

Mechanism and origins of gold-catalyzed domino cyclization to spiroindolines: the role of periplanar cooperation and hydrogen bonding interactions

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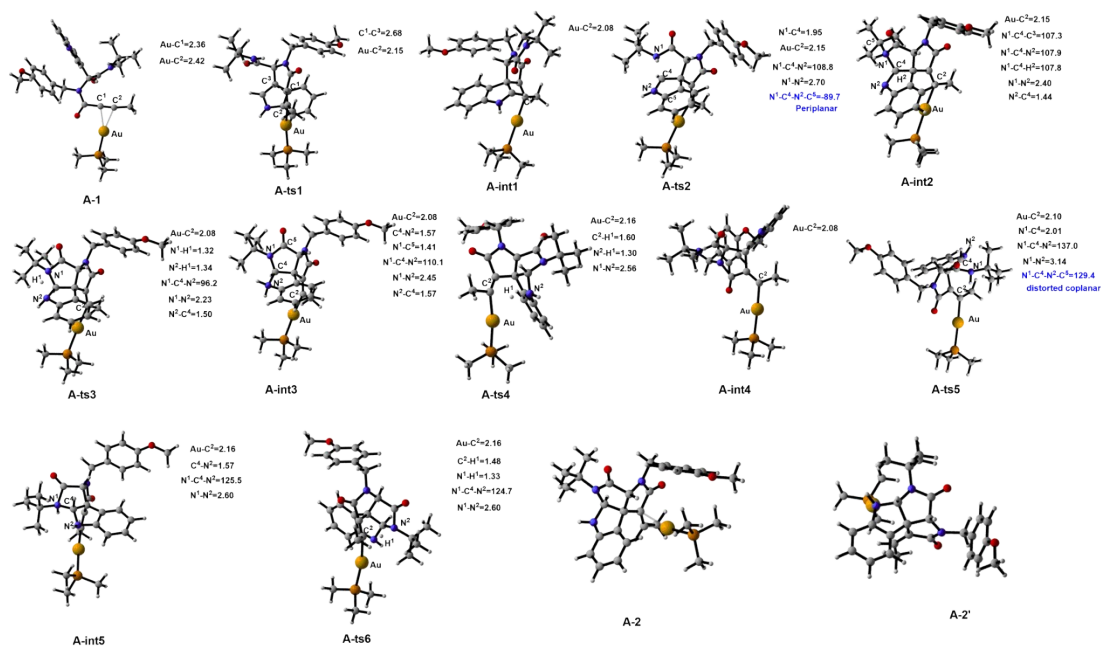


Fig. S1 optimized intermediates and transition structures in Fig. 1a. The selected bond distances are in Å.

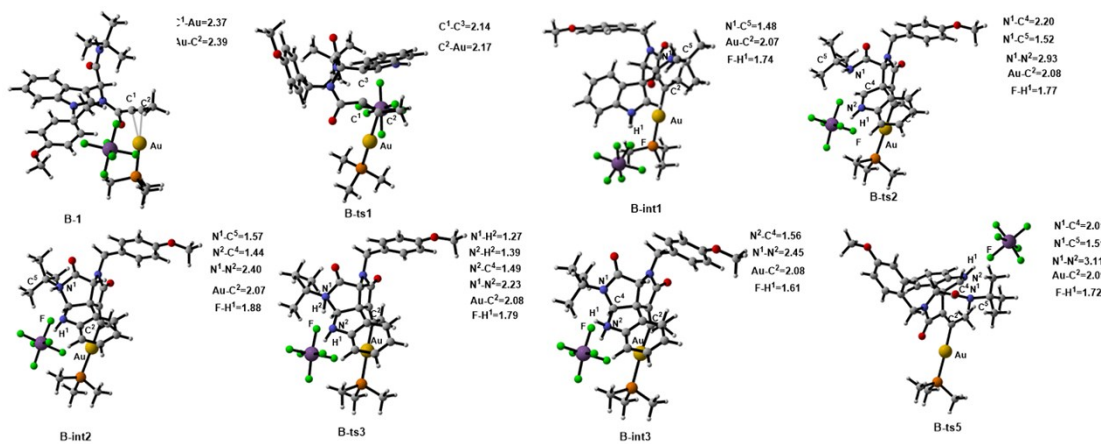


Fig. S2 optimized intermediates and transition structures in Fig. 1b. The selected bond distances are in Å.

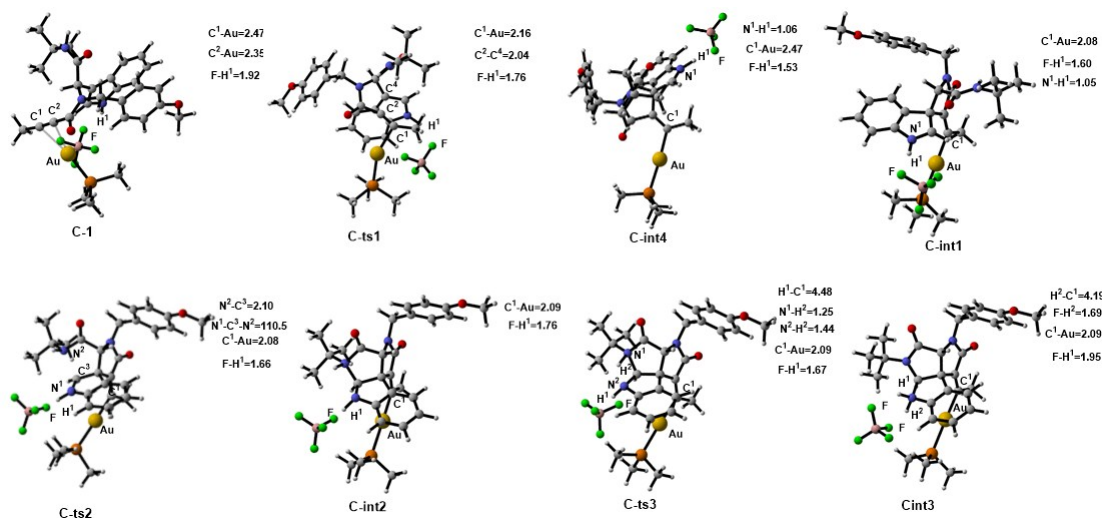


Fig. S3 optimized intermediates and transition structures in Fig. 1b. The selected bond distances are in Å.

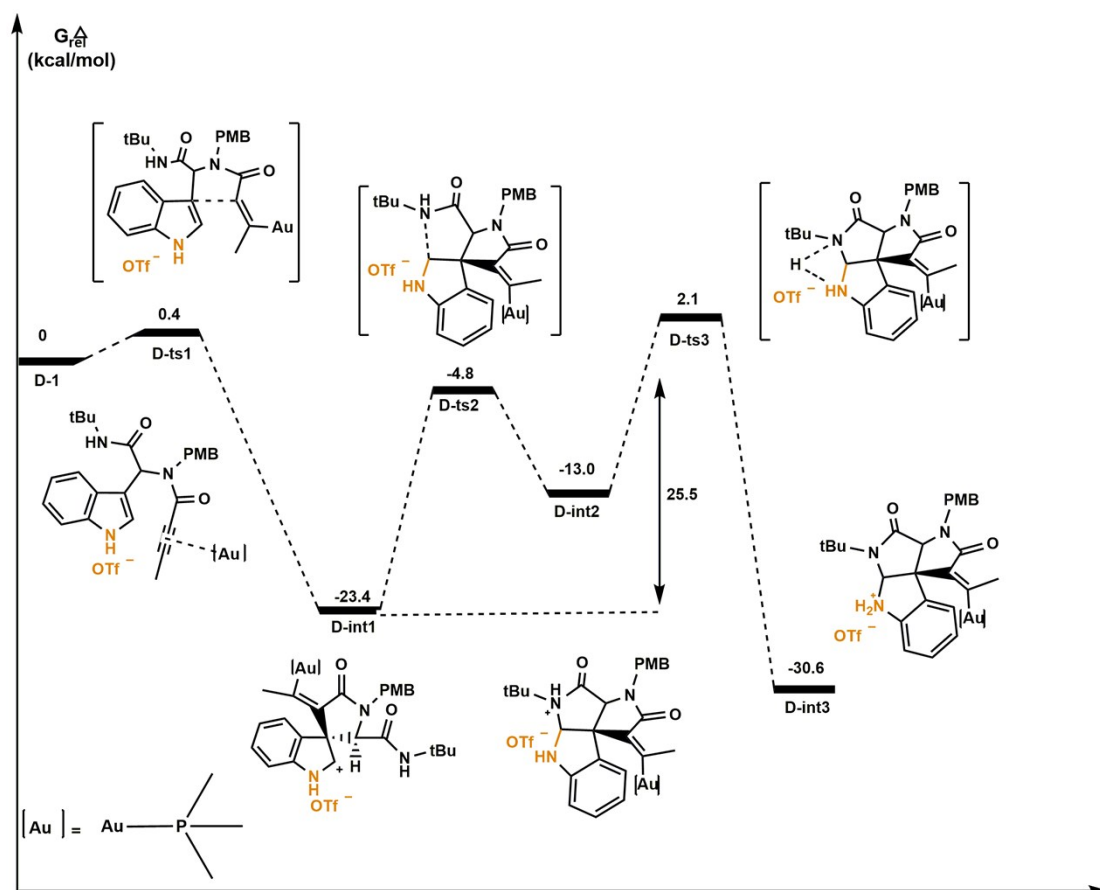


Fig. S4. Energy profiles for catalyzed by $[\text{Au}(\text{PMe}_3)\text{OTf}]$.

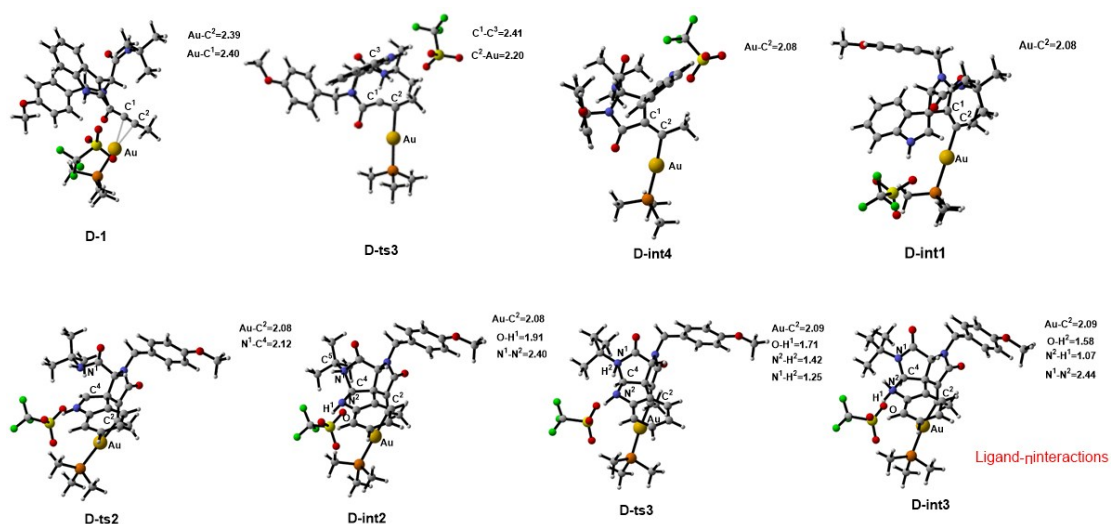


Fig. S5 optimized intermediates and transition structures in Fig. S4. The selected bond distances are in Å.

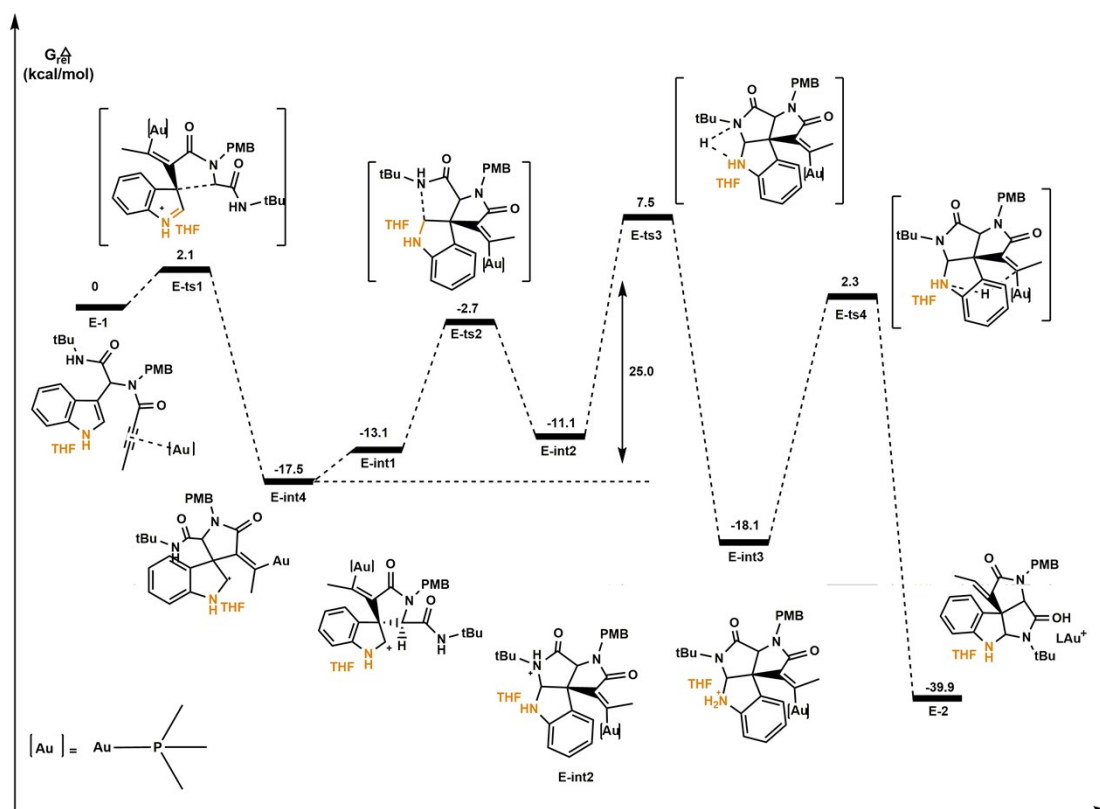


Fig. S6. DFT-computed free energy profiles for [Au(P(CH₃)₃)⁺]-catalyzed preferred pathway in THF solvent. Energy values are in kcal/mol.

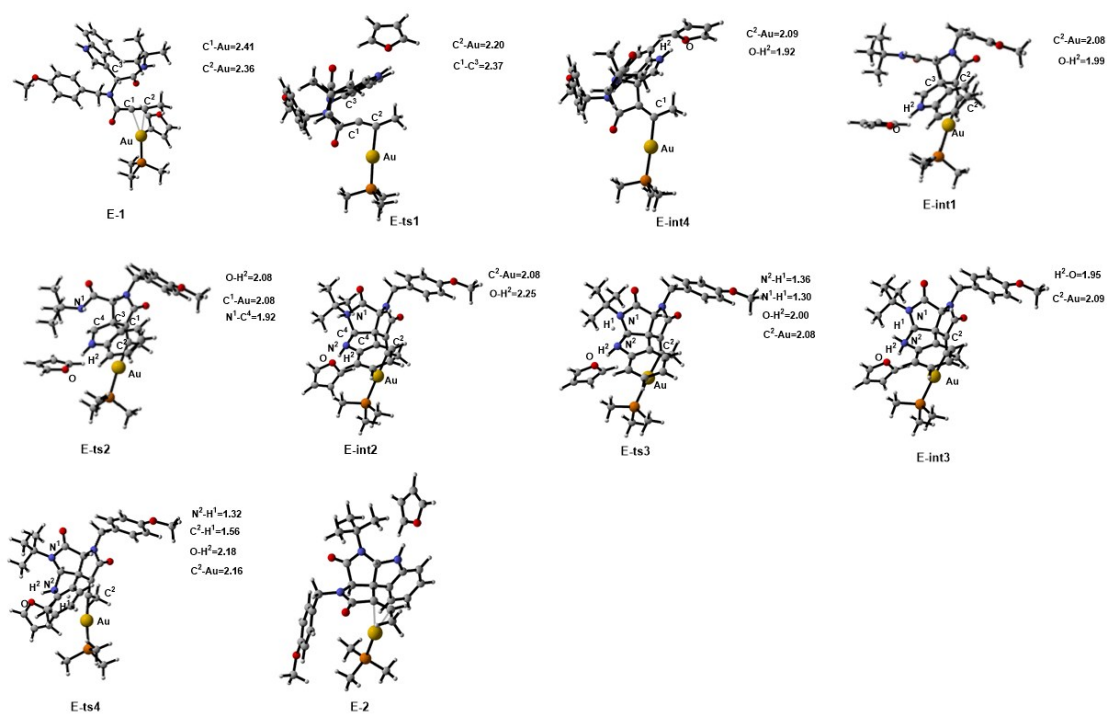


Fig. S7 optimized intermediates and transition structures in Fig. S6. The selected bond distances are in Å.

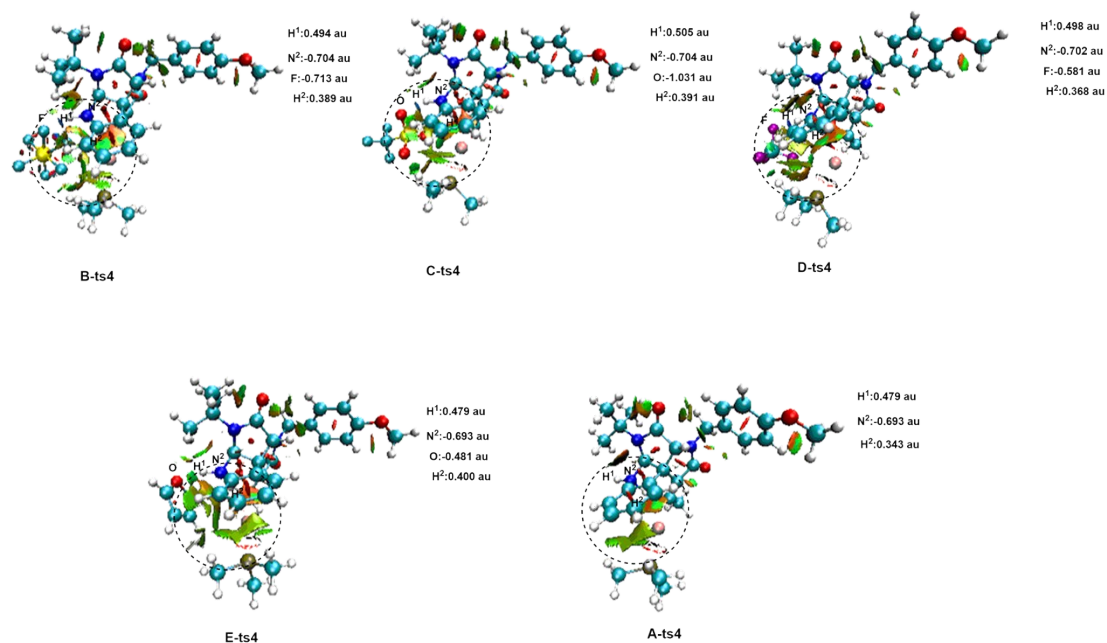


Figure S4. Noncovalent interaction (NCI) plot for the rate-determining transition states. The green, blue and red regions respectively represent attractive, strongly and repulsive interactions

Table S1. Thermodynamic properties (relative free energies and activation free energies in gas phase and in solution) of the structures in Figure 1

System	$\Delta E_{\text{gas}}^{\text{rel}}$	$\Delta G_{\text{gas}}^{\text{rel}}$	$\Delta E_{\text{gas}}^{\ddagger}$	$\Delta G_{\text{gas}}^{\ddagger}$	$\Delta E_{\text{sol}}^{\text{rel}}$	$\Delta G_{\text{sol}}^{\text{rel}}$	$\Delta E_{\text{sol}}^{\ddagger}$	$\Delta G_{\text{sol}}^{\ddagger}$
A-1	0	0			0	0		
A-ts1	9.6	11.1	9.6	11.1	16.0	10.2	16.0	10.2
A-int1	-19.4	-16.9			-13.1	-15.6		
A-ts2	-1.4	-0.1	18.0	16.7	0.2	-3.2	13.3	12.4
A-int2	-10.0	-7.7			-8.5	-7.9		
A-ts3	8.1	11.5	18.1	19.2	13.7	10.5	22.2	18.4
A-int3	-14.4	-12.1			-19.3	-18.3		
A-ts4	1.7	5.0	16.1	17.1	6.8	3.8	26.1	22.1
A-2	-44.0	-39.5			-40.3	40.5		
A-int4	-21.0	-19.8			-13.2	-17.1		
A-ts5	29.8	31.7	50.8	51.6	37.9	33.1	51.1	50.2
A-int5	13.4	15.8			16.2	14.9		
A-ts6	23.7	28.0	10.2	12.2	29.4	25.3	13.2	10.4
A-2'	-19.1	-15.6			-20.1	-21.3		

Table S2. Thermodynamic properties (relative free energies and activation free energies in gas phase and in solution) of the structures in Figure 3

System	$\Delta E_{\text{gas}}^{\text{rel}}$	$\Delta G_{\text{gas}}^{\text{rel}}$	$\Delta E_{\text{gas}}^{\ddagger}$	$\Delta G_{\text{gas}}^{\ddagger}$	$\Delta E_{\text{sol}}^{\text{rel}}$	$\Delta G_{\text{sol}}^{\text{rel}}$	$\Delta E_{\text{sol}}^{\ddagger}$	$\Delta G_{\text{sol}}^{\ddagger}$
B-1	0	0			0	0		
B-ts1	0.3	1.1	0.3	1.1	5.0	1.6	5.0	1.6
B-int1	-15.2	-16.5			-13.1	-17.1		
B-ts2	0.8	0.1	16.0	16.5	6.0	-1.0	19.1	16.1
B-int2	-9.3	-8.6			-8.7	-10.8		
B-ts3	5.0	4.5	14.3	13.1	12.4	3.9	21.1	14.7

B-int3	-22.2	-21.9			-24.0	-25.4		
B-int4	-4.1	-7.4			-8.0	-12.7		
B-ts5	48.7	46.1	52.8	53.5	43.5	38.7	51.5	51.4

Table S3. Thermodynamic properties (relative free energies and activation free energies in gas phase and in solution) of the structures in Fig.S4

System	$\Delta E^{\text{rel}}_{\text{gas}}$	$\Delta G^{\text{rel}}_{\text{gas}}$	$\Delta E^{\ddagger}_{\text{gas}}$	$\Delta G^{\ddagger}_{\text{gas}}$	$\Delta E^{\text{rel}}_{\text{sol}}$	$\Delta G^{\text{rel}}_{\text{sol}}$	$\Delta E^{\ddagger}_{\text{sol}}$	$\Delta G^{\ddagger}_{\text{sol}}$
D-1	0	0			0	0		
D-ts1	9.4	5.8	9.4	5.8	8.4	0.4	8.4	0.4
D-int4	-12.6	-14.7			-14.2	-18.3		
D-int1	-21.8	-24.6			-18.4	-23.4		
D-ts2	-5.0	-5.9	16.7	18.7	0	-4.8	18.4	18.6
D-int2	-13.4	-13.6			-12.8	-13.0		
D-ts3	0.2	0.3	13.6	13.9	7.0	2.1	19.7	15.1
D-int3	-29.9	-30.3			-30.5	-30.6		

Table S4. Thermodynamic properties (relative free energies and activation free energies in gas phase and in solution) of the structures in Fig.1c

System	$\Delta E^{\text{rel}}_{\text{gas}}$	$\Delta G^{\text{rel}}_{\text{gas}}$	$\Delta E^{\ddagger}_{\text{gas}}$	$\Delta G^{\ddagger}_{\text{gas}}$	$\Delta E^{\text{rel}}_{\text{sol}}$	$\Delta G^{\text{rel}}_{\text{sol}}$	$\Delta E^{\ddagger}_{\text{sol}}$	$\Delta G^{\ddagger}_{\text{sol}}$
C-1	0	0			0	0		
C-ts1	8.5	9.4	8.5	9.4	15.0	9.6	15.0	9.6
C-int4	-5.6	-8.6			-12.4	-15.6		
C-int1	-21.5	-21.0			-20.0	-20.9		
C-ts2	-2.8	-2.0	18.7	19.0	1.2	-1.2	21.2	19.7
C-int2	-10.8	-8.3			-11.7	-8.8		
C-ts3	2.1	3.7	12.9	12.0	9.0	5.0	20.8	13.8
C-int3	-31.4	-29.1			-29.1	-27.0		

Table S5. Thermodynamic properties (relative free energies and activation free energies in gas phase and in solution) of the structures in Figure 7

System	$\Delta E_{\text{gas}}^{\text{rel}}$	$\Delta G_{\text{gas}}^{\text{rel}}$	$\Delta E_{\text{gas}}^{\ddagger}$	$\Delta G_{\text{gas}}^{\ddagger}$	$\Delta E_{\text{sol}}^{\text{rel}}$	$\Delta G_{\text{sol}}^{\text{rel}}$	$\Delta E_{\text{sol}}^{\ddagger}$	$\Delta G_{\text{sol}}^{\ddagger}$
E-1	0	0			0	0		
E-ts1	3.7	2.1	3.7	2.1	10.2	3.5	10.2	3.5
E-int4	-18.9	-17.5			-10.6	-12.9		
E-int1	-10.8	-13.1			-10.4	-17.2		
E-ts2	-1.9	-2.7	8.9	10.3	-1.5	-6.3	8.9	10.8
E-int2	-9.6	-11.1			-8.8	-12.3		
E-ts3	7.7	7.5	17.3	18.6	12.8	6.5	21.6	18.8
E-int3	-16.6	-18.1			-21.5	-24.2		
E-ts4	2.8	2.3	19.4	20.3	6.7	-0.3	28.1	23.8
E-2	-39.9	-39.4			-37.9	-41.3		

Complete list of authors for references with more than 10 authors

[19] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C.

Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian 09, Revision A.01; Gaussian, Inc., Wallingford CT, 2016.

The Cartesian coordinates of the stationary points discussed in the text

A-1

C	4.1044274	-1.3754477	-2.8450986
C	5.3175124	-0.9490437	-2.2756946
C	5.3706524	-0.4661417	-0.9798036
C	4.1728874	-0.4133277	-0.2679476
C	2.9386924	-0.8244227	-0.8222026
C	2.9174584	-1.3232447	-2.1354606
N	3.9262934	0.0321813	1.0140924
C	2.5878864	-0.0599077	1.2735064
C	1.9392534	-0.5862417	0.1851024
O	-0.4101156	-1.8279427	-1.8747086
C	0.0795264	-1.9938037	-0.7661256
C	0.4613284	-0.7697667	0.0868014
N	0.2491004	-3.2503777	-0.2669876
N	-0.2135446	0.4231163	-0.4652466
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C	-2.2636366	-0.5068717	0.3565704
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C	-3.4043556	-2.6330677	1.5194594
O	-2.2181496	1.4907093	-0.8175266
C	0.9277594	-3.8740387	0.8976024

C	0.3283654	-5.2763177	0.9909874
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C	0.6479564	-3.1382037	2.2027394
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C	2.7348364	2.4312133	-1.2499926
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C	1.0363884	3.0415463	0.3267544
C	0.4895564	1.3023383	-1.4148066
O	4.1491124	4.8884813	0.9852434
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H	6.3067914	-0.1353097	-0.5360516
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H	-3.8802116	-2.3928447	2.4755684
H	-2.5854856	-3.3389507	1.7020244
H	-0.7543116	-5.2359177	1.1643804
H	0.7882064	-5.8307517	1.8156924
H	0.5087214	-5.8463267	0.0705584
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H	-7.9189166	-0.3669197	-1.2770326
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C	-1.5620928	-1.1160949	-1.6490624
C	-0.3474988	-1.0411719	-0.9341724
C	0.1854832	-2.2034299	-0.3631304
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O	1.6026352	2.5304661	-2.2315334
N	1.7463122	3.2438181	-0.0660414
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C	-2.4541928	1.1785711	3.3184226
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C	1.9994882	5.3560271	1.0510116
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C	0.6712622	5.2182681	-1.0579424
C	3.3266832	-3.3173559	1.7341356

C	4.0148062	-3.7136829	0.5777736
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O	4.2167612	-5.0393729	0.4456796
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H	1.7820102	2.9392621	0.8972446
H	-1.6513238	1.4475921	4.0109376
H	-3.1580518	2.0105911	3.2191636
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H	1.0958432	5.1754711	1.6476916
H	2.1142912	6.4389301	0.9370066
H	2.8699872	4.9858791	1.6079056
H	3.1267112	4.4653561	-2.0939384
H	3.2933022	6.0352961	-1.2775734
H	4.0503202	4.5919011	-0.5758954
H	0.5844772	4.7553211	-2.0450304
H	0.7509442	6.3034271	-1.1912954

H	-0.2404588	5.0117061	-0.4827004
H	3.0237942	-4.0870219	2.4393186
H	4.9898782	-3.0308619	-1.2315284
H	4.5182382	-0.6583219	-0.8056574
H	2.5344172	-1.6762899	2.8643206
H	3.1776752	0.7217621	2.3138206
H	3.7177602	1.1108881	0.6680506
H	5.0089152	-6.5788619	-0.5809584
H	5.9585202	-5.0735059	-0.6931794
H	4.4333512	-5.2443079	-1.6153764
P	-5.3627868	-1.0033469	-0.1188754
C	-5.7600788	-0.6674859	-1.8679444
H	-4.9871308	-1.0850149	-2.5202154
H	-6.7228118	-1.1233549	-2.1274504
H	-5.8204598	0.4128951	-2.0323644
C	-6.8374008	-0.4270689	0.7848446
H	-7.7363868	-0.9222919	0.3996706
H	-6.7293978	-0.6548709	1.8495976
H	-6.9443558	0.6558981	0.6707366
C	-5.3968508	-2.8167329	0.0459736
H	-6.3298158	-3.2212659	-0.3634394
H	-4.5385998	-3.2477429	-0.4788564
H	-5.3199098	-3.0835399	1.1045616
A- intl			
C	2.3923592	-2.8092234	2.3261747
C	2.9484192	-2.4139454	3.5431917
C	2.7299112	-1.1348294	4.0521647

C	1.9402532	-0.2989654	3.2845477
C	1.3722572	-0.6695894	2.0684697
C	1.5986972	-1.9425594	1.5731657
N	1.5270792	1.0334586	3.5543417
C	0.8009672	1.5220816	2.5811007
C	0.6333692	0.5154686	1.4846827
N	1.3422822	3.1757166	-0.9229153
C	1.5660282	2.5063346	0.2071867
C	1.3408862	0.9924826	0.1637807
O	1.9834702	2.9917136	1.2654807
N	0.5104252	0.5297026	-0.9093173
C	-0.7508568	0.1314186	-0.4794613
C	-0.8048018	0.2680816	0.9984067
O	-1.6059558	-0.2905464	-1.2386323
C	-1.9225468	0.0664586	1.7255997
C	-1.9256378	0.1012446	3.2159827
Au	-3.7287938	-0.3305904	0.7592857
C	3.6511572	-2.7051464	-1.4229673
C	2.8504972	-3.8520714	-1.3895373
C	1.4813082	-3.7493854	-1.6555643
C	0.9275512	-2.5028494	-1.9349943
C	1.7133592	-1.3506104	-1.9548333
C	3.0847632	-1.4739674	-1.7059743
C	1.0768642	-0.0060994	-2.1555513
O	3.4872302	-5.0031234	-1.0877943
C	2.7370392	-6.1974094	-1.0823503
C	1.5584492	4.6322466	-1.1315913

C	1.1843332	4.9092436	-2.5805143
C	3.0265542	4.9642206	-0.8932403
C	0.6562302	5.4249056	-0.1922643
H	2.5830692	-3.8126144	1.9526247
H	3.5619352	-3.1118894	4.1058567
H	3.1592132	-0.8180384	4.9989347
H	1.1750332	-2.2615804	0.6214607
H	1.7434562	1.5383516	4.4061857
H	0.2672512	2.4579656	2.6853657
H	0.8763792	2.6547246	-1.6580183
H	2.3449642	0.5404666	0.1064277
H	-2.6081948	0.8811236	3.5775697
H	-0.9429528	0.2574216	3.6856197
H	-2.3297188	-0.8405304	3.6079167
H	4.7151312	-2.8146374	-1.2306283
H	0.8449142	-4.6293224	-1.6563273
H	-0.1407718	-2.4195134	-2.1315903
H	3.7220752	-0.5897394	-1.7470933
H	1.8067142	0.7163996	-2.5460793
H	0.2405582	-0.0607454	-2.8608883
H	3.4346562	-6.9994214	-0.8362573
H	2.2912542	-6.3990684	-2.0657473
H	1.9396092	-6.1701774	-0.3256283
H	0.1310152	4.6685706	-2.7742703
H	1.8126152	4.3324806	-3.2706743
H	1.3289832	5.9709706	-2.8046573
H	3.3213082	4.7420836	0.1366477

H	3.6688532	4.3956496	-1.5757773
H	3.1948742	6.0312556	-1.0777633
H	0.9084122	5.2282406	0.8538997
H	-0.3976338	5.1722366	-0.3595703
H	0.7823232	6.4974586	-0.3792153
P	-5.7280518	-0.7831464	-0.4336283
C	-5.3794548	-0.9203084	-2.2210063
H	-6.2905328	-1.1429414	-2.7886573
H	-4.9447128	0.0196146	-2.5754243
H	-4.6400928	-1.7110054	-2.3827733
C	-6.5843628	-2.3444834	-0.0268163
H	-6.9128578	-2.3242804	1.0166237
H	-7.4545638	-2.4883974	-0.6780153
H	-5.8943438	-3.1840714	-0.1540033
C	-7.0481768	0.4753726	-0.3338373
H	-6.6544328	1.4450796	-0.6530053
H	-7.8939898	0.1989586	-0.9742943
H	-7.3929048	0.5676176	0.7004547

A- ts2

C	-0.5215771	-2.0620617	2.2140680
C	-1.4861011	-1.3260667	2.9014190
C	-1.9132711	-0.0790817	2.4381500
C	-1.3376161	0.3795793	1.2663130
C	-0.3624151	-0.3342337	0.5752700
C	0.0543099	-1.5685107	1.0415640
N	-1.5856771	1.5829653	0.5590560
C	-0.6956541	1.7470123	-0.4334090

C	0.0324449	0.4234313	-0.6671520
N	0.8421779	2.7208713	0.2564720
C	1.8522119	2.1341373	-0.6029290
C	1.5558439	0.6611523	-0.8045260
O	2.7330359	2.7566403	-1.1239410
N	1.9199139	0.2195603	-2.1128590
C	0.8694179	-0.3540077	-2.8173420
C	-0.3686681	-0.2261247	-1.9979720
O	1.0201639	-0.8994857	-3.8931110
C	-1.5980951	-0.6851687	-2.3220080
C	-1.8840181	-1.2731407	-3.6728280
Au	-3.2514791	-0.8324357	-1.0603790
C	5.3211509	-1.4499257	0.4828770
C	4.9066199	-2.7853197	0.5094680
C	3.9820759	-3.2426807	-0.4350940
C	3.4917519	-2.3631647	-1.3959060
C	3.9065459	-1.0322767	-1.4393500
C	4.8222809	-0.5885177	-0.4806770
C	3.3118479	-0.0869377	-2.4438490
O	5.4497239	-3.5499217	1.4807880
C	5.1278959	-4.9215207	1.5055020
C	0.8159629	4.2152383	0.4885700
C	-0.4126001	4.5089343	1.3413080
C	0.7086539	4.9441303	-0.8431540
C	2.0766589	4.6151213	1.2476600
H	-0.2075291	-3.0266787	2.6027490
H	-1.9048181	-1.7211597	3.8238680

H	-2.6506351	0.5050103	2.9851860
H	0.8138109	-2.1344907	0.5010210
H	-2.3548161	2.2096233	0.7484150
H	-0.9313041	2.4177473	-1.2577480
H	2.1162199	0.1029653	-0.0267590
H	-2.1085821	-2.3430337	-3.5594000
H	-1.0662551	-1.1691597	-4.3883850
H	-2.7977851	-0.8263457	-4.0845400
H	6.0438179	-1.1214737	1.2253210
H	3.6575489	-4.2791757	-0.4418430
H	2.7825619	-2.7237927	-2.1420060
H	5.1549399	0.4500993	-0.5018360
H	3.8863819	0.8444293	-2.5005660
H	3.2713169	-0.5255417	-3.4474640
H	5.6927289	-5.3570997	2.3313400
H	5.4165009	-5.4209517	0.5704640
H	4.0547919	-5.0838617	1.6814560
H	-0.4357581	3.9007413	2.2557080
H	-1.3450781	4.3569413	0.7845070
H	-0.3904571	5.5598943	1.6478810
H	1.5997879	4.8130943	-1.4602720
H	-0.1708151	4.6211603	-1.4143750
H	0.5868469	6.0143973	-0.6440390
H	2.9799379	4.4027763	0.6707980
H	2.1377879	4.0985423	2.2144420
H	2.0475409	5.6912433	1.4520310
P	-5.2030441	-1.2175227	0.2711530

C	-5.7686271	0.1935253	1.2901490
H	-6.6492681	-0.0809377	1.8826900
H	-4.9651891	0.4996763	1.9688330
H	-6.0228261	1.0382823	0.6422780
C	-6.6965011	-1.6927467	-0.6660300
H	-6.4913081	-2.5977887	-1.2459320
H	-7.5370571	-1.8810157	0.0121240
H	-6.9657721	-0.8936217	-1.3633710
C	-4.9954721	-2.5684647	1.4830600
H	-4.1491911	-2.3391637	2.1392420
H	-5.9032771	-2.7013627	2.0831660
H	-4.7724631	-3.4997087	0.9531800
H	0.8577939	2.2367603	1.1615070

A- int2

C	1.2458851	-2.3010150	-2.4365196
C	2.1584241	-1.5205840	-3.1477076
C	2.3687401	-0.1799920	-2.8241226
C	1.6417771	0.3482640	-1.7663216
C	0.7239081	-0.4178390	-1.0547936
C	0.5165541	-1.7490760	-1.3846536
N	1.6885631	1.6821430	-1.2827136
C	0.7347051	1.8072340	-0.2175216
C	0.0737811	0.4069160	0.0219864
N	-0.3715939	2.7611640	-0.6843816
C	-1.6330989	1.9009930	-0.8985256
C	-1.4357259	0.5926170	-0.1916486
O	-2.5404839	2.3189980	-1.5399016

N	-1.9842699	0.7286970	1.1328514
C	-1.1240989	0.2032890	2.1127564
C	0.1868131	-0.0508800	1.4684414
O	-1.4890059	0.0324680	3.2588674
C	1.3030901	-0.5440150	2.0518754
C	1.3423971	-0.9139980	3.5025044
Au	3.0783951	-0.9147080	1.0255014
C	-5.2933249	-1.6180770	-1.0002736
C	-5.2590299	-2.8133490	-0.2734486
C	-4.6378559	-2.8460290	0.9784174
C	-4.0638629	-1.6870750	1.4898944
C	-4.0998709	-0.4886600	0.7781444
C	-4.7196069	-0.4724210	-0.4762646
C	-3.4367079	0.7384820	1.3330114
O	-5.8491159	-3.8739120	-0.8627016
C	-5.8850259	-5.0934330	-0.1564356
C	-0.5407599	4.0996750	0.1105754
C	0.8117931	4.7965800	0.0520424
C	-0.9667529	3.7922420	1.5319474
C	-1.5836919	4.9416340	-0.6079236
H	1.0949931	-3.3410490	-2.7124166
H	2.7036531	-1.9577640	-3.9814206
H	3.0563031	0.4380500	-3.3982116
H	-0.1905949	-2.3511990	-0.8156336
H	2.6159681	2.0387680	-1.0764176
H	1.1595741	2.2122020	0.7030524
H	-1.9181329	-0.2117000	-0.7718156

H	1.5859471	-1.9807090	3.5980064
H	0.4134211	-0.7130130	4.0409934
H	2.1705191	-0.3863150	3.9936504
H	-5.7867429	-1.6192190	-1.9685896
H	-4.6071279	-3.7606290	1.5629074
H	-3.5857069	-1.7102580	2.4688164
H	-4.7565209	0.4575620	-1.0450816
H	-3.8518159	1.6475010	0.8729564
H	-3.5719299	0.8171430	2.4175504
H	-6.4163439	-5.8031640	-0.7925696
H	-6.4232339	-4.9924980	0.7960034
H	-4.8741439	-5.4767290	0.0415964
H	1.1426951	4.9539870	-0.9825556
H	1.5975221	4.2658900	0.5995404
H	0.7106861	5.7828920	0.5165884
H	-1.9443749	3.2995020	1.5708264
H	-0.2476649	3.1682970	2.0749354
H	-1.0482919	4.7414420	2.0723714
H	-2.5858619	4.5104680	-0.5551716
H	-1.3289849	5.0996340	-1.6629606
H	-1.6138819	5.9236710	-0.1242446
P	5.1329141	-1.4730350	-0.0715106
C	5.7927101	-0.1944060	-1.2011136
H	6.7179401	-0.5362070	-1.6797446
H	5.0460611	0.0201630	-1.9739126
H	5.9972781	0.7235360	-0.6409316
C	6.5374371	-1.8342920	1.0390274

H	6.2746371	-2.6629840	1.7036524
H	7.4297671	-2.1034490	0.4617994
H	6.7562851	-0.9572720	1.6557994
C	5.0125451	-2.9588830	-1.1276596
H	4.2378371	-2.8009870	-1.8865086
H	5.9714241	-3.1688560	-1.6160386
H	4.7225351	-3.8184630	-0.5154456
H	-0.0902419	3.0460410	-1.6330806

A- ts3

C	-1.0987295	-2.2777749	2.4537624
C	-1.9519095	-1.4647139	3.2038854
C	-2.1690365	-0.1352089	2.8469444
C	-1.5106315	0.3313051	1.7201034
C	-0.6562935	-0.4574969	0.9634534
C	-0.4404235	-1.7791809	1.3328784
N	-1.5742535	1.6733031	1.1900674
C	-0.7237315	1.6986941	-0.0490146
C	-0.0538065	0.3083351	-0.1814396
N	0.2744215	2.6777501	0.4611524
C	1.5664975	1.9829991	0.5957254
C	1.4437115	0.5921641	0.0133124
O	2.5429765	2.4958101	1.0572004
N	1.9764005	0.6337821	-1.3277826
C	1.1490085	-0.0251789	-2.2462806
C	-0.1593915	-0.2622869	-1.5835016
O	1.5161245	-0.3083599	-3.3693736
C	-1.2732255	-0.8049359	-2.1220156

C	-1.3158295	-1.2928559	-3.5368146
Au	-3.0434585	-1.0696289	-1.0555986
C	5.4078365	-1.3454519	0.9797424
C	5.4215755	-2.6051169	0.3715544
C	4.7922175	-2.7855389	-0.8633786
C	4.1612445	-1.7073659	-1.4758056
C	4.1482325	-0.4457019	-0.8825906
C	4.7783795	-0.2817019	0.3561244
C	3.4263595	0.6948571	-1.5414546
O	6.0640525	-3.5780509	1.0528174
C	6.1555035	-4.8538399	0.4617104
C	0.2740635	4.1052921	-0.1046646
C	-1.1669285	4.6019071	-0.1372246
C	0.8738275	4.0626251	-1.5006786
C	1.0753375	5.0022671	0.8296564
H	-0.9412965	-3.3099249	2.7549004
H	-2.4421075	-1.8673709	4.0868124
H	-2.8115135	0.5120711	3.4405264
H	0.2195635	-2.4093539	0.7393204
H	-2.5200755	2.0427751	1.0792144
H	-1.2625855	2.0153181	-0.9436056
H	1.9700345	-0.1377129	0.6505984
H	-1.5624835	-2.3630209	-3.5473276
H	-0.3833215	-1.1380419	-4.0849086
H	-2.1392085	-0.8014739	-4.0716906
H	5.9095975	-1.2313739	1.9370954
H	4.7991835	-3.7522849	-1.3580006

H	3.6766505	-1.8450269	-2.4421716
H	4.7765335	0.6992241	0.8323514
H	3.7973685	1.6580461	-1.1669376
H	3.5537795	0.6793421	-2.6291676
H	6.7255245	-5.4754879	1.1542184
H	6.6814065	-4.8158009	-0.5022076
H	5.1637145	-5.3032229	0.3106144
H	-1.6132225	4.6182601	0.8657024
H	-1.8135265	4.0349281	-0.8166766
H	-1.1650475	5.6343901	-0.5011766
H	1.9182205	3.7314921	-1.4797126
H	0.3143815	3.3989851	-2.1722046
H	0.8531265	5.0682531	-1.9347066
H	2.1352365	4.7472971	0.8507974
H	0.6867695	4.9522041	1.8538264
H	0.9744355	6.0361011	0.4816434
P	-5.0844555	-1.4883809	0.1343834
C	-5.6409875	-0.1173169	1.2115044
H	-6.5565135	-0.3879509	1.7504924
H	-4.8513405	0.1064231	1.9383634
H	-5.8327905	0.7750211	0.6070284
C	-6.5489555	-1.8571319	-0.8920016
H	-6.3493515	-2.7365329	-1.5119046
H	-7.4254275	-2.0507829	-0.2626156
H	-6.7585905	-1.0121569	-1.5549316
C	-4.9739825	-2.9067069	1.2809154
H	-4.1700635	-2.7236769	2.0029954

H	-5.9208505	-3.0540799	1.8135634
H	-4.7302405	-3.8136609	0.7190824
A- int3			
C	-0.9398949	-1.9726458	2.7104110
C	-1.8991959	-1.1464588	3.3029700
C	-2.2349209	0.0766192	2.7274380
C	-1.5597279	0.4187262	1.5682110
C	-0.5960779	-0.3670958	0.9681290
C	-0.2805329	-1.5922338	1.5459470
N	-1.8116719	1.6133592	0.7506070
C	-0.6162699	1.6992122	-0.2683680
C	-0.0057189	0.2709962	-0.2515130
N	0.3562381	2.6123222	0.1994110
C	1.6114941	1.9916082	0.3288200
C	1.4927161	0.5449952	-0.1108640
O	2.6398641	2.5427172	0.6370290
N	1.9894471	0.4307782	-1.4629740
C	1.1440391	-0.3043318	-2.2878650
C	-0.1602429	-0.4494878	-1.5773400
O	1.4709841	-0.7103628	-3.3864790
C	-1.2927209	-1.0189398	-2.0371720
C	-1.3697109	-1.6552078	-3.3922350
Au	-3.0758029	-1.1543208	-0.9687450
C	5.5246121	-1.1617548	0.9509310
C	5.5974081	-2.4740868	0.4719070
C	4.9677001	-2.8097058	-0.7294590
C	4.2788991	-1.8303398	-1.4388370

C	4.2086891	-0.5176028	-0.9761690
C	4.8380101	-0.1978138	0.2322120
C	3.4263881	0.5145042	-1.7377420
O	6.2942741	-3.3409918	1.2399140
C	6.4485761	-4.6618698	0.7763070
C	0.2701871	4.0873972	-0.1144510
C	-1.1917369	4.5225592	-0.1787460
C	0.9400061	4.3160032	-1.4654920
C	0.9467951	4.8876742	0.9940330
H	-0.6956929	-2.9230608	3.1771990
H	-2.3822309	-1.4548638	4.2263140
H	-2.9749019	0.7325952	3.1819660
H	0.4678871	-2.2352178	1.0869620
H	-2.6899219	1.4949292	0.2233060
H	-1.0755249	1.9594442	-1.2295910
H	2.0245531	-0.1238858	0.5852900
H	-1.6483879	-2.7127038	-3.2907870
H	-0.4353359	-1.5872458	-3.9550880
H	-2.1776169	-1.1929788	-3.9747590
H	6.0271821	-0.9275578	1.8858570
H	5.0181181	-3.8201728	-1.1241710
H	3.7924091	-2.0884698	-2.3793370
H	4.7823291	0.8243862	0.6073590
H	3.7693181	1.5267642	-1.4909620
H	3.5194761	0.3716792	-2.8195160
H	7.0582231	-5.1812388	1.5177890
H	6.9619411	-4.6925878	-0.1947390

H	5.4812631	-5.1764348	0.6849120
H	-1.6884739	4.4560392	0.8011550
H	-1.7831909	3.9901892	-0.9338280
H	-1.2217989	5.5813462	-0.4554920
H	1.9966601	4.0309902	-1.4310880
H	0.4498381	3.7349762	-2.2580350
H	0.8861481	5.3750382	-1.7413450
H	2.0158921	4.6819292	1.0517930
H	0.4972011	4.6564392	1.9674970
H	0.8020591	5.9562432	0.7981930
P	-5.1753109	-1.4810838	0.1629040
C	-5.8558209	-0.0203358	1.0319220
H	-6.7974189	-0.2689358	1.5353730
H	-5.1357879	0.3254302	1.7823350
H	-6.0395339	0.7869402	0.3155150
C	-6.5486019	-2.0239168	-0.9102310
H	-6.2756459	-2.9593458	-1.4082750
H	-7.4604999	-2.1812708	-0.3225220
H	-6.7391259	-1.2696728	-1.6797490
C	-5.0963049	-2.7560348	1.4683200
H	-4.3403619	-2.4705418	2.2075680
H	-6.0680889	-2.8726758	1.9621190
H	-4.7985099	-3.7121778	1.0269770
H	-1.8585139	2.4828292	1.2910610
A- ts4			
C	-1.7407574	-0.4062973	2.9762040
C	-2.7486254	0.5515827	2.8947550

C	-2.8248854	1.4276157	1.8053530
C	-1.8470814	1.2954657	0.8422200
C	-0.8331884	0.3435807	0.8994190
C	-0.7704634	-0.5241803	1.9749210
N	-1.6960304	1.9887317	-0.4139610
C	-0.2301244	1.9909977	-0.6920610
C	0.0394076	0.5029027	-0.3149020
N	0.7034866	2.7217197	0.1139570
C	1.8513956	1.9309847	0.2716910
C	1.5316306	0.4889607	-0.1388490
O	2.9394436	2.3168317	0.6312320
N	1.9936736	0.1770627	-1.4788010
C	1.0179386	-0.3557563	-2.3055110
C	-0.2975454	-0.2121563	-1.5887140
O	1.2129766	-0.8309633	-3.4064550
C	-1.5649034	-0.2589923	-2.0712010
C	-1.8414584	-0.5730733	-3.5183760
Au	-3.1816224	-0.9925523	-0.8433060
C	5.2494606	-1.7529703	1.0301200
C	5.1740116	-3.0842673	0.6057960
C	4.5342176	-3.3941173	-0.5972020
C	3.9823716	-2.3707803	-1.3618830
C	4.0607506	-1.0413483	-0.9534640
C	4.6991836	-0.7455603	0.2564940
C	3.4229756	0.0431907	-1.7730190
O	5.7451696	-3.9934673	1.4254950
C	5.7417626	-5.3438303	1.0245990

C	0.8171156	4.2187557	0.0772600
C	-0.5698824	4.8166757	-0.1306440
C	1.7354916	4.6366187	-1.0667800
C	1.3478776	4.6987487	1.4244650
H	-1.6971594	-1.0630303	3.8416280
H	-3.4782984	0.6343457	3.6966750
H	-3.6046564	2.1829387	1.7370410
H	0.0178206	-1.2697323	2.0504960
H	-1.9986464	1.0602777	-1.2755370
H	-0.1211044	2.2057767	-1.7661380
H	1.9342136	-0.2140473	0.6064470
H	-2.1134774	-1.6301193	-3.6402990
H	-0.9700594	-0.3952623	-4.1570410
H	-2.6956524	0.0077727	-3.8832350
H	5.7570516	-1.5406693	1.9674850
H	4.4711936	-4.4194403	-0.9492750
H	3.4873426	-2.6102103	-2.3032000
H	4.7573216	0.2911897	0.5897350
H	3.9043906	1.0111077	-1.5855840
H	3.4825046	-0.1711713	-2.8455000
H	6.2637156	-5.8998753	1.8052790
H	6.2693116	-5.4838823	0.0709580
H	4.7192786	-5.7361363	0.9283640
H	-1.2626994	4.5097207	0.6656400
H	-0.9894854	4.5796847	-1.1187280
H	-0.4924064	5.9078337	-0.0850800
H	2.7493756	4.2553127	-0.9174290

