	-8.25193200	6.77634600	-0.70157400
H	-10.37113100	5.54046000	-0.79651500
C	-0.83686600	-1.43748200	-0.37407900
C	-0.83059100	-2.86220600	-0.38529000
C	0.39923200	-0.72127300	-0.32426500
C	-0.83033400	2.86049300	-0.39189500
C	-0.83681900	1.43537600	-0.36973800
C	0.39841100	0.71957600	-0.34177200
C	-10.65216900	-2.84345200	-0.81170300
C	-10.67707300	-1.43210800	-0.80677600
C	-11.89362700	-0.68521200	-0.87683800
C	-10.65253800	2.84285600	-0.80243000
C	-10.67724800	1.43132900	-0.80204400
C	-11.89380400	0.68456500	-0.87409400
H	-11.59549700	3.38257900	-0.85673500
H	-12.83302700	1.22928700	-0.92731400
H	-12.83278100	-1.22990500	-0.93161300
H	-11.59507800	-3.38309700	-0.86775800
C	-5.23532700	1.33374300	2.46456000
C	-5.12223400	-1.27349000	2.46909000
C	-7.40127500	-0.06642600	2.33281100
O	-4.66803300	-2.09795300	3.15001800
O	-4.84977600	2.19480900	3.14332100

O	-8.39936000	-0.10835400	2.92994900	C	7.78944900	5.00506400	-0.31248500
C	0.40549500	3.57013500	-0.36956400	C	6.58519800	5.68591800	-0.32505400
C	1.63215400	2.87156300	-0.33487700	C	9.01916600	1.42516500	-0.29588000
C	0.40490200	5.01638400	-0.39285000	C	9.01898500	-1.42799900	-0.29513200
C	-0.83157000	5.69422400	-0.43239500	C	10.25016700	-0.71464700	-0.28989200
C	1.63162300	1.43098400	-0.30053300	C	9.01792100	-2.85281300	-0.29652100
C	1.63139800	-1.43475700	-0.30983900	C	10.25031100	0.71168100	-0.29016000
C	2.87248900	-0.71685300	-0.29098300	C	7.79418800	-3.56356900	-0.30284600
C	1.63158800	-2.87401400	-0.32355400	C	6.58452000	-5.68848600	-0.31672900
C	2.87412800	0.71503300	-0.30923200	C	7.78895800	-5.00772000	-0.30703000
C	0.40481500	-3.57277700	-0.36398900	H	6.58684300	6.77355800	-0.32949700
C	-0.83232000	-5.69645100	-0.42460700	H	6.58602500	-6.77616000	-0.32030600
C	0.40421400	-5.01883600	-0.38419900	C	10.27035200	3.55840200	-0.29380100
H	-0.83188000	6.78152600	-0.44620900	C	11.46053600	2.84126500	-0.28646200
H	-0.83294400	-6.78373800	-0.43799900	C	10.23610200	5.00139900	-0.29689800
C	2.86756300	3.56980800	-0.33291700	C	9.06314600	5.68618700	-0.30621200
C	4.09959900	2.86014600	-0.32033900	C	11.48530800	1.42767700	-0.28489400
C	2.86942700	5.01337900	-0.35297200	C	11.48514400	-1.43080100	-0.28449200
C	4.10778800	1.42844300	-0.30049800	C	12.70286000	-0.68749500	-0.27835200
C	1.63885400	5.69397100	-0.37942600	C	11.46022400	-2.84434100	-0.28580000
C	4.10757000	-1.43094800	-0.30162300	C	12.70294400	0.68422700	-0.27839800
C	5.32683000	-0.71758400	-0.29931600	C	10.26999100	-3.56140700	-0.29202400
C	4.09895800	-2.86232300	-0.31022100	C	9.06255500	-5.68902900	-0.30166000
C	2.86740400	-3.57255300	-0.32525200	C	10.23561300	-5.00435400	-0.29432000
C	5.32750000	0.71493600	-0.30530800	H	9.06149300	6.77328200	-0.30818900
C	1.63807100	-5.69691400	-0.36737400	H	11.18297200	5.53570000	-0.29157100
C	2.86874900	-5.01594000	-0.34193500	H	12.40529300	3.38082800	-0.28199900
H	1.64026900	6.78128000	-0.39093600	H	13.64368600	1.22914300	-0.27331800
H	1.63950300	-6.78421800	-0.37865000	H	13.64353000	-1.23253100	-0.27311400
C	5.33072200	3.56560000	-0.31881700	H	12.40492800	-3.38399700	-0.28123500
C	6.56005400	2.85506400	-0.30987600	H	11.18242900	-5.53876100	-0.28949000
C	5.33115000	5.00878800	-0.33009400	H	9.06074200	-6.77614000	-0.30292100
C	6.56115400	1.42507900	-0.30286300	Cr	1.58611100	0.01067900	1.57669900
C	4.11172000	5.69050900	-0.34822100	C	0.06970300	-0.13288900	2.60052200
C	6.56095200	-1.42772800	-0.30261300	C	2.42658700	-1.20659600	2.66558500
C	7.78594100	-0.71655100	-0.29817200	C	2.16550100	1.37924300	2.65355300
C	6.55956000	-2.85760500	-0.30454600	O	2.96758600	-1.98691400	3.33719400
C	7.78621000	0.71385000	-0.29981200	O	-0.90574000	-0.22307600	3.22611800
C	5.33034900	-3.56801300	-0.31246700	O	2.53864100	2.25739700	3.31887000
C	4.11104800	-5.69314700	-0.33608600				
C	5.33059100	-5.01116100	-0.32118200	<b>18-e</b>			
H	4.11356500	6.77790500	-0.35740600	C	-7.18618100	0.71791500	-0.50433400
H	4.11309000	-6.78058800	-0.34460200	C	-5.95522800	1.42945200	-0.44737300
C	7.79454600	3.56081400	-0.30668100	C	-7.18551600	-0.71974900	-0.49134900
C	9.01827900	2.84999700	-0.29867400	C	-4.71124400	0.71419600	-0.43190400

C	-5.95467400	-1.43275200	-0.45570400	H	-8.45441000	6.77528500	-0.61492900
C	-4.71233900	-0.71591700	-0.41901700	H	-10.57468800	5.53942300	-0.68335400
Cr	-6.02983700	0.00402600	1.42372800	C	-1.02627200	-1.43091500	-0.38324300
C	-3.47680600	1.42905800	-0.40861900	C	-1.02727000	-2.86066000	-0.39014000
C	-3.48581900	2.86051100	-0.43051500	C	0.20210500	-0.72078200	-0.35886600
C	-5.95433300	2.86929300	-0.48044900	C	-1.02772300	2.85911900	-0.39210500
C	-4.72577100	3.56877700	-0.46176000	C	-1.02648300	1.42909200	-0.38061400
C	-5.95401800	-2.87171000	-0.47362200	C	0.20145200	0.71907500	-0.36301200
C	-7.18682800	-3.56881300	-0.53102500	C	-10.85548900	-2.84425600	-0.68310300
C	-8.42613700	-1.43617000	-0.56088300	C	-10.88050400	-1.43297300	-0.68010500
C	-8.41712300	-2.85474700	-0.57202600	C	-12.09813700	-0.68623800	-0.73595300
C	-2.25744100	0.71685000	-0.39717200	C	-10.85617500	2.84184500	-0.68236600
C	-2.25759100	-0.71871900	-0.39340500	C	-10.88084200	1.43034500	-0.67970400
C	-3.47654300	-1.43103900	-0.41146000	C	-12.09840500	0.68338600	-0.73522000
C	-4.72521100	-3.57128600	-0.45912900	H	-11.79970800	3.38154600	-0.72557700
C	-3.48550600	-2.86224500	-0.42571200	H	-13.03823600	1.22802200	-0.77738500
C	-9.64645200	-0.71793300	-0.61952800	H	-13.03782400	-1.23114500	-0.77798600
C	-9.64690600	0.71546100	-0.62106300	H	-11.79894800	-3.38412300	-0.72632200
C	-8.42644800	1.43385100	-0.55892400	C	-5.43429400	1.35667500	2.51422400
C	-7.18713800	3.56612400	-0.53331600	C	-5.24376100	-1.23969000	2.52488400
C	-8.41759700	2.85268500	-0.57544000	C	-7.56273500	-0.10338800	2.42125100
C	-2.26227500	-3.56918700	-0.41522600	O	-4.74375000	-2.04024700	3.20359600
C	-2.26258700	-5.01502500	-0.43100600	O	-5.05664400	2.22704700	3.18654900
C	-3.50077200	-5.69313300	-0.46209400	O	-8.54861400	-0.17154600	3.03569700
C	-7.18272200	-5.01006300	-0.54969900	C	0.20124900	3.56808000	-0.38049700
C	-8.45581600	-5.69072100	-0.60241500	C	1.42836100	2.86105600	-0.35773200
C	-5.97567600	-5.69003400	-0.52028900	C	0.20197400	5.01563000	-0.39779300
C	-9.66482000	-3.56345900	-0.63309500	C	-1.03249300	5.69403400	-0.42363100
C	-9.62871900	-5.00647300	-0.64216900	C	1.42035100	1.43394600	-0.33700000
C	-4.72482300	-5.01201700	-0.47921300	C	1.42056500	-1.43557300	-0.34295700
H	-3.50156500	-6.78047600	-0.47463300	C	2.66003500	-0.71990700	-0.30950800
H	-5.97602200	-6.77755100	-0.53237300	C	1.42888000	-2.86224300	-0.35481600
H	-8.45405800	-6.77771600	-0.61086500	C	2.65811800	0.71904000	-0.32681700
H	-10.57412200	-5.54166500	-0.68230500	C	0.20162900	-3.56954300	-0.37987900
C	-2.26261400	3.56745000	-0.41720800	C	-1.03189900	-5.69547900	-0.41931700
C	-2.26299000	5.01344500	-0.43459600	C	0.20252000	-5.01696400	-0.39535000
C	-9.66544600	3.56109400	-0.63410100	H	-1.03325500	6.78134100	-0.43494800
C	-9.62931200	5.00415800	-0.64363900	H	-1.03259300	-6.78279700	-0.42977900
C	-4.72529600	5.00970000	-0.48434400	C	2.66802600	3.57012800	-0.35383300
C	-3.50149700	5.69094800	-0.46794400	C	3.89317000	2.87150700	-0.33920600
C	-5.97624000	5.68740000	-0.52634500	C	2.66800700	5.01461600	-0.37623200
C	-7.18319500	5.00762300	-0.55413000	C	3.89241300	1.42980500	-0.30428200
C	-8.45629100	5.68829200	-0.60631100	C	1.43581700	5.69410300	-0.39469500
H	-3.50263900	6.77829900	-0.48091900	C	3.89234900	-1.43347100	-0.32013400
H	-5.97664000	6.77493400	-0.53850000	C	5.13217200	-0.71516700	-0.31847200