H	1.3604276	4.2752697	-2.0335590
H	1.7885886	5.7299377	-1.1202430
H	2.3522806	4.3192307	1.6203430
H	0.6838756	4.3756427	2.2348810
H	1.3830416	5.7941757	1.4263130
P	-4.9219564	-2.0881523	0.3208880
C	-6.1604084	-0.9594543	1.0432820
H	-6.9262924	-1.5268193	1.5849760
H	-5.6641144	-0.2702203	1.7342700
H	-6.6372704	-0.3756743	0.2502040
C	-5.8953194	-3.2563123	-0.6844100
H	-5.2377434	-4.0301883	-1.0917210
H	-6.6738884	-3.7282453	-0.0738430
H	-6.3629424	-2.7260033	-1.5194300
C	-4.3301774	-3.0730983	1.7371200
H	-3.8026244	-2.4157963	2.4365140
H	-5.1712984	-3.5546173	2.2494160
H	-3.6316284	-3.8395323	1.3879850
H	-2.1961964	2.8673567	-0.5345390
A-2			
C	-1.1068597	-3.1564879	2.7324637
C	-2.4041387	-3.6653259	2.6985807
C	-3.3426737	-3.2096039	1.7751767
C	-2.9460757	-2.2308899	0.8709607
C	-1.6415477	-1.7280349	0.8808867
C	-0.7219617	-2.1761589	1.8169297
N	-3.6787357	-1.6366279	-0.1490793

C	-3.0084577	-0.4360619	-0.5934753
C	-1.5108447	-0.7225409	-0.2299973
N	-3.3185327	0.8016901	0.1285427
C	-2.1859167	1.4672191	0.5299577
C	-0.9721447	0.6481651	0.1281727
O	-2.1020187	2.5729811	1.0308647
N	-0.4621307	1.1537251	-1.1425143
C	-0.2229917	0.1802631	-2.0716273
C	-0.7392847	-1.1067619	-1.4687173
O	0.3443093	0.3237051	-3.1400563
C	-0.6808947	-2.3568479	-2.0308053
C	-0.2114797	-2.6953029	-3.4059293
Au	1.3568893	-1.9155729	-0.7699933
C	2.8173803	2.9105441	1.4159797
C	3.9818713	2.5838621	0.7104777
C	3.8981963	2.2296981	-0.6392563
C	2.6515983	2.1908821	-1.2637943
C	1.4880113	2.5219421	-0.5719063
C	1.5880593	2.8848161	0.7773287
C	0.1502243	2.4770331	-1.2568553
O	5.1298503	2.6198081	1.4230237
C	6.3390243	2.3708861	0.7446567
C	-4.5867277	1.5685231	-0.1155213
C	-5.6954267	0.6288811	-0.5781453
C	-4.3104057	2.6046901	-1.2034263
C	-5.0394247	2.2289521	1.1831977
H	-0.4047537	-3.5100889	3.4822477

H	-2.6985927	-4.4249509	3.4184667
H	-4.3568007	-3.6014739	1.7698177
H	0.2800433	-1.7455119	1.8619607
H	-3.1654017	-0.2900299	-1.6740413
H	-0.1940777	0.6596891	0.9085167
H	0.4174193	-3.5923389	-3.4020933
H	0.3133823	-1.8625559	-3.8779253
H	-1.0913867	-2.9419649	-4.0154833
H	2.9123093	3.1994661	2.4596017
H	4.7939243	2.0214561	-1.2190263
H	2.5851673	1.9209541	-2.3176213
H	0.6838073	3.1613831	1.3209767
H	-0.5421527	3.2066831	-0.8214543
H	0.2464013	2.6791541	-2.3283943
H	7.1372003	2.4784271	1.4807667
H	6.5030703	3.0883731	-0.0704283
H	6.3670953	1.3502681	0.3308767
H	-5.9809047	-0.0783429	0.2106587
H	-5.4494647	0.0835841	-1.4979163
H	-6.5835807	1.2304251	-0.7983063
H	-3.5444747	3.3173491	-0.8809303
H	-3.9759217	2.1218511	-2.1318943
H	-5.2224757	3.1686641	-1.4293953
H	-4.3151397	2.9635351	1.5381087
H	-5.1847477	1.4736961	1.9643517
H	-5.9980767	2.7329521	1.0129997
P	3.4577763	-1.8809969	0.2683777

C	3.9822123	-3.4803809	0.9593987
H	4.9395893	-3.3667789	1.4811527
H	3.2265843	-3.8407789	1.6645567
H	4.0928103	-4.2179519	0.1590097
C	4.7999843	-1.3368519	-0.8288073
H	4.5757483	-0.3218299	-1.1745393
H	5.7510093	-1.3378739	-0.2824873
H	4.8761493	-2.0012989	-1.6942653
C	3.4430453	-0.7148319	1.6647857
H	2.8296483	-1.1216329	2.4756107
H	4.4622913	-0.5484149	2.0356377
H	3.0193633	0.2446951	1.3445927
H	-4.6873747	-1.6618689	-0.1308973
H	-1.1574487	-3.1559059	-1.4526693

A- int4

C	2.3923592	-2.8092234	2.3261747
C	2.9484192	-2.4139454	3.5431917
C	2.7299112	-1.1348294	4.0521647
C	1.9402532	-0.2989654	3.2845477
C	1.3722572	-0.6695894	2.0684697
C	1.5986972	-1.9425594	1.5731657
N	1.5270792	1.0334586	3.5543417
C	0.8009672	1.5220816	2.5811007
C	0.6333692	0.5154686	1.4846827
N	1.3422822	3.1757166	-0.9229153
C	1.5660282	2.5063346	0.2071867
C	1.3408862	0.9924826	0.1637807

O	1.9834702	2.9917136	1.2654807
N	0.5104252	0.5297026	-0.9093173
C	-0.7508568	0.1314186	-0.4794613
C	-0.8048018	0.2680816	0.9984067
O	-1.6059558	-0.2905464	-1.2386323
C	-1.9225468	0.0664586	1.7255997
C	-1.9256378	0.1012446	3.2159827
Au	-3.7287938	-0.3305904	0.7592857
C	3.6511572	-2.7051464	-1.4229673
C	2.8504972	-3.8520714	-1.3895373
C	1.4813082	-3.7493854	-1.6555643
C	0.9275512	-2.5028494	-1.9349943
C	1.7133592	-1.3506104	-1.9548333
C	3.0847632	-1.4739674	-1.7059743
C	1.0768642	-0.0060994	-2.1555513
O	3.4872302	-5.0031234	-1.0877943
C	2.7370392	-6.1974094	-1.0823503
C	1.5584492	4.6322466	-1.1315913
C	1.1843332	4.9092436	-2.5805143
C	3.0265542	4.9642206	-0.8932403
C	0.6562302	5.4249056	-0.1922643
H	2.5830692	-3.8126144	1.9526247
H	3.5619352	-3.1118894	4.1058567
H	3.1592132	-0.8180384	4.9989347
H	1.1750332	-2.2615804	0.6214607
H	1.7434562	1.5383516	4.4061857
H	0.2672512	2.4579656	2.6853657

H	0.8763792	2.6547246	-1.6580183
H	2.3449642	0.5404666	0.1064277
H	-2.6081948	0.8811236	3.5775697
H	-0.9429528	0.2574216	3.6856197
H	-2.3297188	-0.8405304	3.6079167
H	4.7151312	-2.8146374	-1.2306283
H	0.8449142	-4.6293224	-1.6563273
H	-0.1407718	-2.4195134	-2.1315903
H	3.7220752	-0.5897394	-1.7470933
H	1.8067142	0.7163996	-2.5460793
H	0.2405582	-0.0607454	-2.8608883
H	3.4346562	-6.9994214	-0.8362573
H	2.2912542	-6.3990684	-2.0657473
H	1.9396092	-6.1701774	-0.3256283
H	0.1310152	4.6685706	-2.7742703
H	1.8126152	4.3324806	-3.2706743
H	1.3289832	5.9709706	-2.8046573
H	3.3213082	4.7420836	0.1366477
H	3.6688532	4.3956496	-1.5757773
H	3.1948742	6.0312556	-1.0777633
H	0.9084122	5.2282406	0.8538997
H	-0.3976338	5.1722366	-0.3595703
H	0.7823232	6.4974586	-0.3792153
P	-5.7280518	-0.7831464	-0.4336283
C	-5.3794548	-0.9203084	-2.2210063
H	-6.2905328	-1.1429414	-2.7886573
H	-4.9447128	0.0196146	-2.5754243

H	-4.6400928	-1.7110054	-2.3827733
C	-6.5843628	-2.3444834	-0.0268163
H	-6.9128578	-2.3242804	1.0166237
H	-7.4545638	-2.4883974	-0.6780153
H	-5.8943438	-3.1840714	-0.1540033
C	-7.0481768	0.4753726	-0.3338373
H	-6.6544328	1.4450796	-0.6530053
H	-7.8939898	0.1989586	-0.9742943
H	-7.3929048	0.5676176	0.7004547

A- ts5

C	-1.2960467	-0.9208338	-4.0326671
C	-0.9788647	0.1434472	-4.8744221
C	-0.6581347	1.4030892	-4.3626381
C	-0.6919037	1.5412022	-2.9894561
C	-0.9985547	0.4815402	-2.1273811
C	-1.2852437	-0.7686088	-2.6448241
N	-0.5042107	2.7439062	-2.2208211
C	-0.7790297	2.4530532	-0.9343571
C	-0.6693627	0.9610832	-0.7379871
N	0.1131593	2.6951012	0.8539459
C	-0.9765707	1.9282002	1.4624919
C	-1.3939297	0.7267902	0.5822929
O	-1.5270647	2.2453242	2.4795399
N	-0.8511527	-0.4850478	1.1263409
C	0.3800063	-0.7877878	0.5991269
C	0.7187853	0.2747872	-0.4063581
O	1.0453643	-1.7511718	0.9404389

C	1.9690583	0.4263292	-0.8944121
C	2.3850373	1.4521322	-1.9018361
Au	3.4622563	-0.9042798	-0.2583481
C	-5.2746077	-1.5964038	1.5536889
C	-5.3138557	-2.6503368	0.6347079
C	-4.1221947	-3.2534258	0.2187309
C	-2.9118097	-2.7986568	0.7307769
C	-2.8620817	-1.7565688	1.6546859
C	-4.0601477	-1.1579388	2.0542859
C	-1.5386137	-1.2560178	2.1536859
O	-6.5420727	-3.0103898	0.2087369
C	-6.6469177	-4.0938718	-0.6865301
C	0.5340743	4.0277612	1.4002679
C	1.6494423	4.5073062	0.4801239
C	1.0655843	3.8549752	2.8201999
C	-0.6382027	4.9971362	1.3586299
H	-1.5498177	-1.8850888	-4.4640831
H	-0.9826467	-0.0043868	-5.9508141
H	-0.4133567	2.2344662	-5.0186541
H	-1.5129487	-1.6026468	-1.9829911
H	-0.7722287	3.6387662	-2.6121281
H	-1.5924627	3.0292832	-0.4906571
H	0.9231593	2.0780102	0.6928639
H	-2.4920297	0.6876142	0.5313749
H	3.4244713	1.7578982	-1.7476511
H	1.7651083	2.3541242	-1.9465711
H	2.3554183	0.9855172	-2.8981641

H	-6.2155307	-1.1477588	1.8608969
H	-4.1314147	-4.0788848	-0.4868421
H	-1.9799427	-3.2723188	0.4161949
H	-4.0345247	-0.3387718	2.7742219
H	-1.6680757	-0.6335638	3.0507849
H	-0.8538267	-2.0737218	2.4065939
H	-7.7113377	-4.2283068	-0.8853631
H	-6.2440507	-5.0183848	-0.2504751
H	-6.1292177	-3.8878858	-1.6340141
H	1.3008733	4.6105652	-0.5555851
H	2.5042223	3.8178182	0.4905569
H	2.0082033	5.4866252	0.8139699
H	0.2808953	3.5352042	3.5097549
H	1.8828433	3.1234462	2.8465249
H	1.4666183	4.8126952	3.1713659
H	-1.4774997	4.6581192	1.9725279
H	-0.9843807	5.1669142	0.3304189
H	-0.3101187	5.9664592	1.7489969
P	5.0708423	-2.4731968	0.4917779
C	4.2723383	-3.6980548	1.5851739
H	4.9952443	-4.4364248	1.9512479
H	3.8123793	-3.1785088	2.4317409
H	3.4738233	-4.2039898	1.0333619
C	5.8841923	-3.4854338	-0.7925181
H	6.4683373	-2.8413318	-1.4565631
H	6.5464533	-4.2295348	-0.3345421
H	5.1239613	-3.9973848	-1.3902011

C	6.4621263	-1.8287058	1.4844959
H	6.0729063	-1.2832158	2.3494819
H	7.1002193	-2.6497888	1.8319109
H	7.0585773	-1.1380608	0.8809209

A- int5

C	0.8711191	-3.3891185	0.8210818
C	-0.2588859	-3.4836515	1.6315148
C	-1.0743989	-2.3764765	1.8729048
C	-0.7203799	-1.1760165	1.2787968
C	0.4154341	-1.0726545	0.4669678
C	1.2120171	-2.1773335	0.2202638
N	-1.4196619	0.0737475	1.3769558
C	-0.4167949	1.0106225	0.9654138
C	0.4136411	0.3075465	-0.1151302
N	-0.6763339	2.3343335	0.3388728
C	0.9077791	2.6390135	0.0212748
C	1.5974181	1.2680525	-0.1840642
O	1.3074761	3.7422355	-0.0646342
N	2.1020361	1.2272225	-1.5131492
C	1.1771451	0.6687105	-2.3901432
C	-0.0475199	0.3424655	-1.5896392
O	1.4074011	0.4894185	-3.5678472
C	-1.2642229	0.0594025	-2.1180712
C	-1.4989909	0.1405635	-3.5988152
Au	-2.9397879	-0.6442365	-1.0903652
C	6.0356031	-0.0003685	0.5454848
C	6.0585031	-1.3317385	0.1182438

C	5.2551281	-1.7285745	-0.9565742
C	4.4445631	-0.7913325	-1.5878032
C	4.4163221	0.5399405	-1.1719082
C	5.2219591	0.9198495	-0.0949902
C	3.4920771	1.5132775	-1.8454252
O	6.8824991	-2.1526515	0.8007318
C	6.9856341	-3.4945625	0.3813088
C	-1.5003379	3.4147015	1.0423838
C	-2.9164009	2.8680595	1.1901848
C	-1.5323559	4.6395975	0.1363308
C	-0.8806329	3.7224745	2.3936708
H	1.4897521	-4.2669765	0.6574538
H	-0.5073439	-4.4355045	2.0942098
H	-1.9430739	-2.4517805	2.5257088
H	2.0932521	-2.0871605	-0.4151302
H	-1.7886899	0.2452855	2.3079028
H	0.2655311	1.2380875	1.8098558
H	-1.1073619	2.1327105	-0.5841882
H	2.3808361	1.1172245	0.5757538
H	-1.5583319	-0.8843225	-3.9923862
H	-0.7166989	0.6574815	-4.1596982
H	-2.4751209	0.5924115	-3.8091992
H	6.6749281	0.2831965	1.3772528
H	5.2695961	-2.7533535	-1.3159892
H	3.8285831	-1.0963295	-2.4352832
H	5.2226071	1.9592055	0.2350558
H	3.7270781	2.5487285	-1.5614622

H	3.5440371	1.4446325	-2.9383512
H	7.7105801	-3.9701935	1.0437198
H	7.3444461	-3.5673305	-0.6544562
H	6.0240991	-4.0203695	0.4665568
H	-2.9756749	2.0105405	1.8666098
H	-3.3356799	2.5657775	0.2216478
H	-3.5515049	3.6607025	1.6003328
H	-0.5572199	5.1184895	0.0367388
H	-1.9063089	4.3835695	-0.8632402
H	-2.2276639	5.3685675	0.5654608
H	0.1479921	4.0874975	2.3058778
H	-0.8994029	2.8567325	3.0672278
H	-1.4670109	4.5135505	2.8727168
P	-4.8773459	-1.6069505	-0.0888112
C	-5.3020399	-0.9430545	1.5627298
H	-6.1767859	-1.4558435	1.9797058
H	-4.4522369	-1.0771935	2.2405858
H	-5.5182669	0.1273015	1.4831218
C	-6.4336589	-1.4456035	-1.0301312
H	-6.3120889	-1.9031175	-2.0167002
H	-7.2593579	-1.9375145	-0.5028232
H	-6.6733089	-0.3873245	-1.1712682
C	-4.7211819	-3.4049935	0.1941658
H	-3.8387879	-3.6039275	0.8112328
H	-5.6145799	-3.8030665	0.6894398
H	-4.5836419	-3.9122985	-0.7657742

A- ts6

C	-1.7661072	-3.2160060	-0.6788311
C	-0.6419242	-3.6426030	-1.3821301
C	0.4178528	-2.7754090	-1.6595951
C	0.3106498	-1.4690200	-1.2135901
C	-0.8153762	-1.0374090	-0.4961491
C	-1.8579482	-1.9022540	-0.2152411
N	1.2626328	-0.4138670	-1.3865311
C	0.4684848	0.7737360	-1.1669831
C	-0.5102302	0.3636610	-0.0730811
N	0.9846088	2.0382110	-0.5922081
C	-0.3117502	2.6880990	-0.1849741
C	-1.4054682	1.5867400	-0.0207281
O	-0.4188032	3.8506830	0.0530099
N	-1.9753402	1.6196070	1.3004209
C	-1.2326122	0.8516770	2.1709229
C	-0.0096772	0.4567320	1.3771879
O	-1.5034522	0.6096180	3.3269079
C	1.2607238	0.7054860	1.7729189
C	1.5782688	1.1745000	3.1688309
Au	2.9345608	-0.3809720	0.9523849
C	-5.6923092	0.1731820	-0.7630301
C	-5.9732072	-0.9728730	-0.0112321
C	-5.4310032	-1.1101750	1.2709579
C	-4.6101132	-0.1081540	1.7802429
C	-4.3220202	1.0375290	1.0385299
C	-4.8801922	1.1641290	-0.2383511
C	-3.3479222	2.0497190	1.5688919

O	-6.7766722	-1.8798030	-0.6033801
C	-7.1322702	-3.0324390	0.1264159
C	2.0067718	2.9103600	-1.3039741
C	3.0773198	2.0066190	-1.9039801
C	2.6348458	3.8113370	-0.2473331
C	1.3448278	3.7159650	-2.4156401
H	-2.5786552	-3.9118950	-0.4895521
H	-0.5901022	-4.6698250	-1.7341511
H	1.2819608	-3.1108830	-2.2313871
H	-2.7314482	-1.5591960	0.3412159
H	1.7408018	-0.4434610	-2.2810391
H	-0.1118302	1.0227500	-2.0787791
H	1.4411218	1.5077310	0.5442189
H	-2.1682912	1.6509790	-0.8105811
H	2.0402958	0.3655560	3.7490229
H	0.6957798	1.5055090	3.7266009
H	2.3151928	1.9858080	3.1351409
H	-6.1409672	0.2633540	-1.7487111
H	-5.6513002	-1.9812380	1.8808759
H	-4.1824072	-0.2181710	2.7765089
H	-4.6926012	2.0667460	-0.8216091
H	-3.4921432	3.0400120	1.1193139
H	-3.4232722	2.1557350	2.6563339
H	-7.7942592	-3.6136980	-0.5173241
H	-7.6656382	-2.7760830	1.0518839
H	-6.2511002	-3.6403640	0.3770639
H	2.6999878	1.4327770	-2.7600411

H	3.5018318	1.3179190	-1.1609331
H	3.8884538	2.6392550	-2.2804421
H	1.8918928	4.4558150	0.2285539
H	3.1381718	3.2152750	0.5257909
H	3.3883708	4.4509600	-0.7199151
H	0.6461448	4.4619500	-2.0291991
H	0.8172318	3.0648440	-3.1250071
H	2.1211118	4.2455120	-2.9789941
P	4.6934588	-1.8389840	0.3917469
C	5.1504908	-1.7581640	-1.3746931
H	5.9162688	-2.5054730	-1.6133321
H	4.2605598	-1.9478780	-1.9848781
H	5.5337138	-0.7615170	-1.6156571
C	6.2655568	-1.6262660	1.2875229
H	6.0946108	-1.7443210	2.3617139
H	6.9989608	-2.3695070	0.9537119
H	6.6605428	-0.6215950	1.1098439
C	4.2333988	-3.5838000	0.6542399
H	3.3211578	-3.8072110	0.0910799
H	5.0399528	-4.2504640	0.3275309
H	4.0298458	-3.7550960	1.7156529
A-2'			
C	-0.5524640	-4.4515512	-1.3904064
C	0.6559970	-4.4806922	-2.0841974
C	1.4415260	-3.3333552	-2.2074684
C	0.9659550	-2.1763062	-1.6209094
C	-0.2445740	-2.1299042	-0.9152924

C	-1.0060290	-3.2785612	-0.7855704
N	1.6206670	-0.8609962	-1.6442434
C	0.4361360	-0.0061252	-1.3862934
C	-0.2914680	-0.7737992	-0.2632744
N	0.4859210	1.3637748	-0.9649164
C	-0.7369760	1.5744458	-0.3066344
C	-1.4189820	0.2213808	0.0183326
O	-1.2002840	2.6500058	-0.0044534
N	-1.6760600	0.1726038	1.4363516
C	-0.5578170	-0.2210152	2.1265426
C	0.3375000	-0.8999622	1.1346666
O	-0.3938450	-0.1053542	3.3272406
C	1.3073320	-1.7556622	1.5047086
C	1.8107230	-2.0017442	2.8849466
Au	3.2836870	-0.3824572	-0.2247214
C	-5.8001890	1.3902978	-0.1504394
C	-6.4848180	0.1879138	0.0551976
C	-5.9528720	-0.7729232	0.9195506
C	-4.7497310	-0.5156792	1.5692816
C	-4.0647720	0.6824908	1.3818106
C	-4.6051170	1.6300258	0.5060536
C	-2.7551240	0.9326318	2.0681216
O	-7.6437100	0.0491518	-0.6242754
C	-8.3979490	-1.1227932	-0.4196874
C	1.0513630	2.4830048	-1.7978374
C	2.2003320	1.9678068	-2.6551914
C	1.5842670	3.5441348	-0.8423924

C	-0.0203510	3.0561848	-2.7247724
H	-1.1457200	-5.3586882	-1.3135264
H	0.9922610	-5.4078002	-2.5401494
H	2.3852320	-3.3515812	-2.7495724
H	-1.9368620	-3.2608842	-0.2226534
H	2.0068300	-0.6868572	-2.5718044
H	-0.1934880	-0.1062672	-2.2941874
H	-2.3359160	0.1023928	-0.5747064
H	1.3877110	-2.9399502	3.2688786
H	1.5350790	-1.2056762	3.5772846
H	2.8983420	-2.1455442	2.8701266
H	-6.2375120	2.1208058	-0.8260354
H	-6.4702420	-1.7104612	1.0999276
H	-4.3391470	-1.2627432	2.2489926
H	-4.0727310	2.5668538	0.3433666
H	-2.5079460	2.0026928	2.0553076
H	-2.7655660	0.6061638	3.1145256
H	-9.2929010	-1.0266812	-1.0367554
H	-8.6977070	-1.2323102	0.6318266
H	-7.8445970	-2.0207872	-0.7295124
H	1.8654390	1.2524938	-3.4191254
H	3.0050020	1.5215298	-2.0520764
H	2.6349560	2.8143858	-3.1974064
H	0.7887890	3.9360148	-0.2044454
H	2.3686930	3.1169088	-0.2032814
H	2.0152520	4.3743298	-1.4141454
H	-0.8384690	3.5131278	-2.1635944

H	-0.4319910	2.2771728	-3.3804944
H	0.4240710	3.8253448	-3.3663534
P	5.1208310	0.3112328	1.0150006
C	5.2663700	2.1265388	1.0117426
H	6.1611000	2.4333468	1.5660226
H	5.3338060	2.4935518	-0.0174914
H	4.3823000	2.5671558	1.4836556
C	5.0883700	-0.1524152	2.7742746
H	5.1422500	-1.2408492	2.8758496
H	5.9446360	0.2974348	3.2904926
H	4.1602850	0.1985468	3.2366316
C	6.7164060	-0.2996412	0.3871936
H	6.8574680	0.0276898	-0.6472014
H	7.5346100	0.0887698	1.0048796
H	6.7331710	-1.3932492	0.4123656
H	1.7332630	-2.4090732	0.7363466

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C	4.4048880	-2.2713760	0.5139559
C	3.8707580	-3.3120000	-0.2652061
C	2.7150490	-3.1328960	-1.0071741
C	2.0985050	-1.8839180	-0.9458131
C	2.6075210	-0.8283760	-0.1482731
C	3.7882240	-1.0336440	0.5807039
N	0.9622050	-1.4253030	-1.5774861
C	0.7221080	-0.1428120	-1.1769851
C	1.6976890	0.2726480	-0.3072151
O	3.5111410	2.1596790	1.8325369

C	3.0292440	2.1566840	0.7081449
C	1.6432580	1.5780850	0.4209769
N	3.7411050	2.6843840	-0.3314481
N	0.8283530	1.5261640	1.6498999
C	-0.4097610	2.0730430	1.7033669
C	-0.9620700	2.5734340	0.4211569
C	-1.4678200	2.8462200	-0.6675801
C	-1.8382730	3.1481600	-2.0448741
O	-1.1354930	2.0833240	2.6916809
C	3.6076750	2.7948380	-1.8026051
C	4.5456810	3.9366560	-2.1927021
C	4.0649630	1.5076280	-2.4857641
C	2.1953370	3.1633800	-2.2505271
C	-0.7265080	-2.4072610	1.3316579
C	0.0719780	-3.4631160	1.7682029
C	1.1679730	-3.2015620	2.5952229
C	1.4948270	-1.8949530	2.9210939
C	0.7249670	-0.8202210	2.4666959
C	-0.4005300	-1.1067300	1.7034089
C	1.1717200	0.5985450	2.7428399
O	-0.1251750	-4.7606060	1.4211269
C	-1.1342270	-5.0240350	0.4769009
H	5.3179580	-2.4463520	1.0787939
H	4.3753300	-4.2752090	-0.2876731
H	2.2990780	-3.9353240	-1.6125991
H	4.2002230	-0.2386660	1.2015729
H	0.2733710	-1.9834120	-2.0698141

H	-0.1601260	0.3795840	-1.5243001
H	1.1354480	2.2999040	-0.2245131
H	4.6564950	2.9532020	0.0150239
H	-2.7146630	3.8010840	-2.0960671
H	-2.0670170	2.2102680	-2.5689741
H	-1.0006910	3.6362060	-2.5558621
H	4.2362720	4.8773470	-1.7217381
H	4.5444650	4.0738310	-3.2795991
H	5.5780570	3.7187360	-1.8889661
H	3.4050120	0.6692320	-2.2406401
H	4.0682540	1.6394940	-3.5751991
H	5.0814920	1.2454810	-2.1683151
H	2.2277500	3.4652150	-3.3041631
H	1.8042020	4.0085350	-1.6680011
H	1.5059080	2.3140510	-2.1854151
H	-1.5592440	-2.5597140	0.6496849
H	1.7821860	-4.0379380	2.9194439
H	2.3940380	-1.7008770	3.5059639
H	-1.0188030	-0.3082490	1.3024659
H	0.7018260	1.0039460	3.6452299
H	2.2540530	0.6502620	2.8843859
H	-1.0931660	-6.0949020	0.2659079
H	-0.9785920	-4.4622310	-0.4563421
H	-2.1333920	-4.7750180	0.8646029
Au	-3.2166050	1.7990590	0.5451949
P	-4.9996270	0.5345530	1.3194519
C	-4.3756120	-1.0880740	1.8561699

H	-3.5303840	-0.9576960	2.5402249
H	-5.1749420	-1.6539130	2.3494039
H	-4.0353920	-1.6298880	0.9672079
C	-6.3041010	0.1611270	0.1101539
H	-7.0709540	-0.4676790	0.5775149
H	-6.7554450	1.0877000	-0.2555041
H	-5.8482880	-0.3656610	-0.7326611
C	-5.8459820	1.2384140	2.7722139
H	-6.6182780	0.5492990	3.1338089
H	-5.1116650	1.4130250	3.5645929
H	-6.3062000	2.1950360	2.5077729
Sb	-2.9310250	-1.0670330	-2.1660471
F	-4.0711080	0.2985470	-2.0801721
F	-1.7770500	0.0090370	-2.9899161
F	-2.2304360	-0.5252520	-0.6039391
F	-1.7136820	-2.3641660	-2.1671591
F	-3.6023290	-1.6332460	-3.6793601
F	-4.0619330	-2.0557350	-1.2197651
B- ts1			
C	2.4651196	0.2747779	4.7314709
C	1.6450306	-0.3904661	5.6635329
C	0.5791176	-1.1769061	5.2433539
C	0.3623606	-1.2751791	3.8717849
C	1.1606306	-0.6150611	2.9259569
C	2.2310006	0.1711499	3.3658949
N	-0.6113184	-1.9879601	3.1636489
C	-0.4313394	-1.8188621	1.8380069

C	0.6131976	-0.9258491	1.6019379
C	1.4159776	-0.8414021	0.3202629
N	0.8658896	0.1420769	-0.6127321
C	-0.1560584	0.9393939	-0.2661621
C	-0.7426404	0.7731379	1.0790589
O	-0.6026034	1.8399199	-0.9976771
C	1.5660696	-2.2228641	-0.3482841
O	2.6143466	-2.8503081	-0.1483631
N	0.5387866	-2.6605761	-1.1034271
C	-1.5725084	1.2546339	1.9056739
Au	-2.9595884	2.4236839	0.5906459
C	-2.0265584	1.1252879	3.3289299
C	0.4850996	-3.9750251	-1.8108841
C	-0.8752124	-4.0233351	-2.5280411
C	1.6254766	-4.0654351	-2.8447791
C	0.5785926	-5.1294841	-0.7938331
C	3.9719386	3.3440259	-1.2604061
C	5.2163006	2.7048759	-1.2291571
C	5.2946196	1.3270269	-1.4064681
C	4.1212026	0.5930399	-1.6142351
C	2.8753106	1.2117169	-1.6445971
C	2.8184336	2.6043209	-1.4670841
C	1.6057226	0.4099939	-1.8674821
O	6.3039676	3.5228589	-1.0198501
C	7.6380166	2.9969139	-0.9948401
H	3.2840126	0.8689829	5.0855349
H	1.8508456	-0.2922591	6.7109609

H	-0.0433804	-1.6896311	5.9501069
H	2.8631106	0.6865289	2.6699269
H	-1.3375424	-2.5375451	3.5621009
H	-1.0360414	-2.3399051	1.1359559
H	2.4261236	-0.5580681	0.5739419
H	-0.2513384	-2.0591451	-1.2157151
H	-2.7745344	0.3438949	3.3757909
H	-1.2049864	0.8750049	3.9833279
H	-2.4767734	2.0428459	3.6769779
H	-1.6950634	-3.9968011	-1.8230981
H	-0.9553404	-4.9412031	-3.0969831
H	-0.9883574	-3.1923891	-3.2158481
H	2.5924516	-4.0182311	-2.3659401
H	1.5554056	-5.0033821	-3.3850331
H	1.5494816	-3.2571621	-3.5649661
H	1.5196086	-5.1091121	-0.2640361
H	0.4951376	-6.0792791	-1.3111811
H	-0.2321254	-5.0670141	-0.0763751
H	3.9392266	4.4062399	-1.1288961
H	6.2351976	0.8161039	-1.3888771
H	4.1957316	-0.4695581	-1.7479781
H	1.8686346	3.1017839	-1.4963881
H	0.9310926	0.9335289	-2.5234821
H	1.8387616	-0.5407001	-2.3225301
H	8.2798586	3.8450809	-0.8273741
H	7.8892676	2.5302249	-1.9399081
H	7.7595806	2.2829679	-0.1888201

P	-4.7302354	3.3394509	-0.8019201
C	-4.5041094	2.8442329	-2.5851571
H	-4.5264594	1.7670549	-2.6466581
H	-5.2947074	3.2614869	-3.1964921
H	-3.5465844	3.1947539	-2.9424541
C	-4.8854854	5.1998469	-0.8412301
H	-5.6802324	5.4995969	-1.5127381
H	-5.1013794	5.5712199	0.1509139
H	-3.9548814	5.6351899	-1.1774031
C	-6.4379944	2.7334659	-0.3630701
H	-7.1698834	3.1398909	-1.0499601
H	-6.4482734	1.6558929	-0.4225501
H	-6.6893274	3.0338989	0.6444129
Sb	-3.9971474	-1.7518081	-0.2670031
F	-4.6582534	-0.1300351	-0.9810001
F	-4.2136124	-2.6163331	-1.9158381
F	-5.7127964	-2.2557671	0.2923889
F	-3.7083864	-0.8711861	1.3852619
F	-2.2337324	-1.2480261	-0.7856871
F	-3.1989474	-3.2847531	0.5031299

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C	0.1964092	3.5160819	-0.1766691
C	-0.9882468	3.6979079	0.5380719
C	-1.6950168	2.6134229	1.0582299
C	-1.1399318	1.3698299	0.8238869
C	0.0303812	1.1567009	0.1015529
C	0.7178042	2.2413829	-0.4116011

N	-1.6410498	0.1031639	1.2177989
C	-0.8960398	-0.8576011	0.7830409
C	0.3076002	-0.3311601	0.0605199
C	1.6384742	-0.6710131	0.8215739
N	2.6083422	-0.8151001	-0.2286161
C	2.0400362	-0.9905391	-1.4875931
C	0.5645532	-0.9161131	-1.3248921
O	2.7126252	-1.1265711	-2.4955081
C	1.4686182	-1.9096411	1.7091489
O	0.6288542	-1.8737021	2.6052609
N	2.2636512	-2.9532251	1.4206029
C	-0.3775078	-1.1690611	-2.2613341
Au	-2.4009768	-0.7082311	-2.1369131
C	0.0019642	-1.7389781	-3.5966861
C	2.2175112	-4.2682791	2.0950349
C	3.2728432	-5.1327521	1.4194809
C	2.5472252	-4.0984981	3.5741099
C	0.8356462	-4.8906701	1.9140649
C	4.1356712	3.1266529	-1.4741511
C	4.0641552	3.9041599	-0.3111761
C	4.0529352	3.2836949	0.9375849
C	4.0853482	1.8918349	1.0081589
C	4.1233162	1.1067089	-0.1396831
C	4.1617062	1.7462579	-1.3864041
C	3.9974752	-0.3886881	-0.0703951
O	4.0058002	5.2432639	-0.5028521
C	3.8796252	6.0632909	0.6340859

H	0.7250782	4.3809559	-0.5734681
H	-1.3766308	4.7018459	0.6880289
H	-2.6339058	2.7308049	1.5936629
H	1.6368962	2.1136549	-0.9812151
H	-2.5147048	0.0166189	1.7582119
H	-1.1565738	-1.8992991	0.9304109
H	1.8940912	0.1594029	1.4970129
H	2.8361722	-2.8553311	0.5893999
H	1.0534692	-2.0254561	-3.6809401
H	-0.6378848	-2.6002771	-3.8274931
H	-0.2129438	-0.9962691	-4.3777441
H	3.0555962	-5.2641341	0.3514609
H	3.2941242	-6.1256181	1.8814559
H	4.2717492	-4.6904061	1.5232199
H	1.8147092	-3.4514731	4.0649869
H	2.5383832	-5.0766351	4.0697219
H	3.5447602	-3.6602531	3.6981289
H	0.0668292	-4.2743341	2.3897489
H	0.8116112	-5.8868661	2.3717569
H	0.5978552	-4.9980651	0.8483749
H	4.1601842	3.6378949	-2.4332161
H	4.0128612	3.8652329	1.8535699
H	4.0767912	1.4120359	1.9876169
H	4.1843322	1.1396479	-2.2909961
H	4.5568682	-0.8707691	-0.8803471
H	4.3716632	-0.7778721	0.8870519
H	3.8231632	7.0913489	0.2713139

H	4.7464682	5.9679299	1.3032749
H	2.9655012	5.8299179	1.1995489
P	-4.7211898	-0.1544021	-2.3926511
C	-5.9561538	-1.1488571	-1.4863101
H	-5.7684128	-1.1329981	-0.4119091
H	-6.9622048	-0.7576581	-1.6779431
H	-5.8922618	-2.1816041	-1.8450741
C	-5.2126508	-0.4468541	-4.1367071
H	-6.2687398	-0.1940151	-4.2914111
H	-4.5946408	0.1667739	-4.8003171
H	-5.0531318	-1.4990371	-4.3938741
C	-5.1821018	1.5992319	-2.1666041
H	-6.2580548	1.7274649	-2.3334161
H	-4.9344768	1.9244249	-1.1561941
H	-4.6233878	2.1999609	-2.8918391
Sb	-5.2770498	0.8813129	1.8186279
F	-6.2188508	1.2008359	3.2570999
F	-4.8212468	2.5867739	1.6632649
F	-3.7816018	0.6146729	2.7943779
F	-4.1814238	0.5332149	0.4267169
F	-6.6103668	1.1145809	0.6899869
F	-5.6083668	-0.8525841	1.9039059
B-ts2			
C	1.0099721	-3.1634729	2.2063097
C	-0.0947029	-3.0591489	3.0499367
C	-0.9918679	-1.9956529	2.9363227
C	-0.7317949	-1.0653679	1.9470197

C	0.3656571	-1.1516739	1.0956507
C	1.2530041	-2.2043239	1.2205437
N	-1.4990109	0.0598081	1.5635117
C	-0.9285269	0.7129971	0.5694477
C	0.3301111	0.0010071	0.1218117
N	0.0954661	2.5127681	1.3130247
C	1.4448161	2.0475621	1.1524887
C	1.6075641	0.8622931	0.2100127
O	2.3634201	2.4811601	1.8054127
N	1.8970421	1.2494331	-1.1461733
C	1.2565511	0.4311261	-2.0802063
C	0.2109681	-0.3400619	-1.3680533
O	1.5714151	0.4222981	-3.2576503
C	-0.7598889	-1.1157889	-1.9056983
C	-0.8399579	-1.3523109	-3.3832833
Au	-2.3641229	-1.9318009	-0.8641793
C	6.0985611	0.2929191	0.4300427
C	6.4257671	-0.7839449	-0.3982743
C	5.7050431	-0.9981119	-1.5752443
C	4.6717391	-0.1293059	-1.9146603
C	4.3434461	0.9546171	-1.1014823
C	5.0669301	1.1481911	0.0796167
C	3.1892651	1.8497481	-1.4626123
O	7.4507631	-1.5639209	0.0254387
C	7.8258591	-2.6513329	-0.7827063
C	-0.3410179	3.8014641	0.6340507
C	-1.7645999	4.0561461	1.1123437

C	-0.2878369	3.6653401	-0.8791253
C	0.5728571	4.9366821	1.0858567
H	1.6886291	-4.0053289	2.3149917
H	-0.2601059	-3.8154179	3.8130937
H	-1.8504889	-1.9020929	3.5973447
H	2.1064851	-2.2902389	0.5488917
H	-2.4981559	0.1946951	1.7346277
H	-1.5404439	1.3483841	-0.0649073
H	2.4443611	0.2734191	0.6268177
H	-0.8385239	-2.4327429	-3.5795703
H	-0.0410729	-0.8774109	-3.9578053
H	-1.8129519	-0.9924999	-3.7460863
H	6.6708521	0.4327911	1.3435697
H	5.9423111	-1.8277829	-2.2347763
H	4.1049811	-0.2923599	-2.8309443
H	4.8012311	1.9745451	0.7387627
H	3.2688931	2.8138171	-0.9397683
H	3.1602331	2.0474471	-2.5398653
H	8.6622161	-3.1400339	-0.2786753
H	8.1517561	-2.3241879	-1.7805603
H	7.0064071	-3.3756179	-0.8985713
H	-1.7996729	4.1645311	2.2047697
H	-2.4639299	3.2709181	0.8089407
H	-2.1307449	4.9936241	0.6792867
H	0.7252721	3.4447401	-1.2348193
H	-0.9744099	2.9047801	-1.2650973
H	-0.5960239	4.6206441	-1.3187793

H	1.6050581	4.7901021	0.7490287
H	0.5854001	5.0310551	2.1790207
H	0.2093811	5.8827951	0.6679617
P	-4.3335419	-2.8443129	0.1280927
C	-4.9362769	-2.1356939	1.7028767
H	-5.7871269	-2.7200239	2.0735957
H	-4.1366829	-2.1517559	2.4516197
H	-5.2495889	-1.1022209	1.5298237
C	-5.8114469	-2.7290419	-0.9367643
H	-5.5958049	-3.1537319	-1.9217223
H	-6.6559509	-3.2590369	-0.4803043
H	-6.0583969	-1.6700309	-1.0591953
C	-4.1836599	-4.6289599	0.5117977
H	-3.3742599	-4.7717709	1.2361637
H	-5.1183969	-5.0277819	0.9241387
H	-3.9246589	-5.1776229	-0.3992053
H	-0.0144059	2.6851681	2.3154187
Sb	-4.7977909	1.4287521	-0.5839513
F	-3.9348419	0.6227821	0.7994657
F	-4.4545069	0.0197541	-1.6098653
F	-6.2572569	0.5995711	-0.0199933
F	-5.6109999	2.2519431	-1.8960743
F	-3.1913269	2.0739551	-1.0366263
F	-5.0529139	2.7981461	0.4943357
B-int3			
C	-0.5254100	3.3757073	1.8545258
C	0.4697800	3.1642503	2.8085238

C	1.1359250	1.9423473	2.8988208
C	0.7908150	0.9457973	1.9946538
C	-0.1971830	1.1513983	1.0354618
C	-0.8680610	2.3609823	0.9618548
N	1.3524380	-0.3476277	1.9029438
C	0.7528450	-1.0117147	0.7781298
C	-0.3397820	-0.0689617	0.1677968
N	0.0223840	-2.2581297	1.3082948
C	-1.4632680	-1.9263547	1.2939478
C	-1.6897200	-0.7818027	0.3510758
O	-2.2289860	-2.5317747	1.9771288
N	-1.9967860	-1.3322357	-0.9435762
C	-1.2726400	-0.6989347	-1.9734412
C	-0.2147450	0.1068573	-1.3382522
O	-1.5656290	-0.8671007	-3.1438962
C	0.7641870	0.8173923	-1.9484242
C	0.8968970	0.8619043	-3.4379252
Au	2.2779360	1.7925673	-0.9147122
C	-6.2548410	-0.1823477	0.3980038
C	-6.5066410	0.8290383	-0.5330082
C	-5.7179160	0.9271133	-1.6817972
C	-4.6919190	0.0109433	-1.8890362
C	-4.4368630	-1.0074717	-0.9716712
C	-5.2283600	-1.0865167	0.1776078
C	-3.2900500	-1.9514787	-1.2022872
O	-7.5313850	1.6628223	-0.2328182
C	-7.8303230	2.6923663	-1.1431302

C	0.4791110	-3.6460067	0.7334848
C	1.9208930	-3.8148217	1.1868148
C	0.3449020	-3.6444047	-0.7761872
C	-0.3958990	-4.7201797	1.3593968
H	-1.0335310	4.3352013	1.8062198
H	0.7240280	3.9606453	3.5048158
H	1.8953180	1.7671093	3.6584548
H	-1.6237980	2.5191723	0.1931248
H	2.3707870	-0.3596617	1.8310428
H	1.4926080	-1.3376017	0.0422348
H	-2.4959330	-0.1391037	0.7428048
H	0.9193370	1.9063273	-3.7758382
H	0.1173080	0.3193223	-3.9790992
H	1.8809860	0.4511263	-3.7062472
H	-6.8812790	-0.2335477	1.2848348
H	-5.8965730	1.7039783	-2.4192662
H	-4.0733750	0.0821533	-2.7835112
H	-5.0316500	-1.8702067	0.9099148
H	-3.3926370	-2.8488517	-0.5730992
H	-3.2444330	-2.2758637	-2.2485852
H	-8.6777300	3.2399393	-0.7257962
H	-8.1116930	2.2948903	-2.1288042
H	-6.9845540	3.3837953	-1.2681622
H	2.0004110	-3.7982637	2.2820228
H	2.6073480	-3.0794577	0.7625468
H	2.2737080	-4.7949467	0.8483178
H	-0.6914590	-3.4781537	-1.0930372

H	0.9991660	-2.9131847	-1.2616382
H	0.6533550	-4.6332607	-1.1333072
H	-1.4316910	-4.6792437	1.0100218
H	-0.3975510	-4.6686017	2.4546458
H	0.0180840	-5.6922087	1.0706228
P	4.1335490	2.8446453	0.1408888
C	4.7427910	2.1140563	1.7027088
H	5.5392890	2.7382323	2.1256068
H	3.9179380	2.0394423	2.4201148
H	5.1279140	1.1121213	1.4933778
C	5.6401910	2.8570853	-0.8908042
H	5.4258340	3.3185993	-1.8594042
H	6.4516080	3.3996923	-0.3910422
H	5.9375130	1.8166953	-1.0590072
C	3.8532130	4.5986713	0.5875638
H	3.0171530	4.6507383	1.2945698
H	4.7469210	5.0438463	1.0415418
H	3.5780930	5.1652033	-0.3075972
H	0.2678040	-2.2916787	2.3072538
Sb	4.7048950	-1.3516007	-0.7429802
F	3.7673460	-0.5280277	0.5734118
F	4.4374750	0.0118823	-1.8437142
F	6.1314730	-0.5129807	-0.1121032
F	5.5864740	-2.2237107	-1.9798492
F	3.1263370	-2.0286747	-1.2447612
F	4.9199250	-2.6993667	0.3806898

B-ts3

C	0.3881915	-3.0704225	2.1407193
C	-0.5643805	-2.6770265	3.0822543
C	-1.1674565	-1.4232245	3.0076703
C	-0.7982875	-0.5981685	1.9565883
C	0.1436925	-0.9758925	1.0089523
C	0.7532665	-2.2190135	1.1009363
N	-1.3088905	0.7152955	1.6912963
C	-0.6965715	1.1660645	0.4072473
C	0.3443645	0.1005395	-0.0225787
N	0.0334665	2.3480685	0.9780523
C	1.4716615	2.0786145	0.8994553
C	1.6996845	0.8105155	0.1090023
O	2.3089415	2.7921165	1.3760173
N	2.0354855	1.1910155	-1.2428457
C	1.3457195	0.4207205	-2.1940727
C	0.2526635	-0.2815755	-1.4891867
O	1.6755215	0.4045385	-3.3667657
C	-0.7224225	-1.0536105	-2.0225867
C	-0.7999385	-1.3196615	-3.4937817
Au	-2.2737995	-1.8721755	-0.9095107
C	6.2258285	0.2665805	0.4365263
C	6.5247615	-0.8708845	-0.3180767
C	5.7926725	-1.1488445	-1.4746227
C	4.7750195	-0.2838005	-1.8660967
C	4.4746215	0.8593255	-1.1271997
C	5.2098895	1.1178365	0.0335143
C	3.3443645	1.7568795	-1.5490627

O	7.5364105	-1.6406765	0.1533893
C	7.8851015	-2.7888625	-0.5789117
C	-0.4876565	3.7524135	0.6361213
C	-1.9596905	3.8026045	1.0193063
C	-0.2909745	3.9698065	-0.8556597
C	0.2720565	4.7862985	1.4562203
H	0.8470075	-4.0526365	2.2193043
H	-0.8343995	-3.3524625	3.8904723
H	-1.9006195	-1.1006615	3.7439523
H	1.4774155	-2.5253085	0.3477773
H	-2.3364915	0.7521325	1.6437223
H	-1.4420405	1.4193235	-0.3517127
H	2.4899985	0.2043335	0.5822763
H	-0.7969665	-2.4033675	-3.6716937
H	-0.0010285	-0.8537115	-4.0765917
H	-1.7736705	-0.9691905	-3.8633817
H	6.8086725	0.4566975	1.3342163
H	6.0089675	-2.0259375	-2.0774977
H	4.2008935	-0.4941455	-2.7683937
H	4.9728275	1.9993165	0.6293863
H	3.4324495	2.7388515	-1.0644667
H	3.3411865	1.9093215	-2.6341787
H	8.7137925	-3.2586825	-0.0451427
H	8.2127895	-2.5381525	-1.5980657
H	7.0504425	-3.5022245	-0.6412397
H	-2.0984055	3.6408725	2.0961243
H	-2.5870545	3.1058485	0.4603543

H	-2.3405335	4.8036805	0.7908833
H	0.7655535	3.8756795	-1.1379147
H	-0.8849115	3.2697475	-1.4553637
H	-0.6207715	4.9823185	-1.1140967
H	1.3144685	4.8910325	1.1515583
H	0.2487715	4.5426555	2.5248013
H	-0.2284565	5.7513085	1.3185983
P	-4.1255175	-2.8645875	0.2232033
C	-4.7040225	-2.1040695	1.7822653
H	-5.4781885	-2.7305355	2.2416233
H	-3.8608245	-1.9972235	2.4732713
H	-5.1136785	-1.1150655	1.5587353
C	-5.6564315	-2.9234015	-0.7704757
H	-5.4573955	-3.3998445	-1.7350897
H	-6.4426135	-3.4729195	-0.2389197
H	-5.9798375	-1.8933835	-0.9504817
C	-3.8228965	-4.6063665	0.7047013
H	-2.9755365	-4.6386405	1.3988453
H	-4.7054825	-5.0479175	1.1833403
H	-3.5590155	-5.1907545	-0.1824017
H	-0.5374785	1.8311525	1.9881003
Sb	-4.7622575	1.2750595	-0.7347877
F	-3.7265635	0.5045425	0.5489283
F	-4.5174955	-0.1255385	-1.7926757
F	-6.1282565	0.4260835	0.0074723
F	-5.7386815	2.0816915	-1.9416447
F	-3.2341485	1.9686565	-1.3513797

F	-4.9368785	2.6410275	0.3713743
B-int3			
C	0.9002080	-2.8302316	1.9098172
C	-0.0826870	-2.5761016	2.8704752
C	-0.8480440	-1.4148276	2.8123272
C	-0.5877570	-0.5480496	1.7641102
C	0.3681720	-0.7806866	0.7976062
C	1.1355810	-1.9373446	0.8707522
N	-1.3014370	0.6982354	1.4925612
C	-0.6470000	1.3298814	0.2268812
C	0.4194720	0.2988314	-0.2376668
N	0.0261370	2.5419844	0.5707402
C	1.3865420	2.4801984	0.2867702
C	1.7334820	1.0893354	-0.2138658
O	2.1827820	3.3914734	0.3565482
N	2.1550240	1.1619704	-1.5894958
C	1.4082640	0.3665964	-2.4480278
C	0.2640910	-0.1780366	-1.6741688
O	1.7248040	0.1794644	-3.6116888
C	-0.7285440	-0.9799136	-2.1178828
C	-0.8429940	-1.3602506	-3.5639158
Au	-2.2207220	-1.8168086	-0.9380798
C	6.2189980	0.4899484	0.4476002
C	6.4522690	-0.8130736	0.0011992
C	5.7275270	-1.3161766	-1.0817678
C	4.7841040	-0.5068766	-1.7089418
C	4.5520510	0.7991974	-1.2814648