C	3.89334200	-2.87325100	-0.33410800	C	8.86344300	-5.68823800	-0.41837300
C	2.66805600	-3.57239800	-0.35404400	C	10.03637200	-5.00348300	-0.42888400
C	5.13384000	0.71466000	-0.33650900	H	8.86128500	6.77493100	-0.41879900
C	1.43614000	-5.69603300	-0.39047800	H	10.98252300	5.53788000	-0.43560300
C	2.66851300	-5.01665800	-0.37364200	H	12.20644700	3.38255900	-0.44537700
H	1.43622100	6.78141400	-0.40744900	H	13.44607000	1.23029300	-0.45838900
H	1.43608700	-6.78334600	-0.40258400	H	13.44596700	-1.23059900	-0.46022300
C	5.12915100	3.56884200	-0.35772700	H	12.20641400	-3.38261000	-0.45030400
C	6.36208200	2.85811400	-0.36716600	H	10.98301000	-5.53798500	-0.44189900
C	5.13064700	5.00958500	-0.37770000	H	8.86187100	-6.77528600	-0.42315300
C	6.37060900	1.42881300	-0.34860400	Cr	3.88836200	0.00640700	1.56435600
C	3.90811800	5.69123500	-0.38293300	C	2.40950000	-0.21466700	2.62696300
C	6.37060200	-1.42988700	-0.35444900	C	4.81283800	-1.17066200	2.62858700
C	7.58784400	-0.71696600	-0.37224500	C	4.42969400	1.39732800	2.63204000
C	6.36200400	-2.85878900	-0.36411600	O	5.40610600	-1.92586000	3.28458900
C	7.58850400	0.71614500	-0.37627500	O	1.45845300	-0.35652500	3.28080200
C	5.12975900	-3.57077300	-0.35853400	O	4.77801200	2.28977900	3.29187100
C	3.90860500	-5.69363900	-0.37927200				
C	5.13109500	-5.01119900	-0.37595400	<b>18-f</b>			
H	3.91013400	6.77862600	-0.39421800	C	7.38771500	-0.72072100	-0.40418500
H	3.91081800	-6.78098500	-0.39100100	C	6.15640500	-1.43348600	-0.38851000
C	7.59433100	3.56293600	-0.38704500	C	7.38886100	0.71696200	-0.41984700
C	8.82060500	2.85117400	-0.40022600	C	4.91370100	-0.71644400	-0.37188000
C	7.58916900	5.00682500	-0.39781000	C	6.15733100	1.42876600	-0.38294600
C	6.38426800	5.68707100	-0.39423900	C	4.91291800	0.71394100	-0.38788000
C	8.82312500	1.42786800	-0.39502300	Cr	6.20028000	0.00657600	1.49386600
C	8.82310500	-1.42844100	-0.39798000	C	3.67829100	-1.43105000	-0.38370300
C	10.05244300	-0.71408800	-0.41424900	C	3.68699200	-2.86204500	-0.39515900
C	8.82054100	-2.85156600	-0.40204500	C	6.15572300	-2.87218100	-0.40355300
C	10.05266200	0.71376800	-0.41355000	C	4.92621700	-3.57143600	-0.40810500
C	7.59453900	-3.56360200	-0.38934100	C	6.15722600	2.86837400	-0.41799500
C	6.38493800	-5.68821000	-0.39309700	C	7.39068700	3.56504600	-0.45238000
C	7.58961900	-5.00736400	-0.39960200	C	8.62984300	1.43256700	-0.45546100
H	6.38535100	6.77464900	-0.40287300	C	8.62152200	2.85138500	-0.47454900
H	6.38660800	-6.77578500	-0.40230800	C	2.45886400	-0.71808500	-0.38444600
C	10.07110100	3.55994200	-0.41877000	C	2.45876900	0.71649500	-0.38982200
C	11.26203800	2.84263400	-0.43223500	C	3.67904900	1.42873700	-0.38312000
C	10.03595900	5.00321600	-0.42369000	C	4.92835700	3.56803800	-0.41827800
C	8.86296600	5.68787900	-0.41481500	C	3.68838100	2.85992200	-0.40570600
C	11.28708100	1.42969200	-0.43083100	C	9.85113100	0.71384500	-0.49771600
C	11.28703400	-1.42992700	-0.43294400	C	9.85038200	-0.71941400	-0.49390000
C	12.50540700	-0.68554200	-0.44820100	C	8.62899000	-1.43739100	-0.45342100
C	11.26195700	-2.84274900	-0.43668700	C	7.38892100	-3.56969300	-0.44047500
C	12.50547400	0.68529500	-0.44689400	C	8.61986700	-2.85597900	-0.46269700
C	10.07123400	-3.56032800	-0.42266000	C	2.46469400	3.56673600	-0.40928900

C	2.46594300	5.01249400	-0.42512300	O	4.86701300	-2.02500100	3.25212600
C	3.70478700	5.69020800	-0.44170800	O	8.68956200	-0.17951500	3.14963900
C	7.38723400	5.00664100	-0.47496300	C	-0.00104900	-3.56687200	-0.40503500
C	8.66114400	5.68700200	-0.50891500	C	-1.22936900	-2.85880800	-0.40165100
C	6.18017300	5.68652800	-0.46564700	C	-0.00137000	-5.01420700	-0.41704200
C	9.87028400	3.55954900	-0.51510600	C	1.23221700	-5.69382600	-0.42201800
C	9.83446100	5.00263800	-0.52748900	C	-1.22734500	-1.42801400	-0.39196600
C	4.92852600	5.00904400	-0.44134600	C	-1.22660400	1.42872800	-0.39212600
H	3.70599300	6.77758200	-0.45422300	C	-2.45884100	0.71802000	-0.38447500
H	6.18091300	6.77406400	-0.47863700	C	-1.22799400	2.85943800	-0.39823500
H	8.65959200	6.77398400	-0.51914800	C	-2.45879200	-0.71654500	-0.38987100
H	10.78041300	5.53772100	-0.55372100	C	0.00104100	3.56676300	-0.40512900
C	2.46266300	-3.56832800	-0.40318400	C	1.23539400	5.69298200	-0.42733900
C	2.46327900	-5.01414700	-0.41637800	C	0.00136300	5.01410000	-0.41716800
C	9.86825500	-3.56503700	-0.50323100	H	1.23211200	-6.78119400	-0.43021200
C	9.83189200	-5.00810100	-0.51083100	H	1.23597200	6.78034000	-0.43619100
C	4.92583900	-5.01238600	-0.42594800	C	-2.46473100	-3.56682700	-0.40919900
C	3.70160800	-5.69286700	-0.42713100	C	-3.68842300	-2.85999700	-0.40564900
C	6.17722500	-5.69067500	-0.44608600	C	-2.46597300	-5.01258500	-0.42496600
C	7.38466500	-5.01113100	-0.45719400	C	-3.67907000	-1.42880200	-0.38313200
C	8.65836500	-5.69203200	-0.48867700	C	-1.23540900	-5.69308300	-0.42717400
H	3.70202700	-6.78025100	-0.43804800	C	-3.67827900	1.43095800	-0.38378600
H	6.17749200	-6.77822400	-0.45672400	C	-4.91364200	0.71636400	-0.37210600
H	8.65652100	-6.77904500	-0.49566000	C	-3.68698600	2.86195900	-0.39524500
H	10.77767900	-5.54356600	-0.53518000	C	-2.46266200	3.56821700	-0.40326200
C	1.22733700	1.42794000	-0.39200700	C	-4.91293000	-0.71402400	-0.38792800
C	1.22935700	2.85870800	-0.40168900	C	-1.23221700	5.69371600	-0.42213600
C	0.00007100	0.71723000	-0.39093800	C	-2.46327000	5.01403000	-0.41646700
C	1.22800200	-2.85954300	-0.39818700	H	-1.23600100	-6.78044800	-0.43597100
C	1.22661800	-1.42881700	-0.39205300	H	-1.23212900	6.78107900	-0.43035700
C	-0.00007100	-0.71727500	-0.39099000	C	-4.92839300	-3.56809900	-0.41817600
C	11.06143100	2.84004400	-0.54386200	C	-6.15725700	-2.86841000	-0.41794200
C	11.08587800	1.42850100	-0.53848500	C	-4.92856900	-5.00909900	-0.44116800
C	12.30399200	0.68124900	-0.57404300	C	-6.15734800	-1.42885900	-0.38300000
C	11.05962500	-2.84612800	-0.53563700	C	-3.70483100	-5.69029300	-0.44150100
C	11.08496800	-1.43480400	-0.53436300	C	-6.15637100	1.43341000	-0.38853100
C	12.30344700	-0.68835900	-0.57257900	C	-7.38769400	0.72068300	-0.40437700
H	12.00352500	-3.38625400	-0.56329200	C	-6.15570200	2.87211300	-0.40361500
H	13.24355000	-1.23351500	-0.59924600	C	-7.38885100	-0.71699900	-0.41985000
H	13.24445300	1.22567500	-0.60265500	C	-4.92619500	3.57134000	-0.40816200
H	12.00560400	3.37955500	-0.57347500	C	-3.70159100	5.69274900	-0.42720100
C	5.38742800	-1.23008000	2.58137800	C	-4.92580700	5.01227300	-0.42599100
C	5.59306400	1.36259900	2.57172100	H	-3.70604600	-6.77767200	-0.45395100
C	7.71516700	-0.10712300	2.51752700	H	-3.70201400	6.78013100	-0.43811600
O	5.20640100	2.23436200	3.23771100	C	-7.39070300	-3.56507500	-0.45235300



C	-8.62152000	-2.85139900	-0.47458700	C	-4.38090800	0.71734400	-0.30623500
C	-7.38728000	-5.00666600	-0.47485200	C	-5.62126500	-1.43191900	-0.33912500
C	-6.18022800	-5.68658100	-0.46545300	C	-4.38092400	-0.71681200	-0.30711400
C	-8.62983400	-1.43259300	-0.45557000	Cr	-5.69624600	-0.00068700	1.36015600
C	-8.62894900	1.43737300	-0.45342900	C	-3.14164300	1.43300300	-0.27236000
C	-9.85036200	0.71939600	-0.49395800	C	-3.15143500	2.86187500	-0.28596500
C	-8.61982500	2.85595500	-0.46269300	C	-5.62093300	2.87397600	-0.35502400
C	-9.85111500	-0.71385500	-0.49778900	C	-4.39448000	3.57281600	-0.32471800
C	-7.38886700	3.56963100	-0.44046100	C	-5.62102500	-2.87338700	-0.35711800
C	-6.17716900	5.69058600	-0.44608200	C	-6.85436000	-3.56958600	-0.42399100
C	-7.38460400	5.01107100	-0.45715000	C	-8.09951900	-1.43426100	-0.47162100
H	-6.18097100	-6.77412100	-0.47838100	C	-8.08842700	-2.85363100	-0.48270200
H	-6.17741500	6.77813400	-0.45668700	C	-1.92407900	0.72019700	-0.24954400
C	-9.87029000	-3.55955200	-0.51515300	C	-1.92411100	-0.71980200	-0.24998000
C	-11.06142200	-2.84004200	-0.54394100	C	-3.14171200	-1.43253800	-0.27297800
C	-9.83449000	-5.00263700	-0.52747900	C	-4.39462700	-3.57228100	-0.32671000
C	-8.66119500	-5.68700800	-0.50882300	C	-3.15155900	-2.86140500	-0.28740200
C	-11.08586600	-1.42849600	-0.53856900	C	-9.31808700	-0.71788300	-0.54384700
C	-11.08494600	1.43479800	-0.53436500	C	-9.31806800	0.71873400	-0.54327000
C	-12.30344200	0.68836500	-0.57259500	C	-8.09947700	1.43502600	-0.47054800
C	-11.05960000	2.84614500	-0.53558000	C	-6.85425200	3.57027600	-0.42152600
C	-12.30398600	-0.68124600	-0.57410400	C	-8.08834600	2.85440400	-0.48056600
C	-9.86821000	3.56503300	-0.50316300	C	-1.92737900	-3.56809700	-0.25985100
C	-8.65828900	5.69200300	-0.48856800	C	-1.92836300	-5.01515800	-0.26937100
C	-9.83182600	5.00810200	-0.51070800	C	-3.16738900	-5.69386400	-0.31212400
H	-8.65965400	-6.77399200	-0.51901500	C	-6.84987300	-5.00993800	-0.44159200
H	-10.78045200	-5.53769900	-0.55372700	C	-8.12322200	-5.68945300	-0.50805100
H	-12.00560500	-3.37953600	-0.57354800	C	-5.64257800	-5.69273600	-0.39767900
H	-13.24444600	-1.22567800	-0.60271400	C	-9.33411800	-3.56198800	-0.55441500
H	-13.24354100	1.23353800	-0.59923900	C	-9.29624800	-5.00517200	-0.56114600
H	-12.00350400	3.38627600	-0.56321100	C	-4.39270100	-5.01461200	-0.34469700
H	-10.77761300	5.54358000	-0.53501300	H	-3.16663500	-6.78150400	-0.32302800
H	-8.65641700	6.77901600	-0.49550700	H	-5.64412300	-6.78042800	-0.40973200
Cr	-6.20035500	-0.00632100	1.49398500	H	-8.12221900	-6.77671400	-0.51760300
C	-5.39238400	1.23364800	2.58128300	H	-10.24064900	-5.54161000	-0.61375500
C	-7.71570400	0.10165000	2.51748300	C	-1.92719900	3.56849400	-0.25873500
C	-5.58767000	-1.35983800	2.57192000	C	-1.92811100	5.01555500	-0.26792000
O	-8.69051900	0.17041100	3.14938400	C	-9.33401700	3.56285000	-0.55185300
O	-4.87508200	2.03075400	3.25187200	C	-9.29609900	5.00603800	-0.55770500
O	-5.19728000	-2.22998300	3.23785600	C	-4.39249700	5.01515600	-0.34216100
<b>19-a</b>				C	-3.16712900	5.69434700	-0.30988800
C	-6.85772800	0.71634100	-0.40363800	C	-5.64236700	5.69337000	-0.39445600
C	-5.62122000	1.43251900	-0.33811100	C	-6.84970800	5.01063900	-0.43840300
C	-6.85774100	-0.71565900	-0.40447200	C	-8.12304200	5.69024500	-0.50431800
				H	-3.16632400	6.78199200	-0.32053800