C	5.2760680	1.2822044	-0.1883228
C	3.4862410	1.6312464	-1.9403608
O	7.3955540	-1.5106896	0.6834922
C	7.6879190	-2.8146916	0.2499062
C	-0.7219590	3.8477694	0.6498942
C	-2.0943720	3.6188454	1.2749922
C	-0.8829600	4.3870194	-0.7672228
C	0.0337970	4.8326344	1.5381932
H	1.4891270	-3.7412476	1.9787612
H	-0.2477550	-3.2867876	3.6759612
H	-1.6120280	-1.1991006	3.5564742
H	1.8928440	-2.1319616	0.1123542
H	-2.3155090	0.5344714	1.2887202
H	-1.4726180	1.4594524	-0.4834668
H	2.5172010	0.6436644	0.4222222
H	-0.8174530	-2.4541546	-3.6619818
H	-0.0662390	-0.9253106	-4.1978428
H	-1.8316000	-1.0576036	-3.9350398
H	6.7928990	0.8538404	1.2962012
H	5.8952190	-2.3249796	-1.4480728
H	4.2183290	-0.8921496	-2.5577548
H	5.0853550	2.2945374	0.1678782
H	3.5822930	2.6850854	-1.6530468
H	3.5378760	1.5580194	-3.0327738
H	8.4723390	-3.1939436	0.9082682
H	8.0543240	-2.8271896	-0.7868198
H	6.8116710	-3.4758496	0.3217932

H	-2.0182840	3.3072624	2.3276812
H	-2.7277780	2.9247094	0.7180202
H	-2.6346840	4.5712804	1.2796052
H	0.0940370	4.5139364	-1.2465118
H	-1.5025540	3.7184664	-1.3771348
H	-1.3785500	5.3646374	-0.7388298
H	0.9741170	5.1579874	1.0939602
H	0.2538760	4.3840404	2.5151202
H	-0.6066440	5.7068474	1.7038062
P	-3.9755550	-2.9675846	0.2177652
C	-4.5570180	-2.3426426	1.8364352
H	-5.2702770	-3.0493636	2.2775022
H	-3.7053880	-2.2173246	2.5138522
H	-5.0442460	-1.3750046	1.6859072
C	-5.5333110	-3.0965506	-0.7267178
H	-5.3304000	-3.4942146	-1.7256538
H	-6.2466260	-3.7462366	-0.2055568
H	-5.9519650	-2.0914206	-0.8321978
C	-3.5326680	-4.7073256	0.5847282
H	-2.6550270	-4.7230356	1.2401282
H	-4.3614140	-5.2372506	1.0697302
H	-3.2696430	-5.2191266	-0.3465438
Sb	-4.9280290	1.1276454	-0.5497148
F	-3.7916390	0.3623684	0.6802462
F	-4.6587860	-0.2416096	-1.6393018
F	-6.2013660	0.1886364	0.2440942
F	-6.0012360	1.9099504	-1.6842938

F	-3.4578720	1.8956564	-1.2012708
F	-5.1017590	2.4442254	0.6106482
H	-1.2261940	1.3691684	2.2616672
B-ts4			
C	-0.5719712	-1.0828484	3.2463499
C	-1.8394772	-0.5054734	3.2511019
C	-2.2856382	0.2769346	2.1817769
C	-1.3978782	0.4526676	1.1408789
C	-0.1236732	-0.1079344	1.1158889
C	0.3041848	-0.8903324	2.1726839
N	-1.5823922	1.1491976	-0.0992081
C	-0.2543102	1.6104136	-0.5015311
C	0.5410028	0.3169176	-0.1638711
N	0.4558078	2.6513076	0.2069279
C	1.7975498	2.3005896	0.3010369
C	1.9517098	0.8274716	-0.1178471
O	2.7315278	2.9928456	0.6481879
N	2.3801208	0.6544416	-1.4931591
C	1.5873618	-0.2132684	-2.2314721
C	0.3621518	-0.4961844	-1.4118221
O	1.8680878	-0.6267114	-3.3419191
C	-0.8667272	-0.9208644	-1.8005941
C	-1.1650362	-1.2676594	-3.2350031
Au	-2.3303762	-1.9824954	-0.5879561
C	6.3379408	-0.0805624	0.6016829
C	6.6920918	-1.3367464	0.1003699
C	6.0839828	-1.8190504	-1.0601191

C	5.1328538	-1.0364554	-1.7089021
C	4.7817968	0.2213676	-1.2258351
C	5.3924068	0.6879636	-0.0568161
C	3.7225718	1.0308636	-1.9193661
O	7.6308508	-2.0100374	0.8107209
C	8.0302438	-3.2724414	0.3394879
C	-0.1614602	4.0013226	0.3893599
C	-0.8769272	4.4015776	-0.9004611
C	0.8873778	5.0595206	0.7134489
C	-1.1600042	3.9236326	1.5448409
H	-0.2538322	-1.6842024	4.0944579
H	-2.4976902	-0.6618514	4.1029829
H	-3.2809892	0.7088666	2.1472879
H	1.2956958	-1.3382844	2.1755959
H	-1.6202602	0.1095526	-0.9862911
H	-0.2974062	1.8240586	-1.5785211
H	2.6330488	0.3244166	0.5862999
H	-1.2548042	-2.3542254	-3.3674831
H	-0.3869572	-0.9175174	-3.9216291
H	-2.1363502	-0.8411374	-3.5126491
H	6.8255048	0.2674446	1.5088269
H	6.3442448	-2.7920524	-1.4664061
H	4.6498908	-1.4094364	-2.6120871
H	5.1053728	1.6627976	0.3393799
H	3.8603638	2.1011246	-1.7190291
H	3.7471958	0.8723416	-3.0031021
H	8.7858788	-3.6404854	1.0366209

H	8.4713398	-3.2111854	-0.6659091
H	7.1911338	-3.9829694	0.3144809
H	-1.7225862	3.7472936	-1.1452791
H	-0.1826362	4.4162936	-1.7494951
H	-1.2878022	5.4103116	-0.7829561
H	1.4201008	4.8417486	1.6418829
H	1.6296958	5.1616986	-0.0828241
H	0.3648288	6.0168226	0.8265069
H	-0.6689122	3.5541756	2.4524249
H	-2.0173912	3.2779026	1.3233799
H	-1.5581142	4.9242526	1.7511019
P	-3.9357472	-3.3413234	0.4383639
C	-5.5334222	-3.3492684	-0.4349261
H	-6.2656162	-3.9502634	0.1177549
H	-5.8963042	-2.3221914	-0.5471381
H	-5.3948262	-3.7748874	-1.4338911
C	-3.4750712	-5.1071254	0.5487289
H	-2.5590212	-5.2112214	1.1385259
H	-4.2783342	-5.6874004	1.0183539
H	-3.2851482	-5.4999164	-0.4549711
C	-4.3387912	-2.8858324	2.1559839
H	-4.7190922	-1.8603794	2.1537869
H	-5.0937962	-3.5700914	2.5612869
H	-3.4311862	-2.9307844	2.7670039
H	-2.4220482	1.7332606	-0.1984141
Sb	-5.2798332	0.9329176	-0.6610341
F	-3.9198182	0.4075856	-1.6951981

F	-5.7563252	2.1134476	-1.8644651
F	-6.3135842	-0.3261304	-1.3368761
F	-6.5005282	1.4822676	0.4734829
F	-4.1031602	2.1002456	0.0673679
F	-4.7126582	-0.2506304	0.5698479

B-2

C	-1.0014901	-2.8458154	1.9831037
C	-2.3357991	-3.1907224	1.7435867
C	-3.1231551	-2.5148344	0.8184087
C	-2.5273381	-1.4778674	0.0964327
C	-1.1814271	-1.1578114	0.2900537
C	-0.4242151	-1.8045204	1.2575327
N	-3.0765921	-0.6678524	-0.8703723
C	-2.2179341	0.4429366	-1.1630613
C	-0.8157941	-0.0526934	-0.6610493
N	-2.4279941	1.6982006	-0.4246323
C	-1.3256931	2.1223576	0.2528407
C	-0.1774761	1.1651156	-0.0323153
O	-1.1810141	3.1248836	0.9354657
N	0.6963929	1.6957186	-1.0710323
C	0.9369059	0.8324706	-2.0974723
C	0.0674769	-0.3753374	-1.8404523
O	1.7493499	0.9855076	-2.9969973
C	-0.0361491	-1.4912934	-2.6343673
C	0.5655269	-1.6783624	-3.9884433
Au	1.7213289	-1.8195634	-1.0390113
C	3.7174689	2.0721616	2.2722777

C	4.8480329	1.4814416	1.6985737
C	4.9207979	1.3231986	0.3118287
C	3.8619899	1.7584876	-0.4854863
C	2.7389569	2.3659986	0.0749927
C	2.6789019	2.5108016	1.4657307
C	1.5937379	2.8121686	-0.7947803
O	5.8064009	1.0766076	2.5688967
C	6.9995319	0.5554386	2.0403597
C	-3.6567761	2.5581146	-0.5633303
C	-4.5929721	1.9829386	-1.6203843
C	-3.2319701	3.9524376	-1.0237853
C	-4.3660331	2.6052736	0.7837817
H	-0.4346951	-3.3547754	2.7603697
H	-2.7898271	-3.9907604	2.3240927
H	-4.1785011	-2.7469694	0.6958377
H	0.5883039	-1.4647474	1.4827427
H	-2.2302851	0.6602646	-2.2425753
H	0.3953029	0.9582696	0.8856657
H	0.9742869	-2.6879064	-4.1064333
H	1.3325239	-0.9305694	-4.1992933
H	-0.2344631	-1.5793914	-4.7345743
H	3.6874049	2.1862296	3.3528977
H	5.8051839	0.8994846	-0.1581253
H	3.9141669	1.6400656	-1.5674743
H	1.8026939	2.9821186	1.9120337
H	1.0052159	3.5974296	-0.3069173
H	1.9494669	3.1818506	-1.7619163

H	7.6475989	0.3335726	2.8903847
H	7.5047389	1.2766456	1.3828827
H	6.8254709	-0.3738454	1.4738917
H	-5.0445111	1.0299356	-1.3403833
H	-4.1087321	1.8994786	-2.6021393
H	-5.4325991	2.6774506	-1.7307963
H	-2.5950881	4.4489256	-0.2892453
H	-2.6959571	3.8961496	-1.9810973
H	-4.1295741	4.5627146	-1.1757583
H	-3.7138411	3.0364296	1.5501677
H	-4.6793391	1.6006566	1.0851167
H	-5.2668301	3.2250106	0.6990057
P	3.4014549	-2.6173284	0.3754087
C	3.1533759	-4.3623014	0.8329817
H	3.8948959	-4.6744254	1.5774787
H	2.1459609	-4.4730204	1.2497097
H	3.2341799	-4.9998784	-0.0523633
C	5.1000659	-2.4881214	-0.2646083
H	5.3148599	-1.4313394	-0.4575483
H	5.8147329	-2.8817484	0.4681267
H	5.1933469	-3.0433184	-1.2024093
C	3.4083409	-1.7155484	1.9582857
H	2.5174829	-1.9888894	2.5343697
H	4.3019039	-1.9745184	2.5394527
H	3.3937269	-0.6341364	1.7754907
H	-4.0811941	-0.6773344	-1.0453343
H	-0.7681591	-2.2357664	-2.3025483

Sb	-6.7826321	-0.9716904	0.3712657
F	-7.0552551	0.7386956	0.0026887
F	-5.8102061	-1.0923424	-1.1528023
F	-5.2440401	-0.5164704	1.1616957
F	-6.3696361	-2.6717744	0.6838017
F	-8.2131251	-1.4502094	-0.5307073
F	-7.6511731	-0.8478404	1.8923107

B-int4

C	-1.1950499	2.3061437	-3.2101657
C	-2.5853979	2.4031717	-3.3021877
C	-3.4104989	1.8676777	-2.3157467
C	-2.7679119	1.2564027	-1.2564037
C	-1.3877949	1.1226347	-1.1517447
C	-0.5778069	1.6551047	-2.1400817
N	-3.3512869	0.6356727	-0.1302077
C	-2.4574609	0.1123107	0.6410903
C	-1.0763069	0.3673707	0.1234463
C	-0.2153589	1.2336157	1.1016073
N	1.1303161	0.7673587	0.8951083
C	1.2024121	-0.4456913	0.2288513
C	-0.1804889	-0.8688943	-0.0926207
O	2.2647291	-0.9977283	-0.0237797
C	-0.7277009	1.1098767	2.5408593
O	-1.8490309	1.5384107	2.7957653
N	0.1017421	0.5081917	3.4115133
C	-0.5075839	-2.0614923	-0.6335287
Au	1.0001291	-3.4417043	-0.9774557

C	-1.9041489	-2.3836683	-1.0509947
C	-0.2281769	0.1907527	4.8173153
C	0.9918861	-0.5144953	5.3933823
C	-0.4992939	1.4797657	5.5853903
C	-1.4398399	-0.7358253	4.8652323
C	2.9414941	2.8402087	-2.5360217
C	2.3414801	4.1060307	-2.5359857
C	1.7858071	4.6087397	-1.3600127
C	1.8159801	3.8307557	-0.2035307
C	2.3836351	2.5608697	-0.1965177
C	2.9578841	2.0792987	-1.3809307
C	2.2799521	1.6611537	1.0025733
O	2.3500151	4.7588137	-3.7216737
C	1.7097321	6.0105377	-3.7866557
H	-0.5750229	2.7319867	-3.9967647
H	-3.0330239	2.8939557	-4.1623597
H	-4.4950139	1.8943167	-2.3707677
H	0.5071431	1.5725177	-2.0921407
H	-4.3774439	0.5250717	-0.0287937
H	-2.7402749	-0.4654283	1.5146673
H	-0.3194799	2.2944667	0.8293063
H	0.9635891	0.1417927	3.0238023
H	-2.6882999	-1.9928153	-0.3891237
H	-2.1019679	-1.9504373	-2.0427717
H	-2.0768469	-3.4594923	-1.1428097
H	1.2049741	-1.4453443	4.8517263
H	0.8141771	-0.7711403	6.4432473

H	1.8790781	0.1301337	5.3485853
H	-1.3532979	2.0132787	5.1589223
H	-0.7200869	1.2466257	6.6339303
H	0.3781921	2.1370517	5.5573223
H	-2.3257959	-0.2409343	4.4566303
H	-1.6520349	-1.0202363	5.9028003
H	-1.2482799	-1.6516033	4.2920523
H	3.3794691	2.4800147	-3.4635417
H	1.3264091	5.5920587	-1.3310317
H	1.3798091	4.2292767	0.7131993
H	3.3966011	1.0820167	-1.3872967
H	3.1615961	1.0162677	1.0917023
H	2.1818321	2.2412327	1.9310393
H	1.8025941	6.3540577	-4.8186667
H	2.1844431	6.7457747	-3.1214637
H	0.6437151	5.9319917	-3.5279447
P	2.8120771	-4.9104243	-1.3445077
C	4.3878111	-3.9887383	-1.2421177
H	4.4347141	-3.4751443	-0.2765097
H	5.2529941	-4.6524373	-1.3582457
H	4.4026291	-3.2219023	-2.0231477
C	2.9169341	-5.7688603	-2.9559797
H	3.8399561	-6.3568683	-3.0262537
H	2.0541821	-6.4311413	-3.0754607
H	2.8941351	-5.0301493	-3.7629367
C	3.0301171	-6.2640993	-0.1334147
H	3.9440881	-6.8329323	-0.3426107

H	3.0876271	-5.8414463	0.8743653
H	2.1669391	-6.9353733	-0.1736557
Sb	-5.9893099	-1.4999173	-0.9410717
F	-7.3401309	-1.6659363	0.1682613
F	-5.9255829	0.2870617	-0.5853457
F	-7.0612799	-1.1825223	-2.2943907
F	-5.8781699	-3.2238853	-1.2429937
F	-4.8507089	-1.6327353	0.4425683
F	-4.5718309	-1.1903793	-1.9759007

B-ts5

C	0.1196026	0.7566996	4.4898975
C	-0.7917014	-0.1858644	4.9608625
C	-1.5976634	-0.9177074	4.0861835
C	-1.4648954	-0.6516364	2.7360885
C	-0.5544704	0.2977406	2.2469755
C	0.2627796	0.9906036	3.1203085
N	-2.2303564	-1.1922814	1.6647065
C	-1.8995394	-0.5194894	0.5497765
C	-0.5423234	0.1159626	0.7492855
N	-1.3538494	-1.0021964	-1.3204075
C	-1.0249644	0.3899976	-1.6073945
C	-0.4582094	1.1359916	-0.3721445
O	-1.2041064	0.9195686	-2.6705125
N	0.9473656	1.3885796	-0.5655975
C	1.7007616	0.2999896	-0.1892605
C	0.7850056	-0.6869134	0.4691445
O	2.9006606	0.2059336	-0.4029075

C	1.1821026	-1.9458734	0.7620705
C	0.3141826	-2.9744944	1.4220695
Au	3.1404026	-2.5008564	0.3064925
C	-0.6348054	5.6213656	-1.4153415
C	-0.1469744	6.2590416	-0.2712445
C	0.8608066	5.6535676	0.4837975
C	1.3683026	4.4221626	0.0819215
C	0.8973036	3.7806546	-1.0609165
C	-0.1173394	4.3958436	-1.8002635
C	1.4314966	2.4342026	-1.4549675
O	-0.7118744	7.4529926	0.0225485
C	-0.2626174	8.1323476	1.1692935
C	-2.2562574	-1.7903964	-2.2400345
C	-2.5422584	-3.0901804	-1.5002515
C	-1.5032864	-2.0752624	-3.5355365
C	-3.5394044	-1.0176304	-2.5019345
H	0.7277716	1.3150316	5.1967025
H	-0.8823044	-0.3563104	6.0305935
H	-2.3132834	-1.6499844	4.4503295
H	0.9875226	1.7112686	2.7458125
H	-3.2099424	-1.4863684	1.7441385
H	-2.7285144	-0.0047454	0.0634075
H	-0.4939084	-1.5224004	-1.1051355
H	-1.0207384	2.0682256	-0.2263035
H	0.6969926	-3.9866394	1.2682595
H	-0.7358774	-2.9547374	1.1071725
H	0.3170126	-2.7968664	2.5087755

H	-1.4233864	6.1108336	-1.9807715
H	1.2557736	6.1312186	1.3754815
H	2.1557996	3.9493766	0.6696385
H	-0.5090334	3.8974976	-2.6867345
H	1.1480616	2.2007646	-2.4929275
H	2.5248876	2.3858076	-1.3905385
H	-0.8396414	9.0571716	1.2282305
H	0.8062206	8.3812806	1.1017425
H	-0.4343624	7.5452846	2.0829135
H	-3.1116404	-2.9113754	-0.5833115
H	-1.6092114	-3.6236464	-1.2660095
H	-3.1609084	-3.7378154	-2.1292415
H	-1.2563564	-1.1533014	-4.0694235
H	-0.5791864	-2.6370564	-3.3424295
H	-2.1370934	-2.6910044	-4.1842715
H	-3.3654294	-0.1441024	-3.1359895
H	-4.0410334	-0.7080184	-1.5804265
H	-4.2503574	-1.6810814	-3.0039245
P	5.3716526	-3.0250354	-0.2518645
C	6.1790686	-1.5739884	-1.0150565
H	7.2198896	-1.7890214	-1.2850885
H	5.6166836	-1.2802004	-1.9070015
H	6.1417946	-0.7354454	-0.3124935
C	6.4951816	-3.4698714	1.1207985
H	6.1485776	-4.3922324	1.5965395
H	7.5193066	-3.6116914	0.7552205
H	6.4848206	-2.6727794	1.8704535

C	5.6445516	-4.3619124	-1.4695875
H	5.0895146	-4.1373464	-2.3855305
H	6.7106736	-4.4619304	-1.7061515
H	5.2715406	-5.3084454	-1.0668435
Sb	-6.2791914	-2.0136204	0.1723175
F	-4.5448644	-1.6633594	0.6663795
F	-5.6074784	-2.9008364	-1.2124775
F	-6.1750374	-0.5157254	-0.7721615
F	-7.9281814	-2.3174414	-0.3380585
F	-6.1727744	-3.4846254	1.1397935
F	-6.7774344	-1.0952604	1.5923435

C-1

C	4.4523686	-2.2565144	0.5131612
C	3.9198066	-3.2591964	-0.3155328
C	2.7632906	-3.0471004	-1.0475718
C	2.1435316	-1.8033154	-0.9282568
C	2.6554316	-0.7842244	-0.0836788
C	3.8333236	-1.0247344	0.6384772
N	1.0100976	-1.3114284	-1.5363008
C	0.7830016	-0.0446134	-1.0926768
C	1.7572566	0.3307306	-0.2030578
O	3.5660916	2.1427056	2.0165422
C	3.1090566	2.1612346	0.8819502
C	1.7175456	1.6205426	0.5528222
N	3.8575706	2.6856276	-0.1342788
N	0.8604766	1.5715796	1.7524862
C	-0.3863184	2.1004326	1.7425932

C	-0.8846844	2.5944046	0.4371622
C	-1.3532924	2.8782546	-0.6642808
C	-1.7133284	3.1916556	-2.0415558
O	-1.1587194	2.1086226	2.6956032
C	3.7685246	2.8166326	-1.6073458
C	4.7374836	3.9462546	-1.9551378
C	4.2219496	1.5304636	-2.2954098
C	2.3768336	3.2144386	-2.0919728
C	-0.5687314	-2.4381214	1.4398442
C	0.2994566	-3.4462464	1.8574042
C	1.3835206	-3.1292474	2.6783382
C	1.6324616	-1.8081834	3.0137132
C	0.7968516	-0.7778624	2.5741562
C	-0.3188594	-1.1223014	1.8173092
C	1.1662276	0.6582146	2.8697282
O	0.1797396	-4.7528184	1.5009512
C	-0.7539804	-5.0578744	0.4971952
H	5.3640806	-2.4579044	1.0713452
H	4.4259906	-4.2193784	-0.3845708
H	2.3518996	-3.8201474	-1.6931388
H	4.2409386	-0.2606314	1.2998292
H	0.3439386	-1.7838934	-2.1371528
H	-0.1008864	0.4867036	-1.4217988
H	1.2504486	2.3699416	-0.0924668
H	4.7693566	2.9292196	0.2393572
H	-2.4239524	4.0229566	-2.0879028
H	-2.1850674	2.3152706	-2.5102638

H	-0.8163954	3.4602676	-2.6110248
H	4.4323286	4.8857296	-1.4790228
H	4.7686766	4.0987446	-3.0395738
H	5.7570196	3.7049596	-1.6266138
H	3.5355886	0.7028986	-2.0882838
H	4.2673246	1.6804346	-3.3815928
H	5.2203346	1.2398766	-1.9465808
H	2.4449986	3.5223646	-3.1421968
H	1.9815326	4.0617266	-1.5157298
H	1.6743476	2.3744966	-2.0513218
H	-1.4109394	-2.6345814	0.7799072
H	2.0543956	-3.9288454	2.9826212
H	2.5226746	-1.5643254	3.5938092
H	-0.9975144	-0.3610184	1.4367072
H	0.6193156	1.0489976	3.7343042
H	2.2342326	0.7522616	3.0804842
H	-0.6338274	-6.1195114	0.2687522
H	-0.5742884	-4.4666154	-0.4143368
H	-1.7893994	-4.8797094	0.8239712
Au	-3.1681834	1.8438296	0.5035802
P	-5.1217794	0.7298086	1.0617562
C	-4.6977114	-0.9185314	1.7050232
H	-4.1148624	-0.8015874	2.6247632
H	-5.6062984	-1.4972894	1.9094392
H	-4.0740444	-1.4289804	0.9647842
C	-6.2329154	0.4746196	-0.3550248
H	-7.0220794	-0.2410774	-0.0955718

H	-6.6826854	1.4339566	-0.6298978
H	-5.6474054	0.1094956	-1.2051048
C	-6.1593204	1.4859206	2.3570682
H	-7.0240064	0.8465456	2.5712062
H	-5.5672424	1.6147156	3.2681362
H	-6.5078414	2.4689626	2.0267952
C	-3.6518254	-2.3343934	-2.0339578
F	-3.9913174	-2.6331374	-3.2757378
F	-4.7686484	-2.2200954	-1.3046008
F	-2.9348304	-3.3353204	-1.5267998
S	-2.6854634	-0.7767674	-1.9583128
O	-1.5420754	-1.0386664	-2.8418338
O	-2.3576274	-0.6931584	-0.5189698
O	-3.6229754	0.2628476	-2.4166328
C-ts1			
C	-1.6920928	-1.5757600	-3.8049249
C	-0.6689908	-1.4575400	-4.7591239
C	0.6603552	-1.3390020	-4.3801949
C	0.9365122	-1.3382740	-3.0150409
C	-0.0832678	-1.4276350	-2.0408909
C	-1.4152318	-1.5601440	-2.4457899
N	2.1472212	-1.2616470	-2.3512699
C	1.9337322	-1.2762530	-1.0193239
C	0.5723322	-1.3319290	-0.7535799
C	-0.0804778	-1.5697010	0.5613191
N	-1.0783198	-0.5297180	0.8477941
C	-0.9978538	0.7190820	0.3600751