H	-5.64385900	6.78106900	-0.40608200	H	1.77103300	6.78020200	-0.17451800
H	-8.12199200	6.77751200	-0.51328500	H	1.77066200	-6.78004700	-0.17399100
H	-10.24048600	5.54253800	-0.60992000	C	5.45873500	3.56496500	-0.07715600
C	-0.69183900	-1.42906200	-0.22249500	C	6.68590600	2.85561800	-0.04744900
C	-0.69326800	-2.85975000	-0.22690000	C	5.45953900	5.00719900	-0.07839800
C	0.53640300	-0.71694100	-0.19323600	C	6.68498300	1.42416400	-0.04674900
C	-0.69311800	2.86007900	-0.22630000	C	4.23914600	5.68931900	-0.10909100
C	-0.69176200	1.42939200	-0.22230800	C	6.68491500	-1.42418500	-0.04615400
C	0.53644100	0.71720300	-0.19311400	C	7.91130100	-0.71444300	-0.01740100
C	-10.52797800	-2.84381100	-0.61633800	C	6.68577000	-2.85564600	-0.04616100
C	-10.55315100	-1.43401400	-0.61473600	C	7.91133600	0.71437700	-0.01779800
C	-11.76982100	-0.68435800	-0.68172500	C	5.45855800	-3.56494500	-0.07585900
C	-10.52789300	2.84475100	-0.61427500	C	4.23884700	-5.68927900	-0.10749300
C	-10.55310800	1.43495100	-0.61367600	C	5.45929100	-5.00719900	-0.07656300
C	-11.76979900	0.68538200	-0.68122900	H	4.24080900	6.77696300	-0.11049700
H	-11.46987100	3.38661800	-0.66819300	H	4.24045400	-6.77694200	-0.10858900
H	-12.70972400	1.22946200	-0.73441400	C	7.92096400	3.56127300	-0.01874900
H	-12.70976200	-1.22837100	-0.73532000	C	9.14489700	2.85072800	0.01007200
H	-11.46997100	-3.38561400	-0.67062500	C	7.91648900	5.00459300	-0.01959200
C	0.53702900	3.56734600	-0.19740700	C	6.71174100	5.68512400	-0.04867700
C	1.76470100	2.85950300	-0.16602300	C	9.14523500	1.42603800	0.01060200
C	0.53677500	5.01426700	-0.20185500	C	9.14517000	-1.42614700	0.01139800
C	-0.69810500	5.69420200	-0.23761500	C	10.37585900	-0.71340400	0.03960700
C	1.76433700	1.42660700	-0.16425900	C	9.14476900	-2.85084100	0.01168900
C	1.76425900	-1.42640900	-0.16413900	C	10.37589100	0.71325300	0.03916500
C	2.99498200	-0.71501800	-0.13433600	C	7.92080000	-3.56134600	-0.01694500
C	1.76454300	-2.85931000	-0.16585300	C	6.71146700	-5.68518200	-0.04615300
C	2.99502100	0.71515500	-0.13446000	C	7.91625700	-5.00468300	-0.01705800
C	0.53683300	-3.56708600	-0.19759700	H	6.71285500	6.77295900	-0.04940000
C	-0.69841100	-5.69387600	-0.23854400	H	6.71252600	-6.77303100	-0.04639500
C	0.53649700	-5.01401900	-0.20208400	C	10.39637900	3.55907500	0.03878900
H	-0.69704000	6.78179700	-0.24315500	C	11.58688900	2.84197500	0.06640500
H	-0.69739800	-6.78147600	-0.24417900	C	10.36242400	5.00180000	0.03767000
C	2.99862900	3.56666200	-0.13683900	C	9.18938300	5.68617400	0.01010900
C	4.22467000	2.85847100	-0.10626400	C	11.61123900	1.42934100	0.06730000
C	2.99962900	5.01134000	-0.13905900	C	11.61117400	-1.42953500	0.06822400
C	4.22389100	1.42465500	-0.10527600	C	12.82877700	-0.68577000	0.09593600
C	1.76968400	5.69261600	-0.17171900	C	11.58676100	-2.84217000	0.06823200
C	4.22381800	-1.42457500	-0.10490400	C	12.82880800	0.68553900	0.09548000
C	5.45230400	-0.71402800	-0.07536800	C	10.39621700	-3.55923300	0.04095500
C	4.22452100	-2.85839800	-0.10545700	C	9.18912200	-5.68630700	0.01330600
C	2.99843800	-3.56652900	-0.13620600	C	10.36219400	-5.00196300	0.04069600
C	5.45234200	0.71405700	-0.07567300	H	9.18719000	6.77341700	0.00975400
C	1.76936600	-5.69244600	-0.17130200	H	11.30916800	5.53610900	0.05974200
C	2.99935900	-5.01122800	-0.13815300	H	12.53137200	3.38179000	0.08817000

H	13.76922400	1.23082800	0.11701200	C	4.31120400	5.68893400	-0.25431500
H	13.76916800	-1.23108900	0.11783900	C	7.98806300	5.00221400	-0.36042100
H	12.53121700	-3.38201600	0.09041200	C	9.26091700	5.68326900	-0.39754000
H	11.30891000	-5.53630600	0.06326100	C	6.78341800	5.68328100	-0.32760000
H	9.18687800	-6.77355700	0.01356900	C	10.46751000	3.55587100	-0.42338100
C	-6.49141500	-1.23023600	2.94544600	C	10.43384100	4.99846400	-0.42727200
C	-5.07186300	-1.23066400	3.02261000	C	5.53063600	5.00646900	-0.28925600
C	-4.36534600	-0.00219600	3.07413100	H	4.31391000	6.77659000	-0.25833000
C	-5.07194200	1.22631400	3.02490000	H	6.78528900	6.77112400	-0.33009400
C	-6.49149200	1.22593700	2.94774700	H	9.25911600	6.77050900	-0.40076900
C	-7.20015700	-0.00214300	2.92142300	H	11.38055700	5.53255600	-0.45473400
H	-7.02892700	-2.16834900	2.84854300	C	3.06718700	-3.56908800	-0.16992900
H	-4.52705100	-2.16901500	2.98907200	C	3.06715000	-5.01541000	-0.16880100
H	-3.27953500	-0.00216500	3.07138800	C	10.46629500	-3.56327900	-0.39155800
H	-4.52718900	2.16476400	2.99316700	C	10.43208700	-5.00584500	-0.38286800
H	-7.02908300	2.16420200	2.85271300	C	5.52893100	-5.01076300	-0.24186700
H	-8.27932800	-0.00206000	2.80208900	C	4.30901600	-5.69236100	-0.20284600
				C	6.78140900	-5.68843500	-0.27515700
				C	7.98634100	-5.00811100	-0.31436500
<b>19-c</b>				C	9.25892500	-5.68994200	-0.34651000
C	7.98282200	-0.71712300	-0.34051000	H	4.31107400	-6.78006400	-0.20018600
C	6.75530600	-1.42723100	-0.30240000	H	6.78281400	-6.77629200	-0.26882600
C	7.98305700	0.71119300	-0.34740600	H	9.25671300	-6.77718500	-0.34043600
C	5.52418300	-0.71741000	-0.27169100	H	11.37858900	-5.54052200	-0.40629500
C	6.75575400	1.42209600	-0.31671900	C	1.84781200	1.43281100	-0.15219200
C	5.52435000	0.71304500	-0.27925900	C	1.83855100	2.86152000	-0.16100500
C	4.29705100	-1.42933000	-0.22866100	C	0.60912300	0.71787400	-0.09598300
C	4.29624200	-2.86054000	-0.21698000	C	1.83754600	-2.86294700	-0.12821600
C	6.75583200	-2.85866400	-0.29279800	C	1.84747900	-1.43443200	-0.13167700
C	5.52950600	-3.56755100	-0.25090700	C	0.60918300	-0.71757500	-0.08285300
C	6.75676200	2.85351000	-0.32090100	C	11.65763900	2.83828100	-0.45197600
C	7.99277100	3.55881500	-0.35702100	C	11.68206500	1.42539000	-0.44705800
C	9.21598900	1.42252000	-0.38293300	C	12.89901200	0.68146900	-0.47542700
C	9.21558100	2.84805200	-0.38791500	C	11.65668400	-2.84638700	-0.42689600
C	3.06495200	-0.72083700	-0.19278600	C	11.68159400	-1.43352500	-0.43442500
C	3.06499600	0.71805500	-0.20202800	C	12.89878700	-0.69029400	-0.46941700
C	4.29743900	1.42580200	-0.24489300	H	12.60099600	-3.38647900	-0.44927700
C	5.53062300	3.56319000	-0.28658700	H	13.83914500	-1.23565200	-0.49146100
C	4.29718100	2.85697300	-0.24778800	H	13.83955200	1.22629700	-0.50224900
C	10.44657000	0.70941600	-0.41212300	H	12.60215000	3.37781500	-0.47883500
C	10.44632900	-0.71682000	-0.40567500	C	0.59947600	-3.57477200	-0.09000500
C	9.21552300	-1.42919100	-0.36971600	C	-0.63002600	-2.87608400	-0.05312300
C	7.99158300	-3.56473600	-0.32358800	C	0.60074200	-5.02089200	-0.11992100
C	9.21464000	-2.85471000	-0.36169200	C	1.83916800	-5.69620400	-0.14489700
C	3.06829200	3.56658800	-0.20715400	C	-0.62941500	-1.43463600	-0.00929700
C	3.06898000	5.01298200	-0.21399000				

C	-0.62928500	1.43606600	-0.02741000	C	-9.16662700	-0.71224900	-1.25332300
C	-1.87365200	0.72142300	-0.02749500	C	-6.75851000	3.57260900	-0.69632400
C	-0.62884100	2.87713800	-0.07555700	C	-5.55796900	5.69667800	-0.53564400
C	-1.87352000	-0.71990000	-0.02276200	C	-6.75052100	5.01360000	-0.71906700
C	0.60089300	3.57431800	-0.12108800	H	-5.55065100	-6.77865400	-0.63897600
C	1.84170100	5.69468100	-0.18738400	H	-5.55620100	6.78411300	-0.56148800
C	0.60282800	5.02054300	-0.15199900	C	-9.18038600	-3.55558100	-1.28095400
H	1.84147300	-6.78379900	-0.15841100	C	-10.34795400	-2.83657500	-1.53330100
H	1.84482300	6.78220500	-0.20345600	C	-9.14294900	-4.99904500	-1.28670900
C	-1.86330100	-3.57506500	-0.10895200	C	-7.99254900	-5.68459300	-1.05696300
C	-3.09645400	-2.86349100	-0.16756800	C	-10.37343000	-1.42668500	-1.52882200
C	-1.86146300	-5.02103100	-0.16901600	C	-10.37774700	1.44074900	-1.49579600
C	-3.10198500	-1.43784200	-0.09691600	C	-11.56644100	0.69300000	-1.76954900
C	-0.63243200	-5.70214500	-0.14299600	C	-10.35619900	2.85052600	-1.46909000
C	-3.10243400	1.43971100	-0.09216200	C	-11.56429000	-0.67636500	-1.78552000
C	-4.32673800	0.72163500	-0.21984900	C	-9.18972100	3.56682400	-1.20519400
C	-3.09644600	2.86553600	-0.15741100	C	-8.00316000	5.69365500	-0.95683600
C	-1.86226800	3.57668600	-0.11525500	C	-9.15473800	5.01017500	-1.18674000
C	-4.32569800	-0.71933900	-0.22854300	H	-7.98971600	-6.77178100	-1.07418700
C	-0.62993100	5.70265000	-0.16113400	H	-10.06812300	-5.53381300	-1.48802500
C	-1.86007000	5.02260900	-0.17044000	H	-11.26875200	-3.37742000	-1.74187600
H	-0.63173500	-6.78907500	-0.17604800	H	-12.48226900	-1.21985400	-1.99592800
H	-0.62883700	6.78961200	-0.19226200	H	-12.48606600	1.23842600	-1.96733900
C	-4.32539400	-3.57234600	-0.33526200	H	-11.27858500	3.39332200	-1.66516300
C	-5.54480400	-2.87172300	-0.49780400	H	-10.08217300	5.54667200	-1.37241800
C	-4.31697500	-5.01552100	-0.39696900	H	-8.00148000	6.78097900	-0.95832300
C	-5.55274600	-1.43216800	-0.44279500	Cr	-5.96064800	-0.02395900	1.23963700
C	-3.09940500	-5.69591700	-0.28672500	C	-5.47144600	0.92174000	3.11522500
C	-5.55608300	1.43501900	-0.41545500	C	-6.77523300	1.32649700	2.72460000
C	-6.76462600	0.71850700	-0.69154800	C	-7.75043900	0.35194400	2.40297800
C	-5.54892600	2.87551800	-0.45422400	C	-7.42461700	-1.02856000	2.45981800
C	-6.76227600	-0.71333400	-0.70837900	C	-6.13092700	-1.43599900	2.87901300
C	-4.32756400	3.57520500	-0.30211300	C	-5.15989600	-0.46222800	3.21010700
C	-3.09941900	5.69838500	-0.26336800	H	-4.71266700	1.67287000	3.31089700
C	-4.31924600	5.01890600	-0.35506100	H	-7.00371500	2.38122000	2.60708600
H	-3.09716000	-6.78261700	-0.33409800	H	-8.72231300	0.66112800	2.03154500
H	-3.09781300	6.78529700	-0.30531400	H	-8.15026700	-1.76936700	2.14027800
C	-6.75209300	-3.56609600	-0.75814800	H	-5.86756700	-2.48908100	2.88396200
C	-7.96234800	-2.84871700	-1.00544200	Cr	-0.51336500	0.02152700	1.69840700
C	-6.74302300	-5.00697200	-0.79664200	C	-1.34275300	-0.91759500	3.44969900
C	-5.55298200	-5.69148700	-0.60337800	C	0.00995500	-1.33024000	3.31804900
C	-7.97517700	-1.43036300	-0.98932700	C	1.03109800	-0.36293100	3.17523300
C	-7.97919300	1.43911700	-0.95676500	C	0.70677600	1.02059600	3.16195100
C	-9.16882000	0.72393700	-1.23711000	C	-0.63829100	1.43536600	3.34711100
C	-7.96942500	2.85732100	-0.94601700	C	-1.65866200	0.46858700	3.49023800

H	-2.12897000	-1.66359300	3.50410100	H	11.18493800	5.53807200	-0.31796400
H	0.25025900	-2.38657300	3.24863100	C	2.86511100	-3.57566300	-0.29844200
H	2.05347500	-0.67862100	2.99281900	C	2.86648200	-5.01971300	-0.31473400
H	1.48318300	1.75737900	2.98390600	C	10.27285300	-3.56020500	-0.31591500
H	-0.89223700	2.48984600	3.30331400	C	10.23820900	-5.00336200	-0.31673500
H	-4.16059500	-0.78023400	3.47906900	C	5.33100600	-5.01194000	-0.30991800
H	-2.68939400	0.79125700	3.56285900	C	4.11201100	-5.69428500	-0.31544200
<b>19-d</b>				C	6.58655900	-5.68811400	-0.31281200
C	7.78791300	-0.71576900	-0.31008000	C	7.79087100	-5.00729900	-0.31286500
C	6.56246600	-1.42755400	-0.30629800	C	9.06501000	-5.68802500	-0.31552400
C	7.78788800	0.71593100	-0.30998000	H	4.11579600	-6.78199500	-0.32420100
C	5.32664700	-0.71883200	-0.30137100	H	6.58888200	-6.77599900	-0.31549100
C	6.56242300	1.42767800	-0.30610500	H	9.06350600	-6.77529700	-0.31664300
C	5.32662900	0.71892300	-0.30127400	H	11.18514200	-5.53782300	-0.31878600
C	4.11037900	-1.43244700	-0.28922300	C	1.63076400	1.43437700	-0.27628200
C	4.10075700	-2.86291700	-0.29863000	C	1.63090900	2.87738100	-0.29498400
C	6.56180600	-2.85716700	-0.30779400	C	0.39245300	0.71835400	-0.31245000
C	5.33162900	-3.56795000	-0.30426800	C	1.63092300	-2.87737500	-0.29519700
C	6.56172000	2.85727800	-0.30742800	C	1.63078000	-1.43435900	-0.27646900
C	7.79670900	3.56282500	-0.31055000	C	0.39245100	-0.71835200	-0.31251100
C	9.02064900	1.42688300	-0.31263100	C	11.46264000	2.84352000	-0.31717500
C	9.02000000	2.85220800	-0.31289200	C	11.48756000	1.42939200	-0.31708100
C	2.87070200	-0.71717600	-0.28812900	C	12.70503700	0.68614700	-0.31894400
C	2.87069800	0.71721300	-0.28801300	C	11.46275400	-2.84323700	-0.31760300
C	4.11034900	1.43250200	-0.28903100	C	11.48761500	-1.42910600	-0.31729700
C	5.33154100	3.56803300	-0.30383300	C	12.70506400	-0.68581400	-0.31905000
C	4.10070800	2.86296300	-0.29831700	H	12.40770800	-3.38268900	-0.31947100
C	10.25259200	0.71329000	-0.31503500	H	13.64586500	-1.23086800	-0.32057800
C	10.25262000	-0.71304400	-0.31514100	H	13.64581600	1.23123900	-0.32038900
C	9.02070100	-1.42668000	-0.31283400	H	12.40757300	3.38300900	-0.31895600
C	7.79683200	-3.56267700	-0.31103200	C	0.40393000	-3.57587500	-0.32780800
C	9.02010900	-2.85201400	-0.31329500	C	-0.83656100	-2.86337600	-0.35660700
C	2.86507100	3.57570300	-0.29810600	C	0.40299300	-5.02201300	-0.34800100
C	2.86641900	5.01972200	-0.31429800	C	1.63629400	-5.70202900	-0.33305100
C	4.11190600	5.69427900	-0.31483900	C	-0.84535000	-1.43688600	-0.34105000
C	7.79070200	5.00742100	-0.31219100	C	-0.84535000	1.43687700	-0.34104700
C	9.06480400	5.68819300	-0.31472600	C	-2.06582500	0.72376000	-0.38106000
C	6.58639300	5.68817400	-0.31208500	C	-0.83655400	2.86337300	-0.35660900
C	10.27271200	3.56043700	-0.31539500	C	-2.06582800	-0.72378300	-0.38102100
C	10.23802200	5.00358700	-0.31600700	C	0.40391700	3.57588400	-0.32768000
C	5.33087900	5.01198700	-0.30932500	C	1.63624900	5.70200600	-0.33270000
H	4.11567300	6.78196100	-0.32348400	C	0.40297900	5.02201000	-0.34784000
H	6.58870000	6.77603700	-0.31462600	H	1.63743700	-6.78944200	-0.34471400
H	9.06327000	6.77545300	-0.31569400	H	1.63736600	6.78939600	-0.34430000
				C	-2.06655100	-3.57034700	-0.39757500

C	-3.29383300	-2.86216500	-0.43183900	C	-10.69155700	-1.43459400	-0.82484200
C	-2.06615700	-5.01860600	-0.41473100	C	-10.69156100	1.43450700	-0.82510400
C	-3.28623900	-1.43617900	-0.41352900	C	-11.90734700	0.68496500	-0.90268100
C	-0.83730400	-5.69780200	-0.38695800	C	-10.66639700	2.84456700	-0.82657300
C	-3.28623900	1.43615500	-0.41368300	C	-11.90734400	-0.68506700	-0.90255700
C	-4.52386000	0.71803700	-0.45791900	C	-9.47334200	3.56294100	-0.75454600
C	-3.29382600	2.86215600	-0.43208000	C	-8.26248500	5.69035200	-0.69860400
C	-2.06654800	3.57033800	-0.39772200	C	-9.43518800	5.00607300	-0.76141100
C	-4.52386300	-0.71807600	-0.45777700	H	-8.26147700	-6.77766000	-0.70766700
C	-0.83731300	5.69778800	-0.38696200	H	-10.37900900	-5.54271500	-0.82130700
C	-2.06615400	5.01860000	-0.41491200	H	-11.60801500	-3.38622800	-0.88849300
H	-0.83855800	-6.78539100	-0.40181000	H	-12.84688100	-1.22895700	-0.96399300
H	-0.83859500	6.78536700	-0.40181200	H	-12.84688500	1.22884100	-0.96421500
C	-4.53610400	-3.57344100	-0.48268400	H	-11.60802600	3.38613200	-0.88909000
C	-5.76183400	-2.87456000	-0.52385500	H	-10.37902300	5.54264400	-0.82222600
C	-4.53259200	-5.01623500	-0.50360300	H	-8.26150100	6.77762000	-0.70865700
C	-5.76270400	-1.43293800	-0.50590000	Cr	-5.85597600	0.00022300	1.19599900
C	-3.30725100	-5.69547900	-0.46537600	C	-5.25787100	1.22947500	2.86724900
C	-5.76270600	1.43289900	-0.50619400	C	-6.67545600	1.22924800	2.76928000
C	-6.99858000	0.71629400	-0.58055700	C	-7.38350200	0.00068500	2.72871200
C	-5.76183800	2.87453000	-0.52429800	C	-6.67599300	-1.22818800	2.76943100
C	-6.99858200	-0.71634400	-0.58037300	C	-5.25841400	-1.22902300	2.86744100
C	-4.53610400	3.57342000	-0.48309600	C	-4.55264300	0.00006800	2.92468600
C	-3.30725300	5.69547700	-0.46575500	H	-4.71258600	2.16791800	2.84238700
C	-4.53260000	5.01622900	-0.50410100	H	-7.21124200	2.16747900	2.66435900
H	-3.30735000	-6.78310300	-0.48025900	H	-8.46044400	0.00091600	2.59072200
H	-3.30736300	6.78310200	-0.48068500	H	-7.21219200	-2.16619000	2.66463700
C	-6.99506700	-3.57068900	-0.60236800	H	-4.71353600	-2.16770100	2.84270500
C	-8.22799700	-2.85471100	-0.67122300	Cr	1.61564800	-0.00018800	1.42915400
C	-6.98973700	-5.01096400	-0.62040700	C	0.90383100	-1.22881100	3.05289100
C	-5.78246000	-5.69377500	-0.56717900	C	2.32665800	-1.22891700	3.05389300
C	-8.23938900	-1.43495500	-0.66010200	C	3.03416300	-0.00092100	3.07528900
C	-8.23939000	1.43489600	-0.66037800	C	2.32693600	1.22726600	3.05472000
C	-9.45703600	0.71836400	-0.74323300	C	0.90409700	1.22747200	3.05377400
C	-8.22800500	2.85466000	-0.67172600	C	0.19677300	-0.00060200	3.07500700
C	-9.45703200	-0.71843700	-0.74309100	H	0.36135900	-2.16681400	2.98761900
C	-6.99507600	3.57065600	-0.60293900	H	2.86921500	-2.16673000	2.98812600
C	-5.78247200	5.69376900	-0.56785600	H	4.11832500	-0.00102900	3.01468600
C	-6.98975000	5.01094200	-0.62111900	H	2.86971100	2.16499700	2.98974300
H	-5.78420800	-6.78146600	-0.58081900	H	0.36181500	2.16563900	2.98931300
H	-5.78421800	6.78146100	-0.58158300	H	-3.46680800	-0.00016500	2.93742800
C	-9.47332800	-3.56300400	-0.75393300	H	-0.88761900	-0.00046700	3.01714500
C	-10.66638700	-2.84465100	-0.82606800				
C	-9.43517300	-5.00613400	-0.76059600	<b>19-e</b>			
C	-8.26246500	-5.69039300	-0.69774700	C	7.59055600	-0.71917800	-0.37066100