C	0.1495022	1.0254850	-0.5147429
O	-1.7999098	1.6223480	0.6194931
C	0.8524102	-1.7166460	1.7793891
O	0.7184682	-2.6865550	2.5130801
N	1.7019592	-0.6834430	1.9922701
C	0.8796492	1.8317470	-1.1567959
Au	-0.2355408	3.6376790	-0.5951239
C	2.0659592	1.9785080	-2.0211339
C	2.7127222	-0.6150450	3.0749981
C	3.3231912	0.7786620	2.9938171
C	2.0389442	-0.8054860	4.4294171
C	3.7868072	-1.6719190	2.8385201
C	-5.0331388	-1.9262010	-0.4576069
C	-5.0090848	-3.3205090	-0.3246389
C	-4.0774168	-3.9207430	0.5214691
C	-3.1760598	-3.1219550	1.2238981
C	-3.1877688	-1.7370580	1.0960121
C	-4.1307888	-1.1484520	0.2442111
C	-2.1572738	-0.8838400	1.7760321
O	-5.9294208	-3.9937100	-1.0543939
C	-5.9384818	-5.3979500	-0.9659849
H	-2.7213648	-1.6837240	-4.1393829
H	-0.9225178	-1.4685340	-5.8165829
H	1.4579182	-1.2633060	-5.1154139
H	-2.2170848	-1.6540950	-1.7121519
H	3.0790012	-1.0327260	-2.7221489
H	2.7745032	-1.2036750	-0.3398949

H	-0.6381538	-2.5173130	0.5264991
H	1.8282462	-0.0102980	1.2435131
H	1.8662752	1.5114440	-2.9928869
H	2.3410962	3.0219800	-2.1867539
H	2.9134222	1.4535420	-1.5597119
H	3.7957142	0.9451460	2.0173071
H	4.0932972	0.8889800	3.7657141
H	2.5579882	1.5480800	3.1649821
H	1.6120012	-1.8065030	4.5258731
H	2.7795642	-0.6564600	5.2247031
H	1.2383732	-0.0670560	4.5656261
H	3.3454482	-2.6739690	2.8164941
H	4.5287522	-1.6396440	3.6461631
H	4.3094822	-1.4829830	1.8928841
H	-5.7745868	-1.4869660	-1.1202629
H	-4.0406458	-4.9992910	0.6409251
H	-2.4419608	-3.5900260	1.8810731
H	-4.1391488	-0.0641900	0.1323481
H	-2.5847748	0.0549250	2.1398601
H	-1.7018898	-1.4141140	2.6228711
H	-6.7367888	-5.7456270	-1.6245839
H	-6.1456688	-5.7390530	0.0584381
H	-4.9849158	-5.8317630	-1.2990539
P	-1.3219918	5.6222870	-0.0417819
C	-2.7814108	5.2507370	0.9846581
H	-2.4584058	4.7230840	1.8874971
H	-3.3156358	6.1680110	1.2588031

H	-3.4471298	4.5815340	0.4307301
C	-1.9671898	6.5967100	-1.4411859
H	-2.5123838	7.4752930	-1.0766779
H	-1.1389328	6.9209840	-2.0781129
H	-2.6390918	5.9736770	-2.0390609
C	-0.3468438	6.8111610	0.9372541
H	-0.9586488	7.6808500	1.2043541
H	0.0112602	6.3238040	1.8490061
H	0.5219312	7.1401970	0.3594881
C	5.9612792	-1.5154450	-0.7295629
F	4.9598262	-2.4035890	-0.6893029
F	6.5125992	-1.4626980	0.4783011
F	6.8663842	-1.9475120	-1.5945529
S	5.3126642	0.1286410	-1.2184039
O	4.6882202	-0.1552650	-2.5322129
O	6.4775292	1.0008500	-1.2432809
O	4.3157392	0.3975110	-0.1536409
C-int4			
C	-0.2258950	3.1446503	-3.1635131
C	-1.3596740	2.9059273	-3.9418381
C	-2.2250910	1.8516173	-3.6513891
C	-1.8971500	1.0675323	-2.5601421
C	-0.7615940	1.2803583	-1.7795981
C	0.0903580	2.3297123	-2.0748901
N	-2.6002340	-0.0387127	-2.0219721
C	-1.9993610	-0.5002017	-0.9741471
C	-0.7499010	0.2538423	-0.6726251

C	-0.7727920	0.9178393	0.7453599
N	0.5791140	0.7820773	1.2226349
C	1.3603210	-0.0799217	0.4765779
C	0.5152730	-0.6256447	-0.6121661
O	2.5379520	-0.3000947	0.7266179
C	-1.8522440	0.2638743	1.6158349
O	-3.0168890	0.5993673	1.4417229
N	-1.4207250	-0.7104537	2.4394989
C	0.8612450	-1.6591247	-1.4064451
Au	2.6707820	-2.6130667	-1.0473451
C	-0.0344340	-2.1197137	-2.5173731
C	-2.2923740	-1.5851167	3.2557639
C	-1.3710130	-2.5959447	3.9243179
C	-3.0091830	-0.7464937	4.3090369
C	-3.2998310	-2.3026867	2.3631609
C	2.7434560	4.2717803	-0.2622781
C	1.7938880	5.3018113	-0.2736411
C	0.6760640	5.2214103	0.5556499
C	0.5079230	4.1011763	1.3689579
C	1.4282880	3.0582863	1.3696729
C	2.5580120	3.1648273	0.5468099
C	1.1631240	1.7785063	2.1134509
O	2.0501840	6.3261163	-1.1216051
C	1.1057140	7.3665733	-1.1972371
H	0.4277180	3.9806803	-3.4047841
H	-1.5761650	3.5536223	-4.7874141
H	-3.1144470	1.6571933	-4.2443621

H	0.9769100	2.5232283	-1.4712061
H	-3.4517400	-0.5395727	-2.4311671
H	-2.3906470	-1.3844557	-0.4692391
H	-1.0598490	1.9739453	0.6459449
H	-0.4200890	-0.8633507	2.4748779
H	-0.3447490	-1.2796647	-3.1563781
H	0.4488240	-2.8565747	-3.1636341
H	-0.9505270	-2.5948787	-2.1309111
H	-0.8477940	-3.2061917	3.1769419
H	-1.9558070	-3.2704287	4.5589859
H	-0.6261480	-2.0972337	4.5589889
H	-3.6383670	0.0112963	3.8325339
H	-3.6476540	-1.3895357	4.9268629
H	-2.2863440	-0.2463447	4.9656299
H	-3.9888820	-1.5938057	1.8982369
H	-3.8878200	-3.0079377	2.9631599
H	-2.8005670	-2.8738027	1.5690099
H	3.6134550	4.3684153	-0.9070241
H	-0.0679990	6.0118663	0.5744799
H	-0.3709360	4.0413483	2.0117689
H	3.2810320	2.3497273	0.5339999
H	2.0892480	1.3388073	2.5000139
H	0.4768210	1.9374743	2.9570689
H	1.4815470	8.0745623	-1.9383861
H	0.9923470	7.8844343	-0.2342301
H	0.1217660	6.9961793	-1.5200161
P	4.7556950	-3.6058397	-0.5126951

C	5.6001170	-2.6172387	0.7721729
H	4.9509660	-2.5481817	1.6508739
H	6.5636520	-3.0591037	1.0530919
H	5.7520000	-1.6005367	0.3961699
C	6.0035000	-3.7389577	-1.8433661
H	6.9477720	-4.1388007	-1.4546131
H	5.6288310	-4.3965337	-2.6336151
H	6.1788180	-2.7493207	-2.2761931
C	4.7162660	-5.2909647	0.1970909
H	5.7226960	-5.6178927	0.4849429
H	4.0662180	-5.2974987	1.0773779
H	4.3029810	-5.9892617	-0.5369401
C	-5.6742040	-2.0651357	-0.5901901
F	-5.0750970	-0.9710297	-0.1004961
F	-5.8046200	-2.9451987	0.3956749
F	-6.8786620	-1.7236177	-1.0211211
S	-4.6534690	-2.7538787	-1.9482251
O	-4.5637360	-1.5777397	-2.8661811
O	-5.4018500	-3.8853927	-2.4642771
O	-3.3743260	-3.0369847	-1.2660941
C-int1			
C	-1.0237251	-3.4055863	-1.1106368
C	0.1845279	-3.9263923	-0.6477238
C	1.1562189	-3.1044023	-0.0755388
C	0.8433879	-1.7591553	0.0009432
C	-0.3530681	-1.2127323	-0.4609508
C	-1.3062341	-2.0399623	-1.0264308

N	1.6309849	-0.7013083	0.5239112
C	1.0195249	0.4332647	0.4165672
C	-0.3459301	0.2761567	-0.1812578
C	-1.4960881	0.6588247	0.8105582
N	-2.5448691	1.1268397	-0.0559938
C	-2.1077801	1.4500317	-1.3358738
C	-0.6490481	1.1658617	-1.3850298
O	-2.8585521	1.8613497	-2.2044958
C	-1.0065931	1.6809737	1.8424672
O	-0.1113631	1.3455987	2.6123902
N	-1.5986231	2.8875457	1.8036142
C	0.2354999	1.5352627	-2.3372168
Au	2.2253579	0.9211247	-2.3480028
C	-0.1774661	2.3917727	-3.4950638
C	-1.2072871	4.0499387	2.6289562
C	-2.1244311	5.1937467	2.2189052
C	-1.4049901	3.7230687	4.1051202
C	0.2467419	4.4158597	2.3428702
C	-4.9573701	-2.2096903	-1.6156378
C	-4.9088521	-3.1742863	-0.6010528
C	-4.6296951	-2.7879923	0.7093862
C	-4.3747421	-1.4454703	0.9853042
C	-4.3892031	-0.4820853	-0.0178318
C	-4.6987401	-0.8820963	-1.3249448
C	-3.9597521	0.9326697	0.2490592
O	-5.1422851	-4.4494753	-0.9924078
C	-5.0765361	-5.4588443	-0.0140768

H	-1.7655581	-4.0691543	-1.5512388
H	0.3771739	-4.9928123	-0.7331168
H	2.1103009	-3.4743853	0.2924742
H	-2.2534291	-1.6481413	-1.3934458
H	2.6242159	-0.7548153	0.8748472
H	1.4958959	1.3590467	0.7233982
H	-1.8057401	-0.2320533	1.3769542
H	-2.2584571	3.0339227	1.0481232
H	-1.2172841	2.7275197	-3.4536828
H	0.4899599	3.2598547	-3.5720568
H	-0.0334871	1.8282187	-4.4271858
H	-1.9983971	5.4437027	1.1573522
H	-1.8893951	6.0893967	2.8039342
H	-3.1770041	4.9398407	2.3976052
H	-0.7767901	2.8793797	4.4044412
H	-1.1373211	4.5936847	4.7158152
H	-2.4533561	3.4720847	4.3064772
H	0.9171749	3.6022727	2.6354542
H	0.5252859	5.3129447	2.9087512
H	0.3874969	4.6266327	1.2751352
H	-5.1943331	-2.5370063	-2.6248758
H	-4.6011411	-3.5145963	1.5156502
H	-4.1550401	-1.1492753	2.0116882
H	-4.7048191	-0.1355603	-2.1184018
H	-4.5072321	1.6383167	-0.3866008
H	-4.1286791	1.2106607	1.2990332
H	-5.2727841	-6.4022753	-0.5270668

H	-5.8329181	-5.3148423	0.7705492
H	-4.0825421	-5.5044073	0.4545472
P	4.4940779	0.1543147	-2.4769678
C	5.6913879	0.9410747	-1.3522458
H	5.3570809	0.8167707	-0.3181298
H	6.6757419	0.4713847	-1.4579128
H	5.7520189	2.0064267	-1.5987118
C	5.2297759	0.4273747	-4.1321748
H	6.2467309	0.0186017	-4.1694428
H	4.6151209	-0.0603893	-4.8953048
H	5.2644909	1.4998227	-4.3482408
C	4.6495249	-1.6505753	-2.2571458
H	5.7030409	-1.9421453	-2.1820358
H	4.1397159	-1.9844523	-1.3474198
H	4.1810149	-2.1394893	-3.1184208
C	5.3596989	-1.8454483	3.0296562
F	6.0460859	-2.9661303	3.2025642
F	4.2410449	-1.9122693	3.7426512
F	6.0842079	-0.8235783	3.4640002
S	4.9600779	-1.6285153	1.2545762
O	6.2529369	-1.5459213	0.5836482
O	4.1772389	-0.3524363	1.2428372
O	4.1081669	-2.7829823	0.9297782
C-ts2			
C	0.6538583	-3.0287013	2.5428899
C	-0.5012617	-2.7717993	3.2789069
C	-1.3178187	-1.6785873	2.9828069

C	-0.9320757	-0.8765543	1.9235029
C	0.2254223	-1.1113753	1.1840809
C	1.0317503	-2.1919293	1.4897819
N	-1.6030837	0.2342467	1.3679739
C	-0.9013897	0.7685877	0.3820059
C	0.3489803	-0.0543853	0.1127489
N	0.0910543	2.5180687	1.0685609
C	1.4379783	2.0093437	1.1055889
C	1.6501963	0.7626477	0.2625939
O	2.2891933	2.4707837	1.8253779
N	2.0462083	1.0785737	-1.0845131
C	1.4686053	0.2203937	-2.0228991
C	0.3670753	-0.5082143	-1.3502091
O	1.8667983	0.1598897	-3.1737171
C	-0.5451777	-1.3314673	-1.9171691
C	-0.4840487	-1.6845443	-3.3718001
Au	-2.2028067	-2.1130033	-0.9248031
C	6.1603323	0.1797987	0.7244859
C	6.5960423	-0.8508823	-0.1127801
C	5.9754563	-1.0512843	-1.3474011
C	4.9323693	-0.2148523	-1.7340401
C	4.4967383	0.8235797	-0.9126851
C	5.1216093	1.0048747	0.3257359
C	3.3449013	1.6910977	-1.3406071
O	7.6218413	-1.6001763	0.3614109
C	8.1065513	-2.6395353	-0.4514821
C	-0.2325637	3.7751257	0.2761089

C	-1.6894657	4.0901087	0.5900979
C	-0.0439277	3.5452777	-1.2151031
C	0.6698113	4.9100417	0.7488529
H	1.2686363	-3.8895753	2.7922749
H	-0.7695817	-3.4284723	4.1029409
H	-2.2127097	-1.4613613	3.5615239
H	1.9283363	-2.3948043	0.9057479
H	-2.6054567	0.4798797	1.4824959
H	-1.4346007	1.3438197	-0.3712161
H	2.4334623	0.1755647	0.7750799
H	-0.4632667	-2.7771103	-3.4806781
H	0.3660333	-1.2496853	-3.9029541
H	-1.4160607	-1.3617683	-3.8555361
H	6.6578803	0.3106487	1.6820919
H	6.2967853	-1.8460473	-2.0141611
H	4.4403933	-0.3693383	-2.6937421
H	4.7768223	1.7999017	0.9873569
H	3.3811563	2.6633187	-0.8271021
H	3.3707143	1.8759827	-2.4203991
H	8.9245563	-3.1093193	0.0985919
H	8.4910243	-2.2616723	-1.4098481
H	7.3326863	-3.3941613	-0.6540141
H	-1.8370127	4.2559087	1.6657289
H	-2.3676727	3.2971197	0.2553789
H	-1.9808977	5.0110317	0.0724529
H	0.9904923	3.2851317	-1.4654551
H	-0.7051567	2.7678407	-1.6144201

H	-0.2929897	4.4756867	-1.7376721
H	1.7244613	4.7169557	0.5231369
H	0.5801203	5.0690307	1.8306539
H	0.3780803	5.8384187	0.2438529
P	-4.1651877	-3.0324993	0.0836239
C	-4.8163597	-2.1941313	1.5686139
H	-5.7238177	-2.6997013	1.9209339
H	-4.0563147	-2.2306163	2.3569649
H	-5.0373107	-1.1488813	1.3289229
C	-5.6057737	-3.1540213	-1.0287561
H	-5.3374427	-3.7392943	-1.9138121
H	-6.4492897	-3.6315413	-0.5155891
H	-5.8765697	-2.1390863	-1.3353421
C	-3.9120337	-4.7510533	0.6681869
H	-3.1078147	-4.7607303	1.4120889
H	-4.8281287	-5.1557323	1.1155299
H	-3.6081117	-5.3842113	-0.1714451
C	-5.6606937	2.5153777	-0.5251841
F	-5.1114417	3.6420577	-0.0795241
F	-6.7368877	2.2486057	0.2027429
F	-6.0262417	2.6879807	-1.7868321
S	-4.4511187	1.1440397	-0.4039221
O	-3.3128517	1.6187577	-1.2083981
O	-5.1646537	-0.0301723	-0.9115971
O	-4.1680247	1.1006057	1.0573739
H	-0.1493187	2.7361737	2.0390089

C-int2

C	-0.6087146	-3.3489648	-1.9186052
C	0.3995814	-3.1297738	-2.8567562
C	1.0948564	-1.9211138	-2.9040242
C	0.7630404	-0.9418568	-1.9753352
C	-0.2439206	-1.1550088	-1.0346982
C	-0.9405126	-2.3509588	-1.0021992
N	1.3398274	0.3350322	-1.8412662
C	0.7518424	0.9767572	-0.7012772
C	-0.3906016	0.0558172	-0.1531002
N	0.0808124	2.2775982	-1.1832412
C	-1.4051516	1.9744362	-1.2820692
C	-1.7127106	0.8061782	-0.3935642
O	-2.1128546	2.6152032	-1.9957882
N	-2.0825126	1.3333802	0.8950558
C	-1.4203886	0.6705902	1.9487848
C	-0.3432556	-0.1392418	1.3545628
O	-1.7700516	0.8266002	3.1057708
C	0.6015514	-0.8609428	2.0044328
C	0.6738534	-0.9043398	3.4971398
Au	2.1193224	-1.8767498	1.0059258
C	-6.2393596	0.1414102	-0.6576962
C	-6.5551406	-0.8476788	0.2778128
C	-5.8485876	-0.9164098	1.4807998
C	-4.8385526	0.0055022	1.7362388
C	-4.5200016	1.0016832	0.8145688
C	-5.2309236	1.0525442	-0.3880342
C	-3.3881106	1.9494992	1.0971488

O	-7.5563576	-1.6907928	-0.0726392
C	-7.9160586	-2.6991448	0.8391688
C	0.5392414	3.6083022	-0.4829292
C	1.9571634	3.8374362	-0.9838942
C	0.4809954	3.4570662	1.0250468
C	-0.3782826	4.7252572	-0.9502822
H	-1.1382856	-4.2979248	-1.9038632
H	0.6432734	-3.9102148	-3.5749842
H	1.8649774	-1.7412258	-3.6515882
H	-1.7117946	-2.5113868	-0.2493992
H	2.3648994	0.3794082	-1.8052222
H	1.4933474	1.2404202	0.0599848
H	-2.5088816	0.1936222	-0.8480382
H	0.7440034	-1.9437598	3.8423688
H	-0.1542206	-0.4024608	4.0045838
H	1.6198634	-0.4313548	3.7986608
H	-6.8025616	0.1701682	-1.5869412
H	-6.0782276	-1.6758088	2.2224158
H	-4.2810526	-0.0452098	2.6711898
H	-4.9838596	1.8193952	-1.1231652
H	-3.4644626	2.8451292	0.4628538
H	-3.3918476	2.2737082	2.1442068
H	-8.7301486	-3.2607138	0.3764968
H	-8.2679276	-2.2792838	1.7924458
H	-7.0792826	-3.3833868	1.0409248
H	1.9604954	4.0755232	-2.0562772
H	2.6224794	2.9851462	-0.8099152

H	2.3826234	4.6947542	-0.4512792
H	-0.5306946	3.2175292	1.3718818
H	1.1924174	2.7179332	1.4091178
H	0.7616804	4.4247122	1.4560948
H	-1.3902196	4.6342062	-0.5416982
H	-0.4487816	4.7795592	-2.0425002
H	0.0436294	5.6704702	-0.5915132
P	3.8837234	-3.0474078	-0.0960862
C	4.5823134	-2.2502088	-1.5828952
H	5.3910624	-2.8635108	-1.9990062
H	3.7899404	-2.1389988	-2.3317752
H	4.9556194	-1.2583238	-1.3114792
C	5.3460204	-3.3837478	0.9433978
H	5.0479234	-3.9682388	1.8194398
H	6.1079364	-3.9339728	0.3779508
H	5.7446394	-2.4204458	1.2753258
C	3.3922794	-4.7011648	-0.7163072
H	2.5620954	-4.5826268	-1.4227472
H	4.2304234	-5.2028368	-1.2155342
H	3.0453554	-5.3181428	0.1188118
C	5.5385384	2.3260752	0.6407488
F	5.0131604	3.4857132	0.2433278
F	6.5846034	2.0530702	-0.1282582
F	5.9486564	2.4559392	1.8940778
S	4.2841434	0.9931782	0.5166298
O	3.1929864	1.4726262	1.3807018
O	4.9982934	-0.2065128	0.9635208

O	3.9470874	1.0059702	-0.9298222
H	0.3817174	2.3772922	-2.1619212
C-ts3			
C	0.1574378	-2.7710324	2.4636743
C	-0.9131112	-2.2846434	3.2167913
C	-1.4926922	-1.0514234	2.9249053
C	-0.9727162	-0.3382294	1.8557413
C	0.0846088	-0.8135964	1.0884393
C	0.6653438	-2.0357294	1.3944963
N	-1.4216562	0.9357366	1.3986743
C	-0.6571172	1.2492026	0.1656893
C	0.4129248	0.1435136	-0.0257107
N	0.0242308	2.4832736	0.6973413
C	1.4607488	2.2082656	0.7969893
C	1.7539078	0.8663196	0.1650253
O	2.2531328	2.9719536	1.2739973
N	2.2135758	1.1198856	-1.1811127
C	1.6114738	0.2595716	-2.1145537
C	0.4626518	-0.3888894	-1.4476107
O	2.0429438	0.1450946	-3.2488097
C	-0.4544842	-1.2210024	-1.9936977
C	-0.3833402	-1.6322084	-3.4317887
Au	-2.0716002	-2.0041544	-0.9330737
C	6.2185748	0.1284236	0.8285203
C	6.5869658	-1.0035424	0.0960683
C	5.9712048	-1.2686454	-1.1288967
C	4.9997538	-0.3966074	-1.6107547

C	4.6319418	0.7414756	-0.8950897
C	5.2505338	0.9879036	0.3345083
C	3.5530008	1.6474206	-1.4195887
O	7.5466318	-1.7805494	0.6562393
C	7.9648298	-2.9202214	-0.0525887
C	-0.4345872	3.8572596	0.1916253
C	-1.9578272	3.8765736	0.1954153
C	0.1124478	4.0430136	-1.2141577
C	0.0816818	4.9254206	1.1462803
H	0.5951568	-3.7348584	2.7113763
H	-1.2993822	-2.8733434	4.0461183
H	-2.3282512	-0.6584744	3.5005953
H	1.4806538	-2.4196534	0.7832173
H	-2.4602472	1.0003446	1.2965553
H	-1.3014662	1.4195316	-0.7008417
H	2.4941358	0.3112556	0.7652023
H	-0.3523082	-2.7280084	-3.4987527
H	0.4664718	-1.2121544	-3.9763517
H	-1.3164592	-1.3383214	-3.9312507
H	6.7119838	0.3091116	1.7801593
H	6.2424058	-2.1421174	-1.7146047
H	4.5125758	-0.5996044	-2.5640197
H	4.9600218	1.8684566	0.9088913
H	3.6309338	2.6426036	-0.9618177
H	3.6275868	1.7625816	-2.5064057
H	8.7391628	-3.3963934	0.5524063
H	8.3880508	-2.6574014	-1.0328067

H	7.1406518	-3.6325794	-0.2029737
H	-2.3678372	3.6913726	1.1969233
H	-2.4107002	3.1631356	-0.5011787
H	-2.2849402	4.8772716	-0.1077527
H	1.2090098	4.0493086	-1.2248087
H	-0.2400692	3.2576886	-1.8939157
H	-0.2334772	5.0046546	-1.6095207
H	1.1700248	5.0008496	1.1485123
H	-0.2553552	4.7286826	2.1713443
H	-0.3366752	5.8894696	0.8358383
P	-3.8806382	-3.1242224	0.1661523
C	-4.6918762	-2.3962204	1.6304293
H	-5.4476052	-3.0909374	2.0174913
H	-3.9384932	-2.2074084	2.4022873
H	-5.1545762	-1.4469234	1.3479703
C	-5.2714532	-3.5492844	-0.9371217
H	-4.8969742	-4.1155954	-1.7957687
H	-6.0215502	-4.1456624	-0.4035797
H	-5.7157192	-2.6140774	-1.2896167
C	-3.3213512	-4.7541034	0.7973623
H	-2.5347082	-4.5965374	1.5442783
H	-4.1507902	-5.3093134	1.2525753
H	-2.8990632	-5.3406624	-0.0250487
C	-5.6913002	2.1936196	-0.5641737
F	-5.1202832	3.3370096	-0.1844217
F	-6.7496962	1.9756346	0.2042253
F	-6.0886022	2.3160916	-1.8217927

S	-4.4926792	0.8150466	-0.4093667
O	-3.3802062	1.2279866	-1.2817577
O	-5.2487792	-0.3670314	-0.8259177
O	-4.1485142	0.8449196	1.0383993
H	-0.6382112	2.0844276	1.6742653

C-int3

C	0.5421814	-2.6793186	2.1090842
C	-0.4958586	-2.2875796	2.9593762
C	-1.1669466	-1.0851886	2.7512112
C	-0.7550386	-0.3190406	1.6746462
C	0.2509254	-0.6928526	0.8058412
C	0.9224524	-1.8894536	1.0287332
N	-1.3444736	0.9532794	1.2754062
C	-0.6396996	1.3800174	-0.0418198
C	0.4493314	0.2988894	-0.2995408
N	0.0270484	2.6272614	0.1388932
C	1.4051804	2.5045174	0.1429362
C	1.7748274	1.0698614	-0.1943598
O	2.2057104	3.4028954	0.3116802
N	2.3384614	1.0282464	-1.5197948
C	1.6518754	0.2079404	-2.4027328
C	0.4292884	-0.2717876	-1.7099908
O	2.0686384	-0.0455106	-3.5220438
C	-0.5313436	-1.0883556	-2.1963398
C	-0.5176046	-1.5566436	-3.6202618
Au	-2.0795586	-1.8984526	-1.0543328
C	6.2000174	0.3792434	0.8730412