C	6.37548100	-1.43196600	-0.34587700	H	3.90968700	-6.78582100	-0.37216600
C	7.59056900	0.71921400	-0.37061600	H	6.38975400	-6.77760500	-0.38049100
C	5.13296600	-0.71607600	-0.33222800	H	8.86496600	-6.77630700	-0.39991600
C	6.37550200	1.43202000	-0.34579600	H	10.98585600	-5.53993600	-0.42212300
C	5.13297400	0.71614600	-0.33218300	C	1.41443900	1.43424100	-0.34750500
C	3.89415100	-1.43286200	-0.30973200	C	1.42476000	2.86353900	-0.35898100
C	3.89456800	-2.87620000	-0.32682400	C	0.19800500	0.72147200	-0.37259600
C	6.36587900	-2.85972300	-0.35545000	C	1.42476100	-2.86343400	-0.35902200
C	5.12889400	-3.57379000	-0.34287400	C	1.41444000	-1.43414900	-0.34751600
C	6.36592800	2.85978500	-0.35529100	C	0.19801000	-0.72139100	-0.37259500
C	7.59770300	3.56430200	-0.37407900	C	11.26681100	2.84385400	-0.42187600
C	8.82684900	1.42952000	-0.38879500	C	11.29141700	1.43033800	-0.42168600
C	8.82507700	2.85241100	-0.39009000	C	12.51001900	0.68523900	-0.43745800
C	2.65500100	-0.71706800	-0.33357800	C	11.26674900	-2.84388100	-0.42210100
C	2.65500600	0.71715700	-0.33354900	C	11.29138600	-1.43036800	-0.42179900
C	3.89416200	1.43294400	-0.30965700	H	12.21145000	-3.38362100	-0.43516400
C	5.12894400	3.57386800	-0.34272100	H	13.45066300	-1.23050600	-0.44994800
C	3.89459700	2.87629000	-0.32671600	H	13.45069000	1.23043300	-0.44984600
C	10.05726000	0.71448200	-0.40542000	H	12.21152400	3.38357700	-0.43488800
C	10.05724500	-0.71449100	-0.40547300	C	0.20012800	-3.56986600	-0.37964100
C	8.82682100	-1.42950400	-0.38889300	C	-1.03284900	-2.86125700	-0.39567400
C	7.59763600	-3.56425800	-0.37429700	C	0.20074300	-5.01831700	-0.38961600
C	8.82501900	-2.85239100	-0.39028700	C	1.43280800	-5.69718300	-0.38048800
C	2.66873400	3.57521100	-0.34528400	C	-1.03302900	-1.43243000	-0.39003700
C	2.66874100	5.01935900	-0.36198900	C	-1.03304900	1.43250000	-0.39007600
C	3.90794200	5.69844900	-0.36194300	C	-2.26437900	0.72128700	-0.40392000
C	7.59142200	5.00885800	-0.37983400	C	-1.03288800	2.86134300	-0.39570700
C	8.86625600	5.68905700	-0.39656100	C	-2.26436400	-0.72124000	-0.40389400
C	6.38677500	5.68980600	-0.37221700	C	0.20010100	3.56996300	-0.37965000
C	10.07596500	3.56096100	-0.40707800	C	1.43280200	5.69733500	-0.38045600
C	10.03957000	5.00460300	-0.40882700	C	0.20070600	5.01844600	-0.38962900
C	5.13034500	5.01479200	-0.35826500	H	1.43202200	-6.78478800	-0.39129400
H	3.90974500	6.78597100	-0.37198300	H	1.43201200	6.78497000	-0.39126400
H	6.38985700	6.77770500	-0.38016900	C	-2.26717300	-3.56950400	-0.41388300
H	8.86509800	6.77634700	-0.39946700	C	-3.49075300	-2.86241700	-0.42583900
H	10.98597100	5.53992600	-0.42169100	C	-2.26734700	-5.01720600	-0.42488300
C	2.66872000	-3.57511300	-0.34535700	C	-3.48101000	-1.43354600	-0.41157300
C	2.66871700	-5.01923200	-0.36207700	C	-1.03661100	-5.69632800	-0.41167100
C	10.07589000	-3.56096200	-0.40734300	C	-3.48104600	1.43357100	-0.41166400
C	10.03946800	-5.00459900	-0.40919500	C	-4.72160600	0.71686400	-0.42915400
C	5.13027700	-5.01469400	-0.35846000	C	-3.49082600	2.86245400	-0.42595400
C	3.90788900	-5.69832100	-0.36210100	C	-2.26724400	3.56956600	-0.41398000
C	6.38668400	-5.68972000	-0.37249100	C	-4.72158300	-0.71687200	-0.42909000
C	7.59133000	-5.00880300	-0.38012700	C	-1.03669000	5.69646400	-0.41174800
C	8.86614500	-5.68902500	-0.39693800	C	-2.26744600	5.01729800	-0.42500100

H	-1.03691100	-6.78393300	-0.42015800	H	-13.05494700	-1.22900100	-0.74297300
H	-1.03700400	6.78410000	-0.42025300	H	-13.05499500	1.22868800	-0.74304200
C	-4.73534500	-3.57329300	-0.44935600	H	-11.81467300	3.38587800	-0.69516400
C	-5.96119200	-2.87422000	-0.46339700	H	-10.58463600	5.54214400	-0.65519600
C	-4.73326100	-5.01518700	-0.46743200	H	-8.46488900	6.77716800	-0.58857100
C	-5.96161400	-1.43227200	-0.44655900	Cr	-6.01428100	0.00007300	1.25242800
C	-3.50676200	-5.69503300	-0.45161600	C	-5.36207500	1.22848600	2.90499400
C	-5.96165900	1.43222500	-0.44671500	C	-6.78252500	1.22875800	2.85203600
C	-7.19887900	0.71610900	-0.49530100	C	-7.49190100	0.00079300	2.83795300
C	-5.96128700	2.87418200	-0.46358100	C	-6.78356200	-1.22777800	2.85214800
C	-7.19885500	-0.71619200	-0.49522400	C	-5.36311600	-1.22870800	2.90516000
C	-4.73545000	3.57329100	-0.44953800	C	-4.65527800	-0.00041400	2.94261900
C	-3.50690400	5.69511000	-0.45180100	H	-4.81740800	2.16657200	2.86208300
C	-4.73340900	5.01521000	-0.46764300	H	-7.32143800	2.16709500	2.76538800
H	-3.50694200	-6.78267800	-0.46326600	H	-8.57292500	0.00124900	2.73657000
H	-3.50710700	6.78278000	-0.46347600	H	-7.32327800	-2.16565900	2.76563500
C	-7.19596600	-3.57037200	-0.51327200	H	-4.81924600	-2.16725300	2.86238400
C	-8.43059000	-2.85437100	-0.55514900	Cr	3.89571100	-0.00003500	1.38724000
C	-7.19171800	-5.01032900	-0.53049600	C	3.19385300	-1.22803600	3.01861600
C	-5.98329800	-5.69312900	-0.50330800	C	4.61627700	-1.22834400	3.00966100
C	-8.44155000	-1.43474400	-0.54456200	C	5.32469000	-0.00065500	3.02378800
C	-8.44160200	1.43461400	-0.54467100	C	4.61691600	1.22742000	3.01002100
C	-9.66086600	0.71829800	-0.59990000	C	3.19448600	1.22784800	3.01903500
C	-8.43069500	2.85424500	-0.55533000	C	2.48636000	0.00008600	3.04186700
C	-9.66083900	-0.71847800	-0.59985100	H	2.65088000	-2.16603800	2.95786600
C	-7.19609200	3.57029200	-0.51349100	H	5.15806400	-2.16643200	2.94091100
C	-5.98348300	5.69311900	-0.50356800	H	6.40841700	-0.00092200	2.95664200
C	-7.19189200	5.01026300	-0.53075600	H	5.15919400	2.16525800	2.94160200
H	-5.98519500	-6.78083600	-0.51538300	H	2.65199400	2.16616300	2.95863000
H	-5.98540800	6.78084200	-0.51567300	H	-3.56968900	-0.00086900	2.92077800
C	-9.67716400	-3.56279200	-0.60901800	H	1.40176400	0.00038300	2.98967700
C	-10.87183200	-2.84439300	-0.65431200				
C	-9.63943400	-5.00580700	-0.61580600	<b>19-f</b>			
C	-8.46558900	-5.69001000	-0.57897500	C	7.39660900	-0.71584100	-0.41253300
C	-10.89681300	-1.43473900	-0.65293500	C	6.15881300	-1.43203300	-0.38012100
C	-10.89686700	1.43451300	-0.65301900	C	7.39663300	0.71598800	-0.41233700
C	-12.11435600	0.68471100	-0.70300600	C	4.91784100	-0.71686400	-0.38322400
C	-10.87194100	2.84417000	-0.65447400	C	6.15885100	1.43221100	-0.37978100
C	-12.11432900	-0.68498700	-0.70296700	C	4.91785700	0.71707000	-0.38308000
C	-9.67729900	3.56262000	-0.60922400	C	3.67794200	-1.43247200	-0.38296000
C	-8.46579600	5.68989600	-0.57926800	C	3.68830900	-2.86243800	-0.39642500
C	-9.63962100	5.00564000	-0.61607300	C	6.15911900	-2.87363400	-0.39748500
H	-8.46464300	-6.77727300	-0.58823800	C	4.93232500	-3.57293400	-0.40114500
H	-10.58442800	-5.54234000	-0.65490900	C	6.15920700	2.87383300	-0.39689200
H	-11.81454100	-3.38613800	-0.69498000	C	7.39379200	3.56995800	-0.42894300



C	8.64008600	1.43464300	-0.44402400	C	11.09676900	1.43454100	-0.51903000
C	8.62938700	2.85383600	-0.45412000	C	12.31514600	0.68469200	-0.55267000
C	2.46092500	-0.71987600	-0.39215000	C	11.07154400	-2.84397800	-0.52095100
C	2.46091800	0.72009800	-0.39208700	C	11.09669900	-1.43451500	-0.51941100
C	3.67795300	1.43269900	-0.38275900	C	12.31511100	-0.68471800	-0.55285600
C	4.93239100	3.57316900	-0.40056300	H	12.01459900	-3.38595500	-0.54872500
C	3.68833500	2.86269200	-0.39602800	H	13.25608500	-1.22891600	-0.58007900
C	9.86028400	0.71833100	-0.48301500	H	13.25614700	1.22885600	-0.57974400
C	9.86025000	-0.71826500	-0.48320300	H	12.01477100	3.38596000	-0.54781800
C	8.64002600	-1.43453400	-0.44438700	C	0.00005400	-3.56891300	-0.40289900
C	7.39365500	-3.56978200	-0.42972100	C	-1.22876500	-2.86120400	-0.40050400
C	8.62926300	-2.85370700	-0.45481900	C	0.00008200	-5.01658100	-0.41034400
C	2.46486900	3.56966500	-0.40127600	C	1.23439700	-5.69542700	-0.41481900
C	2.46610100	5.01647300	-0.41113100	C	-1.22721100	-1.42987800	-0.39573700
C	3.70475900	5.69483200	-0.41970600	C	-1.22727900	1.43000500	-0.39581800
C	7.38997500	5.01005600	-0.44601500	C	-2.46095400	0.72001400	-0.39209700
C	8.66455400	5.68962400	-0.47656100	C	-1.22890400	2.86135700	-0.40062000
C	6.18165500	5.69302700	-0.43569200	C	-2.46091100	-0.71995900	-0.39201200
C	9.87634000	3.56227500	-0.49076900	C	-0.00006900	3.56910800	-0.40287300
C	9.83870100	5.00538200	-0.49745400	C	1.23427800	5.69578000	-0.41455600
C	4.93122400	5.01506300	-0.41808500	C	-0.00009300	5.01685000	-0.41030800
H	3.70471000	6.78251200	-0.43066600	H	1.23434700	-6.78299600	-0.42201500
H	6.18369500	6.78075800	-0.44728600	H	1.23419600	6.78342000	-0.42172100
H	8.66377200	6.77691300	-0.48542700	C	-2.46478400	-3.56949700	-0.40123400
H	10.78418900	5.54188800	-0.52331600	C	-3.68822600	-2.86255800	-0.39595400
C	2.46489200	-3.56941500	-0.40160200	C	-2.46596900	-5.01623500	-0.41109600
C	2.46613100	-5.01615400	-0.41156200	C	-3.67789800	-1.43259600	-0.38265600
C	9.87617200	-3.56218200	-0.49166400	C	-1.23421500	-5.69546900	-0.41455600
C	9.83847800	-5.00526900	-0.49867400	C	-3.67799800	1.43257700	-0.38291100
C	4.93112800	-5.01477000	-0.41884600	C	-4.91787200	0.71690800	-0.38309800
C	3.70471900	-5.69447800	-0.42036600	C	-3.68843500	2.86256000	-0.39636200
C	6.18149400	-5.69274500	-0.43670600	C	-2.46500100	3.56957400	-0.40156500
C	7.38979400	-5.00984100	-0.44704500	C	-4.91781100	-0.71702800	-0.38291400
C	8.66432000	-5.68945000	-0.47783500	C	-1.23449500	5.69573200	-0.41478100
H	3.70467600	-6.78209800	-0.43142900	C	-2.46627900	5.01637800	-0.41152600
H	6.18351500	-6.78043600	-0.44847200	H	-1.23411900	-6.78303800	-0.42171700
H	8.66349700	-6.77671400	-0.48693000	H	-1.23445000	6.78337000	-0.42198600
H	10.78393700	-5.54179500	-0.52472200	C	-4.93221700	-3.57309400	-0.40045900
C	1.22721700	1.43004800	-0.39577000	C	-6.15903300	-2.87383000	-0.39678500
C	1.22879200	2.86140300	-0.40050600	C	-4.93097000	-5.01493200	-0.41798600
C	-0.00002000	0.71859900	-0.39636400	C	-6.15876400	-1.43223200	-0.37966600
C	1.22884700	-2.86116500	-0.40066100	C	-3.70454300	-5.69460100	-0.41962200
C	1.22724700	-1.42983800	-0.39583400	C	-6.15889300	1.43200600	-0.38007900
C	0.00000500	-0.71842600	-0.39635800	C	-7.39665900	0.71574500	-0.41248000
C	11.07168600	2.84401400	-0.52020100	C	-6.15929600	2.87362500	-0.39745100

C	-7.39659200	-0.71608600	-0.41224900	C	-5.51994700	-1.22790100	2.96638400
C	-4.93251200	3.57299300	-0.40112100	C	-4.81226900	0.00039800	2.99909000
C	-3.70495900	5.69468900	-0.42035700	H	-4.97513400	2.16715400	2.91710900
C	-4.93138400	5.01487900	-0.41883600	H	-7.48060600	2.16708800	2.84397700
H	-3.70446000	-6.78222400	-0.43058400	H	-8.73184500	0.00142900	2.83150700
H	-3.70494100	6.78236500	-0.43143300	H	-7.48179900	-2.16490800	2.84556000
C	-7.39355100	-3.57002300	-0.42886700	H	-4.97632300	-2.16629800	2.91876200
C	-8.62917800	-2.85399700	-0.45409100	Cr	6.18818000	-0.00018000	1.32029900
C	-7.38964200	-5.01008800	-0.44594300	C	5.51921300	-1.22889600	2.96566300
C	-6.18132400	-5.69295100	-0.43560300	C	6.94053400	-1.22894400	2.92620700
C	-8.63998500	-1.43482500	-0.44399100	C	7.64996000	-0.00121200	2.92225300
C	-8.64013000	1.43436000	-0.44439100	C	6.94146700	1.22707300	2.92693600
C	-9.86029800	0.71799700	-0.48323100	C	5.52013700	1.22807700	2.96646000
C	-8.62946500	2.85354100	-0.45482300	C	4.81232800	-0.00015300	2.99927700
C	-9.86022400	-0.71859600	-0.48303100	H	4.97498300	-2.16690500	2.91739900
C	-7.39389400	3.56969900	-0.42972000	H	7.48041500	-2.16710400	2.84398300
C	-6.18183200	5.69279900	-0.43670700	H	8.73189600	-0.00158600	2.83127700
C	-7.39011600	5.00979200	-0.44705000	H	7.48206800	2.16489300	2.84534800
H	-6.18330700	-6.78064500	-0.44720700	H	4.97660800	2.16655300	2.91883900
H	-6.18389800	6.78052600	-0.44847600	H	-3.72686100	0.00010200	2.96786900
C	-9.87607400	-3.56251400	-0.49079100	H	3.72691300	0.00027700	2.96824700
C	-11.07145800	-2.84435400	-0.52027500				
C	-9.83833300	-5.00560700	-0.49747600	<b>20</b>			
C	-8.66415500	-5.68974500	-0.47653500	C	2.45867100	-0.71288400	0.00009300
C	-11.09665200	-1.43488400	-0.51909800	C	1.23243100	-1.42221000	0.00034100
C	-11.09680200	1.43415600	-0.51947600	C	2.45866800	0.71288300	0.00029200
C	-12.31514900	0.68427300	-0.55295300	C	-0.00003100	-0.71115400	-0.00001800
C	-11.07175600	2.84363400	-0.52100800	C	1.23243100	1.42221300	0.00004600
C	-12.31507600	-0.68513800	-0.55277200	C	-0.00002800	0.71115200	0.00046100
C	-9.87644100	3.56193200	-0.49169100	C	-1.23242400	-1.42217600	0.00034500
C	-8.66471400	5.68931500	-0.47784500	C	-1.23220900	-2.85224200	0.00000500
C	-9.83883500	5.00504100	-0.49869100	C	1.23223300	-2.85224600	0.00007300
H	-8.66329600	-6.77701200	-0.48540300	C	-0.00001300	-3.56205300	0.00009400
H	-10.78377900	-5.54216600	-0.52337800	C	1.23223300	2.85224600	0.00022100
H	-12.01450500	-3.38635200	-0.54792700	C	2.46183300	3.55963700	0.00003500
H	-13.25604000	-1.22936100	-0.57988800	C	3.69464800	1.42626300	0.00005900
H	-13.25617000	1.22839500	-0.58021400	C	3.69338300	2.84766500	0.00004000
H	-12.01486300	3.38553300	-0.54879400	C	-2.45866000	-0.71284500	-0.00009000
H	-10.78433700	5.54151400	-0.52473900	C	-2.45866000	0.71284500	0.00031600
H	-8.66396000	6.77660100	-0.48693100	C	-1.23242300	1.42217700	-0.00007500
Cr	-6.18825300	0.00020200	1.32029600	C	-0.00001200	3.56205200	0.00002900
C	-5.51927400	1.22907300	2.96548000	C	-1.23220800	2.85224200	0.00021700
C	-6.94060600	1.22897400	2.92616500	C	4.92560600	0.71352000	0.00001200
C	-7.64989500	0.00115800	2.92235100	C	4.92560600	-0.71352000	0.00002300
C	-6.94127300	-1.22704700	2.92700800	C	3.69464800	-1.42626400	0.00012000

C	2.46183300	-3.55963700	0.00005100	H	-5.84678400	5.53633000	-0.00010900
C	3.69338300	-2.84766600	0.00004300	C	-7.38250000	0.68342700	-0.00012000
C	-2.46180500	3.55963400	-0.00001600	C	-7.38250000	-0.68342400	-0.00010100
C	-2.45516500	4.99787100	-0.00003700	H	-8.32254400	1.22984600	-0.00013600
C	-1.24126300	5.67718000	-0.00003000	H	-8.32254400	-1.22984300	-0.00015300
C	2.45512700	4.99793000	-0.00001900	H	-3.72187300	6.76861500	-0.00012700
C	3.72506800	5.68136000	-0.00008400	H	-1.24110000	6.76511600	-0.00010200
C	1.24131000	5.67719500	-0.00001900	H	1.24104800	6.76513200	-0.00007200
C	4.93941700	3.55766700	-0.00007000	H	3.72190900	6.76864500	-0.00011400
C	4.90167600	4.99868800	-0.00012800	H	5.84678400	5.53638200	-0.00016900
C	-0.00002700	4.99657300	0.00000900	H	7.07892100	3.38131700	-0.00019900
C	-2.46180700	-3.55963500	0.00005400	H	8.32253300	1.22979900	-0.00022900
C	-2.45516500	-4.99787200	-0.00003900	H	8.32253300	-1.22979700	-0.00017300
C	4.93941700	-3.55766800	-0.00002600	H	7.07892100	-3.38131700	-0.00010100
C	4.90167400	-4.99868900	-0.00007000	H	5.84678200	-5.53638300	-0.00010000
C	-0.00002800	-4.99657500	-0.00002700	H	3.72190800	-6.76864700	-0.00012800
C	-1.24126400	-5.67718200	-0.00009800	H	1.24104700	-6.76513300	-0.00012000
C	1.24130900	-5.67719600	-0.00009100	H	-1.24110200	-6.76511800	-0.00012000
C	2.45512600	-4.99793000	-0.00003100	H	-3.72187400	-6.76861600	-0.00009400
C	3.72506700	-5.68136200	-0.00009100				
C	-3.69465900	1.42624500	-0.00005700	<b>21</b>			
C	-3.69340700	2.84764500	0.00005400	C	-2.28221700	0.71723900	-0.40542900
C	-4.92559000	0.71352300	0.00003300	C	-1.05240300	1.42881600	-0.34854500
C	-3.69340800	-2.84764400	-0.00001600	C	-2.28171000	-0.71914200	-0.39484100
C	-3.69466000	-1.42624400	0.00013400	C	0.19099400	0.71250300	-0.32290200
C	-4.92559000	-0.71352100	-0.00004000	C	-1.05146700	-1.43116000	-0.35651700
C	6.13549100	2.83919500	-0.00015100	C	0.19041100	-0.71333700	-0.31110000
C	6.16019000	1.43142200	-0.00010000	Cr	-1.12512300	0.00227600	1.52314000
C	7.38244700	0.68345800	-0.00016400	C	-0.48537900	1.33184600	2.61399600
C	6.13549100	-2.83919600	-0.00006200	C	-2.66000800	-0.06165900	2.52251500
C	6.16019000	-1.43142200	-0.00006200	C	-0.37027800	-1.25958000	2.62167400
C	7.38244600	-0.68345600	-0.00012900	O	0.11432200	-2.06908400	3.30239400
C	-4.93935800	-3.55766900	-0.00003900	O	-3.64612800	-0.10247600	3.13910400
C	-6.13551200	-2.83913900	-0.00005700	O	-0.07566800	2.18539400	3.29020300
C	-4.90167500	-4.99864200	-0.00006400	C	1.42868900	1.42776200	-0.29818500
C	-4.93935700	3.55767000	-0.00005200	C	1.41976100	2.85520700	-0.32190100
C	-6.13551100	2.83914000	-0.00010600	C	-1.05060800	2.86669700	-0.38255400
C	-4.90167400	4.99864300	-0.00010300	C	0.18305100	3.56690400	-0.35922600
C	-3.72503600	-5.68133400	-0.00008500	C	-1.04950500	-2.86852400	-0.37705600
C	-6.16019300	-1.43145700	-0.00006400	C	-2.27576800	-3.56720600	-0.44202500
H	-5.84678400	-5.53633100	-0.00009300	C	-3.52288900	-1.43664600	-0.47060300
H	-7.07890000	-3.38133500	-0.00011800	C	-3.51290900	-2.85208600	-0.48640400
C	-6.16019300	1.43145900	-0.00006400	C	2.64589000	0.71564200	-0.28337800
C	-3.72503500	5.68133300	-0.00007700	C	2.64591200	-0.71571300	-0.27958900
H	-7.07889900	3.38133800	-0.00010800	C	1.42931300	-1.42834400	-0.30153700