C	6.4928694	-0.9214966	0.4556592
C	5.8819434	-1.4379686	-0.6892358
C	4.9914724	-0.6442046	-1.4064028
C	4.7011824	0.6591094	-1.0077838
C	5.3111424	1.1564084	0.1469562
C	3.6976434	1.4761324	-1.7739318
O	7.3773254	-1.6035516	1.2271672
C	7.7230994	-2.9064946	0.8317582
C	-0.6552926	3.9654224	0.1290502
C	-2.1665166	3.7852034	0.0662742
C	-0.1932116	4.7343534	-1.1052608
C	-0.2901356	4.7137694	1.4089442
H	1.0566444	-3.6191376	2.2937362
H	-0.7818086	-2.9241886	3.7931852
H	-1.9840266	-0.7628036	3.3936952
H	1.7151514	-2.1995426	0.3494762
H	-2.4067346	0.8608254	1.1541162
H	-1.4309966	1.3816404	-0.7991978
H	2.4769934	0.6672554	0.5547982
H	-0.4791096	-2.6543556	-3.6478538
H	0.3111564	-1.1556836	-4.2093588
H	-1.4703826	-1.2867756	-4.0950208
H	6.6861944	0.7535804	1.7704782
H	6.0972874	-2.4458006	-1.0325308
H	4.5124684	-1.0399986	-2.3022448
H	5.0736004	2.1680504	0.4770302
H	3.7800184	2.5378384	-1.5105798

H	3.8389244	1.3703714	-2.8556418
H	8.4461484	-3.2730966	1.5635152
H	8.1858194	-2.9209576	-0.1657358
H	6.8511834	-3.5771796	0.8254052
H	-2.5793406	3.2564304	0.9359102
H	-2.5061476	3.2648204	-0.8354968
H	-2.6273006	4.7791814	0.0641692
H	0.8870004	4.9020034	-1.0872888
H	-0.4535076	4.1833604	-2.0168638
H	-0.6947146	5.7085474	-1.1408088
H	0.7895824	4.8581944	1.4917132
H	-0.6432056	4.1703034	2.2963462
H	-0.7787806	5.6951874	1.4083322
P	-3.7177846	-3.1877026	0.1355772
C	-4.4097876	-2.6261226	1.7308332
H	-5.0862156	-3.3915546	2.1308212
H	-3.5894436	-2.4623526	2.4379692
H	-4.9463386	-1.6859086	1.5811202
C	-5.1862706	-3.6585966	-0.8414108
H	-4.8649946	-4.1371706	-1.7719938
H	-5.8221586	-4.3500016	-0.2752588
H	-5.7410316	-2.7471036	-1.0803078
C	-2.9765336	-4.8038076	0.5905542
H	-2.1237866	-4.6278156	1.2564492
H	-3.7063826	-5.4498186	1.0939522
H	-2.6076206	-5.3048636	-0.3102878
C	-5.7780796	2.0301534	-0.1048798

F	-5.1571566	3.1680494	0.2002872
F	-6.6780906	1.7735674	0.8333502
F	-6.3919906	2.1778114	-1.2677328
S	-4.5638076	0.6595194	-0.2105888
O	-3.6059736	1.0962614	-1.2330048
O	-5.3787246	-0.5171026	-0.5056508
O	-3.9707616	0.6526324	1.1668322
H	-1.1761176	1.6792064	1.9772592
C-ts4			
C	-0.5553459	-1.1271575	3.2460763
C	-1.8016689	-0.5066245	3.2555943
C	-2.2185039	0.3070145	2.1964013
C	-1.3210029	0.4671695	1.1600643
C	-0.0669049	-0.1396275	1.1304563
C	0.3304431	-0.9503335	2.1769463
N	-1.4781179	1.1836155	-0.0718257
C	-0.1334299	1.6138405	-0.4520577
C	0.6177931	0.2810005	-0.1412547
N	0.6195911	2.5935955	0.3036503
C	1.9510761	2.2011505	0.3307723
C	2.0507281	0.7282525	-0.0843037
O	2.9091391	2.8965485	0.6079403
N	2.4770031	0.5563185	-1.4613857
C	1.6493651	-0.2661645	-2.2134367
C	0.4144171	-0.5094915	-1.3991967
O	1.9150771	-0.6744715	-3.3297067
C	-0.8261539	-0.8953885	-1.7887287

C	-1.1341719	-1.2359985	-3.2219657
Au	-2.3050689	-1.9473415	-0.5642497
C	6.4114431	-0.3165125	0.6298753
C	6.7168511	-1.5859945	0.1302943
C	6.0875831	-2.0475695	-1.0274087
C	5.1642801	-1.2313545	-1.6750597
C	4.8618781	0.0396575	-1.1937127
C	5.4931581	0.4852555	-0.0276707
C	3.8316571	0.8881215	-1.8843217
O	7.6324011	-2.2926735	0.8388493
C	7.9831531	-3.5695815	0.3681233
C	0.2317411	4.0343035	0.4084333
C	-1.2859899	4.1570855	0.3446403
C	0.8608241	4.8182845	-0.7401087
C	0.7009961	4.5602605	1.7619113
H	-0.2606659	-1.7515545	4.0860693
H	-2.4677879	-0.6529045	4.1031453
H	-3.1981129	0.7796795	2.1706423
H	1.3054391	-1.4334185	2.1761193
H	-1.5451689	0.1516045	-0.9688337
H	-0.1576369	1.8651005	-1.5233387
H	2.7060351	0.1864445	0.6158883
H	-1.2289289	-2.3223695	-3.3537497
H	-0.3569499	-0.8904125	-3.9120917
H	-2.1048379	-0.8070305	-3.4976297
H	6.9145381	0.0149115	1.5347603
H	6.3098211	-3.0304075	-1.4326397

H	4.6653101	-1.5878095	-2.5762247
H	5.2440081	1.4713345	0.3663063
H	4.0065701	1.9519165	-1.6791267
H	3.8503461	0.7329395	-2.9687357
H	8.7285231	-3.9636795	1.0620713
H	8.4209871	-3.5263345	-0.6396667
H	7.1187781	-4.2493715	0.3487763
H	-1.7806599	3.5794975	1.1359243
H	-1.6994909	3.8596595	-0.6273057
H	-1.5543859	5.2090395	0.4907983
H	1.9527271	4.7743685	-0.6946757
H	0.5292811	4.4262935	-1.7106097
H	0.5543311	5.8695675	-0.6839727
H	1.7877731	4.5133315	1.8567903
H	0.2479821	3.9751745	2.5711503
H	0.3826581	5.6035965	1.8731713
P	-3.9631709	-3.2620865	0.4504303
C	-4.3429339	-2.8353945	2.1801663
H	-5.1278909	-3.4953685	2.5688673
H	-3.4387429	-2.9332155	2.7898583
H	-4.6840259	-1.7951205	2.1971763
C	-5.5628929	-3.1507395	-0.4136517
H	-5.4390259	-3.4520605	-1.4581617
H	-6.3046599	-3.7958105	0.0727213
H	-5.8914249	-2.1070275	-0.3775307
C	-3.6003069	-5.0540595	0.5020673
H	-2.6869379	-5.2275775	1.0793553

H	-4.4310549	-5.6025375	0.9621893
H	-3.4413199	-5.4258955	-0.5149027
C	-6.3810449	1.4313085	-1.0145617
F	-6.1781049	2.2975545	-1.9969727
F	-7.0736079	2.0241875	-0.0524587
F	-7.0888789	0.4075355	-1.4836427
S	-4.7832789	0.8142045	-0.3644977
O	-4.1378189	0.1896925	-1.5308407
O	-5.1854379	-0.1162725	0.7038133
O	-4.0983339	2.0376955	0.1187543
H	-2.3138309	1.7866335	-0.1548237
C-2			
C	0.6764961	-2.6914954	-1.8722822
C	1.3283031	-2.0113574	-2.9429912
C	1.3874201	-0.6308744	-3.0005812
C	0.7532751	0.0984816	-1.9855762
C	0.0523141	-0.5469984	-0.9474382
C	-0.0065899	-1.9159944	-0.8855422
N	0.7367051	1.4505016	-1.8372552
C	0.1813651	1.8018386	-0.5235502
C	-0.4681129	0.4888886	0.0071408
N	-0.8900259	2.7737686	-0.5815722
C	-2.1298119	2.1990096	-0.5417672
C	-1.9816259	0.7481256	-0.0987362
O	-3.2058709	2.7307976	-0.7617162
N	-2.4909149	0.5718106	1.2432398
C	-1.5460249	0.2205126	2.1762828

C	-0.2357069	0.2035266	1.4738098
O	-1.7884419	-0.0311604	3.3470198
C	0.9656141	-0.0191804	2.0221618
C	1.2537761	-0.2741804	3.4591738
Au	2.6189621	-2.7637344	-0.6848002
C	-6.0259549	-1.2597564	-0.9831702
C	-6.0115609	-2.5494314	-0.4452452
C	-5.3185739	-2.8008104	0.7408588
C	-4.6535139	-1.7560954	1.3768298
C	-4.6719409	-0.4644694	0.8577058
C	-5.3608209	-0.2308834	-0.3360462
C	-3.9123139	0.6374956	1.5410308
O	-6.6956279	-3.4886494	-1.1471362
C	-6.7239729	-4.7966284	-0.6363012
C	-0.6630079	4.1971686	-0.9614152
C	0.7932481	4.5699566	-0.6992282
C	-1.5432629	5.0959996	-0.0946802
C	-1.0008059	4.3756346	-2.4395312
H	0.4514661	-3.7528954	-1.9718172
H	1.7953611	-2.6038854	-3.7268152
H	1.9369101	-0.1177514	-3.7851132
H	-0.5399569	-2.4131504	-0.0757712
H	0.9872561	2.1523786	0.1288808
H	-2.5050209	0.0866336	-0.8067182
H	1.6475211	-1.2922254	3.5917178
H	0.3642271	-0.1645474	4.0820028
H	2.0429591	0.4067966	3.8050358

H	-6.5691819	-1.0949724	-1.9102792
H	-5.2964969	-3.7954404	1.1768908
H	-4.1082719	-1.9436774	2.3025578
H	-5.3589829	0.7742066	-0.7587012
H	-4.2936089	1.6182126	1.2313718
H	-3.9851719	0.5577186	2.6317938
H	-7.3212379	-5.3904674	-1.3315182
H	-7.1902769	-4.8362944	0.3589678
H	-5.7158099	-5.2319144	-0.5705522
H	1.5172161	3.9909336	-1.2848442
H	1.0493431	4.4647216	0.3618998
H	0.9302971	5.6228836	-0.9697162
H	-2.6043139	4.9034916	-0.2641622
H	-1.3214569	4.9375396	0.9675898
H	-1.3310549	6.1446976	-0.3349192
H	-2.0479989	4.1165646	-2.6264022
H	-0.3636009	3.7393896	-3.0644122
H	-0.8441729	5.4201636	-2.7359632
P	4.6175811	-2.8078954	0.5175898
C	6.0447181	-2.2105204	-0.4341212
H	6.9494681	-2.2714384	0.1830128
H	6.1727551	-2.8264534	-1.3295152
H	5.8739841	-1.1663594	-0.7311602
C	4.5752051	-1.7799574	2.0171098
H	3.8015521	-2.1501914	2.6976058
H	5.5494491	-1.8064114	2.5195008
H	4.3352461	-0.7536694	1.7224158

C	5.1067331	-4.4651784	1.1093418
H	5.2322861	-5.1391244	0.2564128
H	6.0503101	-4.4065064	1.6649098
H	4.3273591	-4.8712104	1.7614418
C	4.1949331	2.2966296	0.7844468
F	2.9723491	2.6881496	1.1551618
F	4.9456611	3.3693726	0.6084728
F	4.7057921	1.5758036	1.7853678
S	4.1144251	1.2857656	-0.7475082
O	3.2635731	0.1478626	-0.3226582
O	5.5107191	0.9370536	-1.0089182
O	3.4734321	2.1914066	-1.7165542
H	1.6047261	1.9266046	-2.0989632
H	1.8288001	0.0053386	1.3469108
D-1			
C	3.9727988	1.7439792	0.9055141
C	3.4206348	2.2849962	2.0789231
C	2.1836798	1.8699292	2.5444601
C	1.5043618	0.9061862	1.7972311
C	2.0322218	0.3647382	0.5964421
C	3.2957218	0.7924822	0.1620791
N	0.2829288	0.3185462	2.0225561
C	0.0251728	-0.5711178	1.0220841
C	1.0546738	-0.5733138	0.1092781
O	3.1337698	-1.3967608	-2.3664979
C	2.4733418	-1.9004988	-1.4670059
C	1.0614978	-1.4330668	-1.1213799

N	3.0154608	-2.9160508	-0.7306859
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C	-0.9275362	-1.2499828	-2.5703779
C	-1.5902452	-2.1257048	-1.5756529
C	-2.1999662	-2.9136298	-0.8567509
C	-2.7922172	-3.8990388	0.0310661
O	-1.5965642	-0.8707118	-3.5229649
C	2.6874498	-3.6747238	0.4999381
C	3.5473508	-4.9355578	0.4166581
C	3.0762478	-2.8779768	1.7435641
C	1.2236498	-4.1011688	0.5768141
C	0.3170368	3.1194072	-0.7393759
C	1.5041508	3.8372402	-0.9041809
C	2.4382528	3.4184102	-1.8520909
C	2.2209058	2.2521292	-2.5664939
C	1.0590188	1.4999962	-2.3874839
C	0.1004028	1.9710042	-1.4938809
C	0.8898018	0.2077732	-3.1377199
O	1.8392578	4.9376602	-0.1850789
C	1.0559848	5.2381282	0.9426091
H	4.9473428	2.0908582	0.5687341
H	3.9775318	3.0361872	2.6348891
H	1.7564898	2.2703212	3.4619161
H	3.7245288	0.3977262	-0.7571869
H	-0.3513902	0.4377852	2.8082051
H	-0.8885532	-1.1553928	1.0531131
H	0.4955808	-2.3346598	-0.8776699

H	3.9769188	-3.0406278	-1.0323729
H	-3.7800112	-4.2119768	-0.3217769
H	-2.8931952	-3.4670648	1.0331521
H	-2.1441842	-4.7808388	0.0860531
H	3.2840008	-5.5329638	-0.4642799
H	3.4044308	-5.5511508	1.3115621
H	4.6139818	-4.6816098	0.3582311
H	2.4744568	-1.9688308	1.8401121
H	2.9292688	-3.4882148	2.6436391
H	4.1318208	-2.5837098	1.6967331
H	1.1199828	-4.8568278	1.3645161
H	0.8914318	-4.5505038	-0.3686919
H	0.5609518	-3.2715708	0.8478001
H	-0.4228202	3.4238072	-0.0034069
H	3.3554878	3.9919302	-1.9600199
H	2.9854768	1.8906852	-3.2540609
H	-0.8137052	1.3950912	-1.3274709
H	0.1754658	0.3153732	-3.9600069
H	1.8469178	-0.1163608	-3.5486589
H	1.5351998	6.0856852	1.4380051
H	1.0171358	4.3857772	1.6388451
H	0.0300078	5.5256492	0.6681811
Au	-3.2587342	-0.6808218	-0.7557679
P	-4.5640372	1.2267282	-0.5121679
C	-3.5509222	2.7181052	-0.2698639
H	-2.8846462	2.8557432	-1.1287389
H	-4.1984432	3.5965472	-0.1627619

H	-2.9556372	2.5697352	0.6351151
C	-5.7359452	1.1695642	0.8748211
H	-6.2388392	2.1394822	0.9707551
H	-6.4823832	0.3926652	0.6817901
H	-5.2007802	0.9221362	1.7982721
C	-5.5806872	1.5943172	-1.9818339
H	-6.1514122	2.5182672	-1.8299409
H	-4.9303782	1.7052862	-2.8549979
H	-6.2727422	0.7676742	-2.1690699
B	-2.9317282	-0.3175548	2.7188891
F	-1.8883792	-0.3608988	3.6365751
F	-4.1620552	-0.1980938	3.3226691
F	-2.8972252	-1.4971368	1.9224301
F	-2.7164912	0.7806882	1.8554891
D-ts1			
C	0.1034781	-2.9170838	-1.6278015
C	1.2961301	-2.7598938	-2.3488625
C	1.7611731	-1.5043808	-2.7158705
C	0.9819811	-0.4186428	-2.3344005
C	-0.1975849	-0.5500088	-1.5892575
C	-0.6493529	-1.8200178	-1.2309735
N	1.1850881	0.9383542	-2.5757935
C	0.1971801	1.6537472	-2.0262745
C	-0.6351479	0.8077102	-1.2672535
N	-2.1778279	3.2430012	0.5448295
C	-2.2223109	2.6257812	-0.6569305
C	-1.9641359	1.1112932	-0.6338685

O	-2.4003559	3.1801412	-1.7323725
N	-1.9312789	0.5172852	0.6989245
C	-0.7104919	0.2792802	1.2751925
C	0.3755791	0.9148512	0.5002845
O	-0.5507829	-0.3017778	2.3373385
C	1.4954011	1.5132862	0.7287005
C	2.3234111	2.5599472	0.0927475
Au	2.6279401	-0.1185768	1.5644745
C	-4.7307559	-2.8119798	-0.6154905
C	-4.0878079	-3.9188118	-0.0529615
C	-3.1836699	-3.7363608	0.9964605
C	-2.9231499	-2.4507708	1.4616935
C	-3.5458989	-1.3381068	0.8976445
C	-4.4604379	-1.5395028	-0.1406975
C	-3.1584779	0.0443122	1.3404745
O	-4.4106259	-5.1199448	-0.5869125
C	-3.7660719	-6.2614918	-0.0776495
C	-2.1251049	4.7066312	0.7337685
C	-1.9993329	4.9392892	2.2331825
C	-3.4052769	5.3476802	0.2103835
C	-0.8989419	5.2652662	0.0160045
H	-0.2435079	-3.9162578	-1.3704615
H	1.8709131	-3.6396788	-2.6303025
H	2.7058681	-1.3695988	-3.2375175
H	-1.5675559	-1.9548018	-0.6648305
H	2.0824151	1.2941702	-2.9316775
H	0.1358221	2.7306172	-2.1316505

H	-1.9388639	2.6645792	1.3403525
H	-2.7737069	0.6340842	-1.2089075
H	2.7028151	3.2606442	0.8445005
H	1.7486801	3.1300982	-0.6519655
H	3.1904201	2.1070442	-0.4044905
H	-5.4368899	-2.9825198	-1.4238425
H	-2.6800409	-4.5818498	1.4557485
H	-2.1975279	-2.2986698	2.2596845
H	-4.9698859	-0.6833758	-0.5840395
H	-3.9498159	0.7712052	1.1098055
H	-2.9769189	0.0698772	2.4209155
H	-4.1467749	-7.1126958	-0.6454485
H	-3.9888309	-6.4142328	0.9880655
H	-2.6755199	-6.2032098	-0.2078515
H	-1.0814509	4.4844112	2.6295105
H	-2.8591869	4.5199312	2.7706465
H	-1.9590709	6.0133872	2.4444705
H	-3.5243349	5.1584982	-0.8597125
H	-4.2782669	4.9456272	0.7382735
H	-3.3721479	6.4312912	0.3769605
H	-0.9744639	5.1011002	-1.0638015
H	0.0129591	4.7790002	0.3891705
H	-0.8107699	6.3433842	0.1964615
P	4.4023891	-1.6427098	1.4612425
C	4.7393441	-2.7456048	2.8790865
H	5.6105201	-3.3784688	2.6709475
H	4.9326861	-2.1469978	3.7743195

H	3.8677651	-3.3795178	3.0677615
C	4.2362031	-2.7560698	0.0294005
H	4.2125801	-2.1380558	-0.8754795
H	5.0854401	-3.4489308	-0.0104245
H	3.2988311	-3.3166748	0.0996875
C	5.9721021	-0.7676618	1.1648435
H	6.2051681	-0.1238668	2.0186095
H	6.7837991	-1.4909788	1.0198725
H	5.8691771	-0.1470598	0.2655215
B	4.5372721	0.4224272	-2.1991715
F	3.6548471	0.0709332	-1.1423175
F	4.8300301	-0.7254558	-2.9155545
F	3.8440971	1.3458522	-3.0205955
F	5.6608511	1.0062762	-1.6545475
D-int4			
C	2.5593247	2.1858650	-2.4545820
C	3.5919877	1.4652120	-3.0563240
C	3.7754797	0.1060710	-2.8061290
C	2.8702247	-0.4686790	-1.9307980
C	1.8216517	0.2237840	-1.3279270
C	1.6551207	1.5736680	-1.5847560
N	2.8047407	-1.8201050	-1.5021300
C	1.8192177	-2.0025450	-0.6896750
C	1.0675077	-0.7322150	-0.4293650
N	0.3460537	-1.7231400	2.8670910
C	1.3498277	-1.4894200	1.9999450
C	1.1709107	-0.2826590	1.0688090

O	2.3668537	-2.1646590	1.8903630
N	-0.0430413	0.4605680	1.2845150
C	-1.0314093	0.1772380	0.3642940
C	-0.4557873	-0.7487930	-0.6457440
O	-2.1558643	0.6587340	0.4220830
C	-1.1842193	-1.3344000	-1.6160690
C	-0.5810283	-2.1701640	-2.6949220
Au	-3.2425203	-1.0315590	-1.6500140
C	2.3163387	4.2987880	1.1257970
C	1.5344067	5.0319530	0.2282760
C	0.1975277	4.6804380	0.0249470
C	-0.3350843	3.5899160	0.7072510
C	0.4398707	2.8405920	1.5906870
C	1.7702287	3.2177370	1.7967870
C	-0.1253203	1.5909520	2.2044590
O	2.1590637	6.0601850	-0.3916780
C	1.4232607	6.8126140	-1.3247880
C	0.2726807	-2.8837610	3.7796720
C	-1.0438583	-2.7517730	4.5329080
C	1.4415057	-2.8458160	4.7581990
C	0.2838197	-4.1771700	2.9692870
H	2.4531477	3.2484480	-2.6650580
H	4.2739297	1.9729710	-3.7334890
H	4.5695547	-0.4821700	-3.2623740
H	0.8521827	2.1464360	-1.1228370
H	3.4574917	-2.5812780	-1.8494150
H	1.5897467	-2.9821280	-0.2848500

H	-0.4668273	-1.1239710	2.7884420
H	2.0620947	0.3482840	1.1986920
H	-1.0049413	-3.1823680	-2.6778550
H	0.5129427	-2.2570550	-2.6669710
H	-0.8518493	-1.7568810	-3.6748050
H	3.3510997	4.5974510	1.2707290
H	-0.4324003	5.2438910	-0.6570750
H	-1.3700363	3.2960840	0.5338760
H	2.3894637	2.6520480	2.4934700
H	0.4058717	1.3235000	3.1287430
H	-1.1882263	1.7147450	2.4430300
H	2.1033847	7.5702110	-1.7186580
H	0.5628787	7.3127550	-0.8574620
H	1.0624077	6.1885270	-2.1557090
H	-1.8993033	-2.7754310	3.8448280
H	-1.0789853	-1.8165950	5.1063160
H	-1.1567033	-3.5831240	5.2370610
H	2.3955817	-2.9034590	4.2270540
H	1.4206077	-1.9210150	5.3471630
H	1.3735247	-3.6944660	5.4493980
H	1.2261767	-4.2861120	2.4243850
H	-0.5464863	-4.1884580	2.2516830
H	0.1704977	-5.0386640	3.6382470
P	-5.5682033	-0.5712050	-1.5975150
C	-5.9300733	0.6661710	-0.3017770
H	-6.9996133	0.9043630	-0.2590630
H	-5.5963103	0.2777240	0.6656110

H	-5.3541273	1.5740800	-0.5072230
C	-6.3034133	0.1575860	-3.1052190
H	-6.2203343	-0.5515430	-3.9343870
H	-7.3590403	0.4071560	-2.9440960
H	-5.7526933	1.0640960	-3.3744030
C	-6.7000803	-1.9528460	-1.2035780
H	-6.4070113	-2.4016920	-0.2496050
H	-7.7367173	-1.6013710	-1.1368810
H	-6.6263763	-2.7206440	-1.9796810
B	5.5510647	-2.9292390	-2.7392930
F	5.4620137	-2.2557650	-3.9526400
F	5.5800087	-1.9981970	-1.6974410
F	4.2957457	-3.6515170	-2.5579180
F	6.5888647	-3.8067890	-2.6919200

D-int1

C	-1.5182711	-3.4303494	0.8096837
C	-0.5591561	-3.7423434	1.7736347
C	0.4805809	-2.8585863	2.0631697
C	0.4964569	-1.6771204	1.3464907
C	-0.4432501	-1.3462014	0.3736747
C	-1.4706781	-2.2298104	0.0958137
N	1.4317759	-0.6214274	1.4339467
C	1.1511979	0.3276546	0.5998197
C	-0.1131091	0.0358376	-0.1556083
C	-1.2684431	1.0389306	0.1888737
N	-2.0297801	1.1108946	-1.0297193
C	-1.3588671	0.6082356	-2.1398653

C	-0.0238731	0.1518496	-1.6743813
O	-1.8610541	0.5689786	-3.2506363
C	-0.6948581	2.3701246	0.6825087
O	-0.0652161	2.3691596	1.7356237
N	-0.9104781	3.4369266	-0.1061463
C	1.0516969	-0.1692564	-2.4265773
Au	2.8278479	-0.8893214	-1.6184353
C	1.0256869	-0.0425284	-3.9188803
C	-0.3325001	4.7800537	0.1168497
C	-0.8058941	5.6467146	-1.0416353
C	-0.8425781	5.3452037	1.4379667
C	1.1912489	4.6890737	0.1165127
C	-4.9242271	-2.1985374	-1.2225113
C	-5.2547981	-2.4484004	0.1154957
C	-5.0787191	-1.4484334	1.0710977
C	-4.5499351	-0.2183494	0.6821297
C	-4.1902701	0.0334256	-0.6377493
C	-4.3974101	-0.9734774	-1.5908583
C	-3.4778751	1.2973487	-1.0288703
O	-5.7330231	-3.6878824	0.3800647
C	-6.0673421	-3.9913494	1.7126037
H	-2.3229931	-4.1329854	0.6021587
H	-0.6217041	-4.6864644	2.3085717
H	1.2382289	-3.0720824	2.8132907
H	-2.2298381	-2.0023954	-0.6511303
H	2.2711999	-0.6263404	2.0581287
H	1.8066699	1.1879957	0.5074807