C	0.18472100	-3.56827000	-0.35820700	H	6.03104700	5.53911300	-0.24850700
C	1.42084600	-2.85572200	-0.31747800	H	7.26288600	3.38322000	-0.21309300
C	-4.74393000	-0.71833800	-0.53471500	C	6.34559400	-1.43048000	-0.22404200
C	-4.74441600	0.71520400	-0.53600700	C	3.91323300	-5.68369900	-0.29746500
C	-3.52370800	1.43406400	-0.46846400	H	7.26430100	-3.38112700	-0.21447600
C	-2.27721000	3.56479100	-0.44280800	H	6.03351800	-5.53758000	-0.24978200
C	-3.51424100	2.84958100	-0.48863700	C	7.56756300	-0.68246800	-0.20106200
C	2.64835600	-3.56178300	-0.30308900	C	7.56730500	0.68460500	-0.20058900
C	2.64202500	-5.00139700	-0.31932600	H	8.50757600	-1.22841400	-0.18351500
C	1.43053500	-5.68072400	-0.35772700	H	8.50710600	1.23090700	-0.18297700
C	-2.26887400	-5.00400400	-0.46518800	H	3.91116700	-6.77077900	-0.30591000
C	-3.53867000	-5.68656900	-0.52689200	H	1.43124200	-6.76837000	-0.37166200
C	-1.05370300	-5.68187400	-0.43104000	H	-1.05215900	-6.76949900	-0.44665700
C	-4.75502300	-3.56268500	-0.55585900	H	-3.53549000	-6.77358900	-0.53969700
C	-4.71459500	-5.00440700	-0.57008100	H	-5.65783900	-5.54288600	-0.61732200
C	0.18640000	-5.00108900	-0.38133400	H	-6.89197100	-3.38440000	-0.66005900
C	2.64679500	3.56176300	-0.30379700	H	-8.13610900	-1.23123600	-0.71461100
C	2.63987100	5.00140300	-0.32060300	H	-8.13685600	1.22642100	-0.71403600
C	-4.75669500	3.55957600	-0.55589900	H	-6.89373400	3.38044700	-0.65881900
C	-4.71676500	5.00134500	-0.56990300	H	-5.66018100	5.53955200	-0.61672600
C	0.18429000	4.99975600	-0.38405700	H	-3.53811900	6.77086400	-0.54075800
C	1.42805900	5.68002700	-0.36047900	H	-1.05496900	6.76755100	-0.44927300
C	-1.05604600	5.67990600	-0.43415700	H	1.42814100	6.76768300	-0.37386500
C	-2.27095900	5.00168000	-0.46727100	H	3.90819600	6.77137700	-0.30606600
C	-3.54098200	5.68383900	-0.52834000				
C	3.88259000	-1.42808900	-0.26610100	<b>22-ts</b>			
C	3.88005600	-2.84842300	-0.27317500	C	1.31011700	1.50078400	-0.36537700
C	5.11223000	-0.71350300	-0.24346400	C	2.52929800	0.77898900	-0.36866400
C	3.87892100	2.84897100	-0.27401000	C	0.06868500	0.80148200	-0.36775500
C	3.88199900	1.42860800	-0.26498100	C	2.51862100	-0.64650800	-0.38635500
C	5.11199800	0.71460700	-0.24361000	C	0.05613000	-0.62921800	-0.41580100
C	-5.94995900	-2.84253600	-0.60987500	C	1.28790200	-1.35344800	-0.38470500
C	-5.97563600	-1.43493000	-0.60366400	Cr	-0.38794000	-0.49385600	1.83869300
C	-7.19750500	-0.68489400	-0.66639100	C	0.95197300	0.14462200	2.89434000
C	-5.95149500	2.83899300	-0.60876400	C	-1.64587900	0.29997100	2.89513600
C	-5.97642500	1.43128200	-0.60320200	C	-0.46743700	-2.01682500	2.83432200
C	-7.19795000	0.68061300	-0.66574400	O	-0.50532400	-3.00054700	3.46018000
C	5.12467900	3.55953000	-0.25485400	O	-2.45918400	0.81544000	3.55331300
C	6.31958800	2.84132300	-0.22860000	O	1.82395300	0.54632700	3.55695200
C	5.08622600	5.00144300	-0.26578000	C	3.74692800	-1.37008300	-0.39575200
C	5.12622200	-3.55845200	-0.25530100	C	4.98253100	-0.66556500	-0.38274200
C	6.32075200	-2.83965200	-0.22988200	C	3.76882700	1.48320200	-0.35939100
C	5.08844600	-5.00033600	-0.26655800	C	4.99345500	0.76073300	-0.36144800
C	3.91074900	5.68429600	-0.29791000	C	-1.18749100	-1.33943500	-0.42889200
C	6.34502500	1.43213800	-0.22353700	C	-2.40928900	-0.61286500	-0.43474500

C	-1.16547500	1.51948100	-0.38483600	C	-6.05330000	2.96666900	-0.44964700
C	-2.39778800	0.81681200	-0.42221800	C	-6.09448700	-2.71039800	-0.57217500
C	3.73335600	-2.79163600	-0.43254900	C	-4.87680100	-4.87978800	-0.62794600
C	2.49706400	-3.49702900	-0.46575200	C	4.99991600	5.04592200	-0.30643800
C	1.27264600	-2.78454000	-0.45497700	C	4.92664100	-4.95031100	-0.48804900
C	-1.19335600	-2.77152000	-0.49645600	C	-3.70609100	-5.57233000	-0.63921000
C	0.03581000	-3.48549900	-0.50772800	C	-7.32764500	-0.54607100	-0.53719100
C	-1.15189800	2.94843100	-0.36832900	C	-7.31684300	0.82037900	-0.50748800
C	0.08706100	3.64561800	-0.35049900	C	-3.62464800	5.79285600	-0.37172000
C	1.31615200	2.92848100	-0.34762500	H	-5.74672800	5.66222000	-0.40198300
C	3.77688200	2.90438000	-0.33962500	H	-3.61431300	6.87977400	-0.35574400
C	2.55089200	3.62605900	-0.33636300	H	-1.13143500	6.85643500	-0.32746300
C	-3.64891500	-1.31921900	-0.47999100	H	1.35093200	6.83824900	-0.30647900
C	-4.87212200	-0.59480000	-0.49039900	H	3.83342500	6.82462900	-0.28974500
C	-3.65388700	-2.73929000	-0.53068100	H	5.94864200	5.57669700	-0.29295100
C	-4.86094700	0.83177500	-0.46396800	H	7.16552700	3.41199300	-0.31473900
C	-2.42724800	-3.46368600	-0.54011200	H	8.39394000	1.25085300	-0.33543100
C	-3.62526200	1.53708400	-0.43359400	H	8.37513800	-1.20801700	-0.37507000
C	-3.61238900	2.95900100	-0.41064600	H	7.11377100	-3.34899700	-0.42743000
C	-2.37720900	3.66247300	-0.38052700	H	5.86838700	-5.49348600	-0.49256300
C	-4.85305100	3.67740500	-0.41934900	H	3.73732600	-6.71206600	-0.56136200
C	-2.35961000	5.10037300	-0.36338000	H	1.25687300	-6.69205300	-0.60800400
C	0.09746100	5.07967800	-0.33572900	H	-1.22818700	-6.67449300	-0.64931900
C	2.55388800	5.06346900	-0.31968300	H	-3.71232700	-6.65865200	-0.67807600
C	5.02733900	3.60498100	-0.32459700	H	-5.82583900	-5.40915400	-0.65911100
C	6.23311100	1.46943700	-0.34596000	H	-7.04129400	-3.24532200	-0.60442800
C	6.21118700	-1.39279700	-0.39091200	H	-8.27158500	-1.08455900	-0.56522600
C	4.97335700	-3.50995900	-0.44467600	H	-8.25238800	1.37405600	-0.51092600
C	2.48097200	-4.93451700	-0.52180600	H	-6.99277500	3.51520600	-0.45518900
C	0.02570000	-4.91721900	-0.56534300				
C	-2.43061700	-4.90076600	-0.59742400	23			
C	-4.90403300	-3.43919100	-0.57606100	C	-2.46447200	0.82419200	-0.37657000
C	-6.11101600	-1.30316100	-0.53277100	C	-1.23809400	1.53474700	-0.34130400
C	-6.08885600	1.55857700	-0.47258200	C	-2.46595300	-0.60297600	-0.40211500
C	-1.22105300	-5.58758400	-0.60994400	C	0.00014400	0.82770600	-0.32136400
C	1.26333100	-5.60507600	-0.56991000	C	-1.24125200	-1.32138900	-0.38486400
C	3.74667200	-5.62560500	-0.52682000	C	0.00012600	-0.60482900	-0.37134300
C	6.17475700	-2.79958000	-0.41990400	Cr	-0.00071500	-0.66444200	1.85568200
C	7.43947300	-0.65448100	-0.37187200	C	-1.30528800	0.05849700	2.90822300
C	7.44984900	0.71201000	-0.35033300	C	-0.00099100	-2.19658900	2.84915200
C	6.21836900	2.87691800	-0.32809200	C	1.30378600	0.05818700	2.90854800
C	3.82833000	5.73763600	-0.30426000	O	2.14671300	0.52526900	3.56492600
C	1.34361400	5.75058100	-0.31922800	O	-0.00111300	-3.18464300	3.46816500
C	-1.14017700	5.76876200	-0.34065600	O	-2.14823600	0.52586600	3.56437500
C	-4.80549600	5.11821300	-0.39762600	C	1.23839900	1.53469900	-0.34126200

C	1.23474900	2.96279100	-0.32326400	C	-6.16191500	1.54200200	-0.42109400
C	-1.23438600	2.96283900	-0.32332400	C	-7.38410200	0.79446800	-0.45668100
C	0.00019600	3.66978800	-0.31116500	C	4.94130600	3.66799100	-0.35926600
C	-1.23403400	-2.75200200	-0.47184900	C	6.13727700	2.94957300	-0.39022100
C	-2.46359500	-3.45405000	-0.51897800	C	4.90312900	5.10877900	-0.33075600
C	-3.69889300	-1.31702700	-0.44897000	C	4.93980400	-3.44701000	-0.54859300
C	-3.69425100	-2.73831700	-0.50247800	C	6.13536600	-2.72695700	-0.53958100
C	2.46474800	0.82409400	-0.37642500	C	4.90270500	-4.88710800	-0.60859500
C	2.46617900	-0.60306400	-0.40202800	C	3.72656100	5.79119200	-0.30601000
C	1.24145000	-1.32143100	-0.38483400	C	6.16222900	1.54176700	-0.42080500
C	0.00006200	-3.45955000	-0.51209700	H	5.84788200	5.64672800	-0.32926500
C	1.23417700	-2.75204200	-0.47181400	H	7.08050200	3.49164600	-0.39039800
C	-4.92851700	-0.60225400	-0.45369900	C	6.16216400	-1.31991800	-0.49480100
C	-4.92822500	0.82382100	-0.41897100	C	3.72739600	-5.57137100	-0.63142300
C	-3.69759600	1.53666400	-0.38664800	H	7.07831900	-3.26867000	-0.57256000
C	-2.46446000	3.66947700	-0.32882200	H	5.84822300	-5.42283500	-0.63891500
C	-3.69541200	2.95807500	-0.35709700	C	7.38457700	-0.57228400	-0.49222400
C	2.46371300	-3.45414100	-0.51888100	C	7.38438700	0.79418500	-0.45634600
C	2.45660100	-4.89079300	-0.59233200	H	8.32442600	-1.11796800	-0.51996400
C	1.24260100	-5.56871800	-0.62529200	H	8.32433400	1.34040900	-0.45456700
C	-2.45653200	-4.89070500	-0.59243000	H	3.72606100	-6.65736200	-0.67903300
C	-3.72735500	-5.57123200	-0.63157600	H	1.24244500	-6.65508500	-0.67770700
C	-1.24255800	-5.56867200	-0.62533700	H	-1.24243600	-6.65503900	-0.67775300
C	-4.93968500	-3.44682400	-0.54879300	H	-3.72605900	-6.65722300	-0.67919300
C	-4.90263500	-4.88692400	-0.60879600	H	-5.84817500	-5.42261200	-0.63915600
C	0.00003600	-4.88953200	-0.58995400	H	-7.07819000	-3.26839800	-0.57284400
C	2.46484700	3.66938400	-0.32870900	H	-8.32421200	-1.11764900	-0.52031700
C	2.45714900	5.10706100	-0.30618000	H	-8.32402600	1.34073200	-0.45495000
C	-4.94091700	3.66818200	-0.35951100	H	-7.08011400	3.49191800	-0.39075000
C	-4.90268300	5.10896900	-0.33099600	H	-5.84741800	5.64695200	-0.32955600
C	0.00022300	5.10366100	-0.29338200	H	-3.72283500	6.87824100	-0.28548200
C	1.24201500	5.78407400	-0.28740100	H	-1.24031900	6.87180700	-0.27124100
C	-1.24155100	5.78412100	-0.28746000	H	1.24083000	6.87176000	-0.27118600
C	-2.45670600	5.10715900	-0.30629700	H	3.72334200	6.87809500	-0.28530600
C	-3.72609400	5.79133800	-0.30619000				
C	3.69909200	-1.31716500	-0.44881400	<b>24-ts</b>			
C	3.69439700	-2.73845600	-0.50233400	C	1.31011700	1.50078400	-0.36537700
C	4.92874500	-0.60244200	-0.45349500	C	2.52929800	0.77898900	-0.36866400
C	3.69577900	2.95793100	-0.35690700	C	0.06868500	0.80148200	-0.36775500
C	3.69790900	1.53652400	-0.38647200	C	2.51862100	-0.64650800	-0.38635500
C	4.92850500	0.82363200	-0.41873500	C	0.05613000	-0.62921800	-0.41580100
C	-6.13521500	-2.72672400	-0.53983200	C	1.28790200	-1.35344800	-0.38470500
C	-6.16196000	-1.31968100	-0.49505900	Cr	-0.38794000	-0.49385600	1.83869300
C	-7.38434400	-0.57200000	-0.49254600	C	0.95197300	0.14462200	2.89434000
C	-6.13690900	2.94981100	-0.39052200	C	-1.64587900	0.29997100	2.89513600

C	-0.46743700	-2.01682500	2.83432200	C	1.26333100	-5.60507600	-0.56991000
O	-0.50532400	-3.00054700	3.46018000	C	3.74667200	-5.62560500	-0.52682000
O	-2.45918400	0.81544000	3.55331300	C	6.17475700	-2.79958000	-0.41990400
O	1.82395300	0.54632700	3.55695200	C	7.43947300	-0.65448100	-0.37187200
C	3.74692800	-1.37008300	-0.39575200	C	7.44984900	0.71201000	-0.35033300
C	4.98253100	-0.66556500	-0.38274200	C	6.21836900	2.87691800	-0.32809200
C	3.76882700	1.48320200	-0.35939100	C	3.82833000	5.73763600	-0.30426000
C	4.99345500	0.76073300	-0.36144800	C	1.34361400	5.75058100	-0.31922800
C	-1.18749100	-1.33943500	-0.42889200	C	-1.14017700	5.76876200	-0.34065600
C	-2.40928900	-0.61286500	-0.43474500	C	-4.80549600	5.11821300	-0.39762600
C	-1.16547500	1.51948100	-0.38483600	C	-6.05330000	2.96666900	-0.44964700
C	-2.39778800	0.81681200	-0.42221800	C	-6.09448700	-2.71039800	-0.57217500
C	3.73335600	-2.79163600	-0.43254900	C	-4.87680100	-4.87978800	-0.62794600
C	2.49706400	-3.49702900	-0.46575200	C	4.99991600	5.04592200	-0.30643800
C	1.27264600	-2.78454000	-0.45497700	C	4.92664100	-4.95031100	-0.48804900
C	-1.19335600	-2.77152000	-0.49645600	C	-3.70609100	-5.57233000	-0.63921000
C	0.03581000	-3.48549900	-0.50772800	C	-7.32764500	-0.54607100	-0.53719100
C	-1.15189800	2.94843100	-0.36832900	C	-7.31684300	0.82037900	-0.50748800
C	0.08706100	3.64561800	-0.35049900	C	-3.62464800	5.79285600	-0.37172000
C	1.31615200	2.92848100	-0.34762500	H	-5.74672800	5.66222000	-0.40198300
C	3.77688200	2.90438000	-0.33962500	H	-3.61431300	6.87977400	-0.35574400
C	2.55089200	3.62605900	-0.33636300	H	-1.13143500	6.85643500	-0.32746300
C	-3.64891500	-1.31921900	-0.47999100	H	1.35093200	6.83824900	-0.30647900
C	-4.87212200	-0.59480000	-0.49039900	H	3.83342500	6.82462900	-0.28974500
C	-3.65388700	-2.73929000	-0.53068100	H	5.94864200	5.57669700	-0.29295100
C	-4.86094700	0.83177500	-0.46396800	H	7.16552700	3.41199300	-0.31473900
C	-2.42724800	-3.46368600	-0.54011200	H	8.39394000	1.25085300	-0.33543100
C	-3.62526200	1.53708400	-0.43359400	H	8.37513800	-1.20801700	-0.37507000
C	-3.61238900	2.95900100	-0.41064600	H	7.11377100	-3.34899700	-0.42743000
C	-2.37720900	3.66247300	-0.38052700	H	5.86838700	-5.49348600	-0.49256300
C	-4.85305100	3.67740500	-0.41934900	H	3.73732600	-6.71206600	-0.56136200
C	-2.35961000	5.10037300	-0.36338000	H	1.25687300	-6.69205300	-0.60800400
C	0.09746100	5.07967800	-0.33572900	H	-1.22818700	-6.67449300	-0.64931900
C	2.55388800	5.06346900	-0.31968300	H	-3.71232700	-6.65865200	-0.67807600
C	5.02733900	3.60498100	-0.32459700	H	-5.82583900	-5.40915400	-0.65911100
C	6.23311100	1.46943700	-0.34596000	H	-7.04129400	-3.24532200	-0.60442800
C	6.21118700	-1.39279700	-0.39091200	H	-8.27158500	-1.08455900	-0.56522600
C	4.97335700	-3.50995900	-0.44467600	H	-8.25238800	1.37405600	-0.51092600
C	2.48097200	-4.93451700	-0.52180600	H	-6.99277500	3.51520600	-0.45518900
C	0.02570000	-4.91721900	-0.56534300				
C	-2.43061700	-4.90076600	-0.59742400	<b>25</b>			
C	-4.90403300	-3.43919100	-0.57606100	C	-2.28221700	0.71723900	-0.40542900
C	-6.11101600	-1.30316100	-0.53277100	C	-1.05240300	1.42881600	-0.34854500
C	-6.08885600	1.55857700	-0.47258200	C	-2.28171000	-0.71914200	-0.39484100
C	-1.22105300	-5.58758400	-0.60994400	C	0.19099400	0.71250300	-0.32290200

C	-1.05146700	-1.43116000	-0.35651700	C	3.88259000	-1.42808900	-0.26610100
C	0.19041100	-0.71333700	-0.31110000	C	3.88005600	-2.84842300	-0.27317500
Cr	-1.12512300	0.00227600	1.52314000	C	5.11223000	-0.71350300	-0.24346400
C	-0.48537900	1.33184600	2.61399600	C	3.87892100	2.84897100	-0.27401000
C	-2.66000800	-0.06165900	2.52251500	C	3.88199900	1.42860800	-0.26498100
C	-0.37027800	-1.25958000	2.62167400	C	5.11199800	0.71460700	-0.24361000
O	0.11432200	-2.06908400	3.30239400	C	-5.94995900	-2.84253600	-0.60987500
O	-3.64612800	-0.10247600	3.13910400	C	-5.97563600	-1.43493000	-0.60366400
O	-0.07566800	2.18539400	3.29020300	C	-7.19750500	-0.68489400	-0.66639100
C	1.42868900	1.42776200	-0.29818500	C	-5.95149500	2.83899300	-0.60876400
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C	-1.05060800	2.86669700	-0.38255400	C	-7.19795000	0.68061300	-0.66574400
C	0.18305100	3.56690400	-0.35922600	C	5.12467900	3.55953000	-0.25485400
C	-1.04950500	-2.86852400	-0.37705600	C	6.31958800	2.84132300	-0.22860000
C	-2.27576800	-3.56720600	-0.44202500	C	5.08622600	5.00144300	-0.26578000
C	-3.52288900	-1.43664600	-0.47060300	C	5.12622200	-3.55845200	-0.25530100
C	-3.51290900	-2.85208600	-0.48640400	C	6.32075200	-2.83965200	-0.22988200
C	2.64589000	0.71564200	-0.28337800	C	5.08844600	-5.00033600	-0.26655800
C	2.64591200	-0.71571300	-0.27958900	C	3.91074900	5.68429600	-0.29791000
C	1.42931300	-1.42834400	-0.30153700	C	6.34502500	1.43213800	-0.22353700
C	0.18472100	-3.56827000	-0.35820700	H	6.03104700	5.53911300	-0.24850700
C	1.42084600	-2.85572200	-0.31747800	H	7.26288600	3.38322000	-0.21309300
C	-4.74393000	-0.71833800	-0.53471500	C	6.34559400	-1.43048000	-0.22404200
C	-4.74441600	0.71520400	-0.53600700	C	3.91323300	-5.68369900	-0.29746500
C	-3.52370800	1.43406400	-0.46846400	H	7.26430100	-3.38112700	-0.21447600
C	-2.27721000	3.56479100	-0.44280800	H	6.03351800	-5.53758000	-0.24978200
C	-3.51424100	2.84958100	-0.48863700	C	7.56756300	-0.68246800	-0.20106200
C	2.64835600	-3.56178300	-0.30308900	C	7.56730500	0.68460500	-0.20058900
C	2.64202500	-5.00139700	-0.31932600	H	8.50757600	-1.22841400	-0.18351500
C	1.43053500	-5.68072400	-0.35772700	H	8.50710600	1.23090700	-0.18297700
C	-2.26887400	-5.00400400	-0.46518800	H	3.91116700	-6.77077900	-0.30591000
C	-3.53867000	-5.68656900	-0.52689200	H	1.43124200	-6.76837000	-0.37166200
C	-1.05370300	-5.68187400	-0.43104000	H	-1.05215900	-6.76949900	-0.44665700
C	-4.75502300	-3.56268500	-0.55585900	H	-3.53549000	-6.77358900	-0.53969700
C	-4.71459500	-5.00440700	-0.57008100	H	-5.65783900	-5.54288600	-0.61732200
C	0.18640000	-5.00108900	-0.38133400	H	-6.89197100	-3.38440000	-0.66005900
C	2.64679500	3.56176300	-0.30379700	H	-8.13610900	-1.23123600	-0.71461100
C	2.63987100	5.00140300	-0.32060300	H	-8.13685600	1.22642100	-0.71403600
C	-4.75669500	3.55957600	-0.55589900	H	-6.89373400	3.38044700	-0.65881900
C	-4.71676500	5.00134500	-0.56990300	H	-5.66018100	5.53955200	-0.61672600
C	0.18429000	4.99975600	-0.38405700	H	-3.53811900	6.77086400	-0.54075800
C	1.42805900	5.68002700	-0.36047900	H	-1.05496900	6.76755100	-0.44927300
C	-1.05604600	5.67990600	-0.43415700	H	1.42814100	6.76768300	-0.37386500
C	-2.27095900	5.00168000	-0.46727100	H	3.90819600	6.77137700	-0.30606600
C	-3.54098200	5.68383900	-0.52834000				



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