H	-1.8703261	0.6368396	1.0175087
H	-1.3780231	3.2521876	-0.9864503
H	0.0974219	0.3776486	-4.3158073
H	1.8793199	0.5601986	-4.2551063
H	1.1750989	-1.0354184	-4.3648933
H	-0.4493271	5.2546416	-2.0031303
H	-0.4162441	6.6642687	-0.9301023
H	-1.9014801	5.7053207	-1.0701043
H	-0.5380011	4.7104747	2.2749147
H	-0.4321921	6.3502056	1.5932317
H	-1.9368271	5.4186277	1.4286597
H	1.5476949	4.0731427	0.9476987
H	1.6252019	5.6907757	0.2201977
H	1.5510089	4.2564436	-0.8257803
H	-5.0885601	-2.9904444	-1.9489973
H	-5.3410371	-1.6129994	2.1117957
H	-4.4142121	0.5601556	1.4337557
H	-4.1120611	-0.7879314	-2.6257613
H	-3.7462011	1.6035306	-2.0464963
H	-3.7200491	2.1225127	-0.3443603
H	-6.4202671	-5.0244333	1.7172627
H	-6.8674041	-3.3387404	2.0900657
H	-5.1961191	-3.9062694	2.3786727
P	4.8769909	-1.7975904	-0.7726003
C	6.2253579	-0.6084354	-0.4846153
H	5.8847729	0.1395526	0.2330037
H	7.1023219	-1.1226204	-0.0745173

H	6.4829979	-0.1320424	-1.4360513
C	5.6213339	-3.0053173	-1.9328863
H	6.5450099	-3.4234284	-1.5145823
H	4.9121539	-3.8164964	-2.1262583
H	5.8480209	-2.5113413	-2.8830673
C	4.6976409	-2.7718394	0.7590017
H	5.6786899	-3.1180694	1.1049227
H	4.2488169	-2.1667144	1.5512837
H	4.0558589	-3.6334883	0.5433727
B	4.4291209	0.2207966	2.6220307
F	3.9247679	0.6235546	1.3547937
F	5.6663909	-0.3617744	2.4563637
F	4.4212779	1.2521426	3.5052077
F	3.5046099	-0.8123934	3.0652357
D-ts2			
C	0.6908555	-2.7336225	2.6229634
C	-0.3869035	-2.3669925	3.4274114
C	-1.2161085	-1.2967805	3.0851024
C	-0.9183025	-0.6288985	1.9108814
C	0.1480565	-0.9869615	1.0916484
C	0.9732215	-2.0376565	1.4446804
N	-1.6179525	0.4325185	1.3001024
C	-1.0290855	0.8143685	0.1779094
C	0.2132655	-0.0346395	-0.0821186
N	-0.0462415	2.6496125	0.4500554
C	1.3120335	2.1815185	0.5538794
C	1.5276705	0.7830065	0.0002134

O	2.1791735	2.8061455	1.1122794
N	2.0605785	0.7944495	-1.3385226
C	1.4641905	-0.1601775	-2.1626146
C	0.2368915	-0.6380355	-1.4838946
O	1.9360685	-0.4698885	-3.2439636
C	-0.7492195	-1.4019965	-2.0086846
C	-0.6590165	-1.9649815	-3.3938676
Au	-2.5520135	-1.7571125	-1.0277256
C	5.8880305	-0.0353365	1.0721344
C	6.1692065	-1.3209675	0.6022374
C	5.5682505	-1.7772015	-0.5731506
C	4.7008995	-0.9400365	-1.2689626
C	4.4219405	0.3488885	-0.8158566
C	5.0213465	0.7858355	0.3693054
C	3.4404835	1.2106665	-1.5626906
O	7.0313725	-2.0477975	1.3545984
C	7.3604925	-3.3408725	0.9121004
C	-0.3721335	3.7036825	-0.5981896
C	-1.8467245	4.0310225	-0.4168636
C	-0.0902865	3.1611375	-1.9901296
C	0.4770595	4.9446075	-0.3434446
H	1.3174185	-3.5720725	2.9156164
H	-0.5854275	-2.9209995	4.3415324
H	-2.0562755	-0.9973895	3.7076864
H	1.8151715	-2.3151365	0.8099064
H	-2.5538105	0.7700845	1.5843604
H	-1.6392845	1.2659505	-0.5957646

H	2.2466535	0.3043515	0.6884874
H	-0.7359195	-3.0594105	-3.3398056
H	0.2566585	-1.6963735	-3.9265186
H	-1.5310785	-1.6434045	-3.9789356
H	6.3636125	0.2918655	1.9931694
H	5.7738265	-2.7718975	-0.9578816
H	4.2304895	-1.2898355	-2.1876706
H	4.7915545	1.7817345	0.7478654
H	3.5456175	2.2653495	-1.2709436
H	3.5911145	1.1382815	-2.6456126
H	8.0659495	-3.7485105	1.6390454
H	7.8378185	-3.3231525	-0.0782556
H	6.4769485	-3.9941655	0.8670904
H	-2.0563885	4.4019005	0.5941344
H	-2.5129225	3.1799445	-0.5895666
H	-2.1296125	4.8224885	-1.1201426
H	0.9731425	2.9356315	-2.1361906
H	-0.6645335	2.2556065	-2.2188476
H	-0.3758625	3.9230435	-2.7237496
H	1.5466975	4.7454255	-0.4692406
H	0.3200335	5.3336645	0.6700974
H	0.1886195	5.7283975	-1.0537286
P	-4.7034545	-2.0808205	-0.0356386
C	-4.8506525	-1.6710765	1.7362074
H	-5.8731785	-1.8626185	2.0832924
H	-4.1489455	-2.2924595	2.3039544
H	-4.6174795	-0.6134325	1.8994304

C	-6.0485705	-1.1541285	-0.8421876
H	-6.0657665	-1.3951475	-1.9096106
H	-7.0121655	-1.4153065	-0.3883356
H	-5.8682215	-0.0844385	-0.7041806
C	-5.2721565	-3.8210855	-0.1059326
H	-4.5652285	-4.4613395	0.4312244
H	-6.2676535	-3.9223755	0.3431154
H	-5.3116535	-4.1514205	-1.1487886
H	-0.2861475	3.0656075	1.3541094
B	-4.6227465	1.9002715	0.8959884
F	-4.5401065	3.2650785	0.8306434
F	-5.9135295	1.4252365	0.8743084
F	-3.9858865	1.4390845	2.1055814
F	-3.8837675	1.3114935	-0.1661436

D-int2

C	0.0061744	-3.2037404	2.0426898
C	-0.9056176	-2.7288274	2.9848668
C	-1.3973286	-1.4245554	2.9282747
C	-0.9587576	-0.6135684	1.8897558
C	-0.0559806	-1.0844774	0.9375177
C	0.4422294	-2.3731304	1.0093918
N	-1.3197106	0.7172346	1.6366678
C	-0.8291166	1.0777856	0.3411948
C	0.2279114	0.0013786	-0.0676662
N	-0.0836906	2.4128546	0.4914338
C	1.3767044	2.0352026	0.7019318
C	1.6086344	0.6580926	0.1440338

O	2.1288194	2.7872436	1.2382928
N	2.1664444	0.8071536	-1.1755022
C	1.4721014	0.0800936	-2.1518082
C	0.2186194	-0.3975974	-1.5354612
O	1.9103134	-0.0470414	-3.2821932
C	-0.8096946	-1.0341204	-2.1430852
C	-0.7738836	-1.3895254	-3.5968222
Au	-2.5627766	-1.5067374	-1.1150082
C	6.0404904	-0.0122794	1.1714048
C	6.3607784	-1.2628054	0.6357978
C	5.7637134	-1.6819084	-0.5558552
C	4.8592774	-0.8434864	-1.1996722
C	4.5412484	0.4100166	-0.6810032
C	5.1381894	0.8105396	0.5174587
C	3.5288504	1.2746236	-1.3772202
O	7.2556724	-1.9936704	1.3427488
C	7.6154394	-3.2577784	0.8423398
C	-0.4121696	3.5494626	-0.5341012
C	-1.8842096	3.8640326	-0.3285062
C	-0.1194196	3.0681686	-1.9406282
C	0.4442054	4.7544966	-0.1798982
H	0.3745144	-4.2239634	2.1112098
H	-1.2388826	-3.3855814	3.7857528
H	-2.1075576	-1.0496714	3.6624658
H	1.1362124	-2.7341624	0.2510808
H	-2.2982046	0.9755606	1.8187358
H	-1.6274696	1.2117766	-0.3953222

H	2.2771354	0.1027116	0.8222008
H	-0.9073166	-2.4743624	-3.7053893
H	0.1425954	-1.0873944	-4.1110843
H	-1.6413566	-0.9435904	-4.1019803
H	6.5154964	0.2858066	2.1025068
H	5.9985844	-2.6492104	-0.9901072
H	4.3903074	-1.1638394	-2.1303032
H	4.8835824	1.7818826	0.9423588
H	3.6111254	2.3178296	-1.0346202
H	3.6712974	1.2638176	-2.4645332
H	8.3390284	-3.6757484	1.5450298
H	8.0823704	-3.1845554	-0.1503452
H	6.7492924	-3.9320654	0.7781718
H	-2.1053586	4.1462696	0.7086157
H	-2.5569706	3.0431966	-0.5900432
H	-2.1458226	4.7195416	-0.9607822
H	0.9479574	2.8688236	-2.0948523
H	-0.6860186	2.1679146	-2.2052532
H	-0.4175746	3.8619186	-2.6340983
H	1.5108434	4.5836406	-0.3535202
H	0.3069154	5.0639926	0.8629967
H	0.1269444	5.5861406	-0.8181232
P	-4.6267766	-2.0177074	-0.0302302
C	-4.7357716	-1.6338244	1.7492768
H	-5.7450466	-1.8512494	2.1193588
H	-4.0038256	-2.2496584	2.2837078
H	-4.5118666	-0.5761124	1.9232478

C	-6.0832386	-1.2087434	-0.7701343
H	-6.1118866	-1.4160744	-1.8442672
H	-7.0011966	-1.5793054	-0.2977852
H	-6.0028436	-0.1316224	-0.5978812
C	-5.0465546	-3.8006834	-0.0887642
H	-4.2564056	-4.3766514	0.4039078
H	-6.0031566	-3.9927914	0.4124127
H	-5.1126286	-4.1286524	-1.1310942
H	-0.3830676	2.7810776	1.4037408
B	-4.5695466	1.8750996	0.9594207
F	-4.5542956	3.2401496	0.7966937
F	-5.8441626	1.3492196	0.9520087
F	-3.9293916	1.5283346	2.1868728
F	-3.8034686	1.2593836	-0.0726272
D-ts3			
C	-0.2009501	-2.7272006	2.4331542
C	-1.1940131	-2.1207076	3.2042203
C	-1.6579071	-0.8422976	2.8996452
C	-1.1106431	-0.2103946	1.7938503
C	-0.1259151	-0.8037496	1.0125943
C	0.3442489	-2.0683356	1.3333012
N	-1.4486931	1.0868864	1.3065772
C	-0.7072611	1.2836914	0.0359402
C	0.2653949	0.0906244	-0.1328248
N	0.0821949	2.4842814	0.4809622
C	1.4956759	2.1097364	0.5489832
C	1.6663849	0.7015414	0.0229142

O	2.3629039	2.8446184	0.9322002
N	2.1700489	0.7997154	-1.3279258
C	1.4894269	-0.0531386	-2.2102018
C	0.2566969	-0.5050146	-1.5302048
O	1.9215109	-0.3049036	-3.3218628
C	-0.7625991	-1.2294636	-2.0469197
C	-0.7278481	-1.7446756	-3.4524528
Au	-2.5139121	-1.6370746	-0.9840118
C	6.0258319	-0.2939096	0.9255902
C	6.2554869	-1.5599226	0.3803062
C	5.6147929	-1.9323546	-0.8036538
C	4.7568909	-1.0338016	-1.4307577
C	4.5275289	0.2352454	-0.9018428
C	5.1690499	0.5893864	0.2889112
C	3.5594929	1.1693384	-1.5736168
O	7.1107389	-2.3530886	1.0715222
C	7.3824219	-3.6321596	0.5553643
C	-0.2963371	3.8653354	-0.0750988
C	-1.8152131	3.9789724	-0.0792208
C	0.2653839	3.9610594	-1.4842508
C	0.2843769	4.9306114	0.8447362
H	0.1469029	-3.7239816	2.6919063
H	-1.6076661	-2.6483606	4.0606213
H	-2.4274801	-0.3552976	3.4948912
H	1.1030089	-2.5407366	0.7111973
H	-2.4674581	1.2844474	1.2474482
H	-1.3654361	1.4646584	-0.8147968

H	2.3439059	0.1302564	0.6792302
H	-0.8380141	-2.8374736	-3.4406438
H	0.1783149	-1.4799716	-4.0038098
H	-1.6069381	-1.3726076	-3.9957298
H	6.5342759	-0.0314566	1.8499042
H	5.7797769	-2.9102626	-1.2464118
H	4.2530819	-1.3185826	-2.3543288
H	4.9833979	1.5729734	0.7211462
H	3.7195969	2.2015054	-1.2346508
H	3.6735879	1.1438354	-2.6629618
H	8.0862829	-4.1031106	1.2446773
H	7.8404849	-3.5797616	-0.4428488
H	6.4740949	-4.2492346	0.4953872
H	-2.2499731	3.8172344	0.9153252
H	-2.3162611	3.3011474	-0.7753458
H	-2.0784981	4.9977914	-0.3826998
H	1.3609219	3.9125844	-1.4899108
H	-0.1238651	3.1617004	-2.1271048
H	-0.0326461	4.9181054	-1.9266188
H	1.3751219	4.9233844	0.8644532
H	-0.0862111	4.8030114	1.8692713
H	-0.0541391	5.9099194	0.4884182
P	-4.5556571	-2.2274636	0.1103492
C	-4.9923721	-1.4128836	1.6844393
H	-5.9789921	-1.7560466	2.0193883
H	-4.2418561	-1.6805206	2.4362642
H	-5.0053471	-0.3276036	1.5471513

C	-6.0481861	-2.0492926	-0.9232478
H	-5.9063161	-2.5860586	-1.8663778
H	-6.9268121	-2.4477696	-0.4015078
H	-6.1890301	-0.9842076	-1.1263108
C	-4.5544641	-4.0014176	0.5727272
H	-3.7239221	-4.1877956	1.2626282
H	-5.4993001	-4.2846946	1.0527502
H	-4.4022011	-4.6150516	-0.3209038
H	-0.5655641	2.1778354	1.5022223
B	-4.5208941	1.8000964	-0.1659928
F	-4.7878551	3.1086274	-0.4610218
F	-5.6129281	0.9661534	-0.3254158
F	-4.0873341	1.7066584	1.2059293
F	-3.4443301	1.3308634	-0.9550158

D-int3

C	0.2751491	-2.1721917	2.7491835
C	-0.7688599	-1.5139197	3.4037555
C	-1.4170610	-0.4319577	2.8132495
C	-0.9679079	-0.0564777	1.5582355
C	0.0577161	-0.6909797	0.8864625
C	0.6990540	-1.7667017	1.4879665
N	-1.5376649	1.0090133	0.7364295
C	-0.7367229	1.0394473	-0.5905335
C	0.3412441	-0.0651177	-0.4439185
N	-0.0625179	2.2726813	-0.7945235
C	1.3059471	2.1699303	-0.6108975
C	1.6716700	0.7013313	-0.4592835

O	2.1041250	3.0844673	-0.6254635
N	2.3608071	0.2295213	-1.6343675
C	1.7405851	-0.8347237	-2.2667715
C	0.4131991	-1.0222407	-1.6212665
O	2.2550161	-1.4557477	-3.1833965
C	-0.5808710	-1.8576977	-1.9865005
C	-0.4550629	-2.7768867	-3.1633375
Au	-2.4049939	-1.9439017	-0.9729525
C	5.9519130	0.4130413	1.2083025
C	6.2814811	-0.9443827	1.2412465
C	5.7926081	-1.8023267	0.2534615
C	4.9858081	-1.2906567	-0.7588915
C	4.6606451	0.0631943	-0.8094705
C	5.1485300	0.9064533	0.1927105
C	3.7492841	0.5824983	-1.8867575
O	7.0770661	-1.3332077	2.2693495
C	7.4536691	-2.6853097	2.3322755
C	-0.7245659	3.5413133	-1.2586755
C	-2.1720989	3.2548213	-1.6407955
C	0.0099521	4.0560773	-2.4945275
C	-0.6739229	4.5651373	-0.1282725
H	0.7641210	-3.0131467	3.2346695
H	-1.0809369	-1.8473537	4.3902085
H	-2.2413899	0.0921973	3.2908125
H	1.5093831	-2.2767157	0.9689405
H	-2.5480080	0.8404063	0.5365175
H	-1.4700339	0.8020543	-1.3675645

H	2.2833051	0.5573033	0.4464635
H	-0.5953349	-3.8159097	-2.8352095
H	0.5058331	-2.6921117	-3.6784385
H	-1.2688650	-2.5826697	-3.8749275
H	6.3423590	1.0568833	1.9923925
H	6.0385241	-2.8603207	0.2587755
H	4.6014780	-1.9543057	-1.5338255
H	4.8839181	1.9639553	0.1709995
H	3.8283420	1.6736533	-1.9672725
H	3.9889661	0.1400173	-2.8602955
H	8.0936401	-2.7902007	3.2108975
H	8.0182181	-2.9935317	1.4403025
H	6.5826170	-3.3475357	2.4446205
H	-2.7751749	2.8696443	-0.8123815
H	-2.2403330	2.5724273	-2.4971405
H	-2.6315400	4.2017333	-1.9443705
H	1.0382951	4.3432263	-2.2655735
H	0.0226021	3.2910963	-3.2805505
H	-0.5195649	4.9339293	-2.8822985
H	0.3554431	4.7188583	0.2096185
H	-1.3026989	4.2575653	0.7151065
H	-1.0633400	5.5246613	-0.4891215
P	-4.5467579	-2.1289857	0.1070605
C	-5.9026020	-1.1442647	-0.6158185
H	-6.8507760	-1.3837827	-0.1196945
H	-5.6752930	-0.0836367	-0.4763165
H	-5.9853530	-1.3609187	-1.6853055

C	-5.1709150	-3.8487107	0.0136755
H	-4.4660489	-4.5220007	0.5117295
H	-6.1530840	-3.9316477	0.4945575
H	-5.2547590	-4.1528147	-1.0345445
C	-4.6185829	-1.7514087	1.8901645
H	-4.4088769	-0.6886317	2.0570625
H	-5.6156409	-1.9847097	2.2833025
H	-3.8692369	-2.3510527	2.4180755
H	-1.5619340	1.9315003	1.1989525
B	-4.2135369	2.1321833	1.6586055
F	-3.9246370	1.3106113	2.7492385
F	-4.1822500	1.2625633	0.4889175
F	-5.4104250	2.7495783	1.7459575
F	-3.1423339	3.0358203	1.4909975
D-ts4			
C	-0.8765524	-0.7836158	3.2613733
C	-2.1018214	-0.1364648	3.1254623
C	-2.4456424	0.5442772	1.9526263
C	-1.4974704	0.5469082	0.9482693
C	-0.2613534	-0.0838738	1.0670783
C	0.0641406	-0.7626168	2.2266063
N	-1.5690374	1.1117512	-0.3671127
C	-0.1964264	1.4431402	-0.7357337
C	0.4995726	0.1553532	-0.2055467
N	0.5487296	2.5169542	-0.1116347
C	1.8549216	2.1028322	0.1055533
C	1.9350746	0.5838002	-0.1246717

O	2.8149636	2.7725312	0.4279433
N	2.4381136	0.2104072	-1.4338777
C	1.6417036	-0.6996248	-2.1096017
C	0.3472846	-0.7942698	-1.3527007
O	1.9632036	-1.2735398	-3.1349887
C	-0.8771594	-1.1999048	-1.7732727
C	-1.0828534	-1.7528258	-3.1605997
Au	-2.5571364	-1.9439148	-0.5647897
C	6.2147286	-0.4939558	0.9828303
C	6.5105336	-1.8209188	0.6568963
C	5.9373786	-2.4031288	-0.4753957
C	5.0797126	-1.6492208	-1.2715797
C	4.7874946	-0.3233308	-0.9629647
C	5.3616356	0.2443432	0.1794773
C	3.8244276	0.4580152	-1.8117297
O	7.3600836	-2.4586118	1.4999853
C	7.6971826	-3.7913868	1.2079503
C	0.0067496	3.9115912	-0.0929987
C	-0.6653474	4.2027902	-1.4343967
C	1.1119936	4.9380842	0.1301783
C	-1.0122004	4.0179182	1.0417773
H	-0.6422314	-1.3021598	4.1877713
H	-2.8092714	-0.1504338	3.9521233
H	-3.4061064	1.0437732	1.8339863
H	1.0258276	-1.2596708	2.3368373
H	-1.6035384	-0.0606528	-1.1611327
H	-0.1636154	1.5332572	-1.8309407

H	2.5343886	0.1333292	0.6818703
H	-1.9973304	-1.3370758	-3.5994947
H	-1.2248514	-2.8412428	-3.1293027
H	-0.2301344	-1.5537698	-3.8182577
H	6.6725946	-0.0682978	1.8721763
H	6.1527746	-3.4323828	-0.7469497
H	4.6238676	-2.0994178	-2.1534397
H	5.1186216	1.2753022	0.4393563
H	4.0158666	1.5349432	-1.7236737
H	3.9028206	0.1735142	-2.8667637
H	8.3866536	-4.1168568	1.9896983
H	8.1956066	-3.8811968	0.2318623
H	6.8140086	-4.4467918	1.2151813
H	-1.5491704	3.5804162	-1.6167347
H	0.0400426	4.0808242	-2.2657317
H	-1.0137024	5.2414802	-1.4378847
H	1.6102786	4.8063662	1.0930913
H	1.8762386	4.8970682	-0.6512347
H	0.6471256	5.9309312	0.1098143
H	-0.5591564	3.7135002	1.9924543
H	-1.9084744	3.4135872	0.8651073
H	-1.3435334	5.0590242	1.1364283
P	-4.6126924	-2.6535438	0.3256983
C	-5.9348344	-2.3732298	-0.8969607
H	-6.9133654	-2.6214418	-0.4690787
H	-5.9030694	-1.3147348	-1.1756087
H	-5.7572074	-2.9839648	-1.7874427

C	-4.7826854	-4.4082238	0.8068193
H	-4.0751264	-4.6411668	1.6082723
H	-5.8026884	-4.6126718	1.1533963
H	-4.5571454	-5.0491148	-0.0510237
C	-5.1645194	-1.7171108	1.7852373
H	-5.2338704	-0.6548228	1.5179053
H	-6.1485434	-2.0811268	2.1052693
H	-4.4448524	-1.8380808	2.6011073
H	-2.3689374	1.7355902	-0.5656357
B	-4.9035474	1.6015782	-0.3260157
F	-5.2869624	1.4510132	1.0100593
F	-4.3454634	0.3705822	-0.7626357
F	-5.9395944	1.9695252	-1.1251087
F	-3.8471254	2.5640862	-0.3808817

D-2

C	0.9269434	-2.6674498	-2.6432602
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C	3.1674404	-2.4820608	-1.6915102
C	2.6614704	-1.5778028	-0.7549942
C	1.3002554	-1.2406478	-0.7507222
C	0.4369344	-1.7560418	-1.7067252
N	3.3178504	-0.9149268	0.2497528
C	2.5142124	0.1417202	0.7705558
C	1.0556844	-0.2958128	0.3954228
N	2.6469364	1.4687052	0.1311508
C	1.4669934	1.9682392	-0.3248962
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O	1.2278864	3.0126322	-0.9125382
N	-0.2789946	1.3860532	1.3194048
C	-0.3963246	0.3706582	2.2213308
C	0.3462554	-0.8023578	1.6226128
O	-1.0315746	0.3977192	3.2643148
C	0.5015384	-2.0480748	2.1808218
C	0.1000504	-2.4608028	3.5582508
Au	-1.5077396	-1.9933628	0.8463958
C	-3.7259666	2.6392782	-1.3253922
C	-4.8146576	2.0421262	-0.6814792
C	-4.6939606	1.6267082	0.6472608
C	-3.4832316	1.8098872	1.3160468
C	-2.3975236	2.4174842	0.6876108
C	-2.5327716	2.8253742	-0.6446022
C	-1.0916246	2.5915922	1.4150968
O	-5.9319276	1.8877002	-1.4351632
C	-7.0730806	1.3486123	-0.8171362
C	3.9875494	2.1391782	0.0158748
C	4.8179674	1.7900692	1.2481708
C	3.8228424	3.6579232	-0.0074852
C	4.6545974	1.6687652	-1.2731492
H	0.2709694	-3.0727668	-3.4102982
H	2.6579394	-3.7213908	-3.3569982
H	4.2301384	-2.7055538	-1.6985892
H	-0.6018746	-1.4223148	-1.7544142
H	2.6751434	0.2494102	1.8535638
H	-0.3883646	0.9327492	-0.7441772

H	-0.3508246	-3.4592978	3.5597328
H	-0.5753586	-1.7374258	4.0192978
H	1.0086184	-2.5307778	4.1713798
H	-3.8481436	2.9550072	-2.3584192
H	-5.5386166	1.1934582	1.1775588
H	-3.3809746	1.4866673	2.3519208
H	-1.6819266	3.2912502	-1.1433832
H	-0.5125006	3.4199733	0.9909948
H	-1.2538956	2.7797872	2.4814308
H	-7.8629366	1.3406543	-1.5706562
H	-7.4001826	1.9555473	0.0385978
H	-6.8999766	0.3168612	-0.4708852
H	5.0460384	0.7276912	1.3588568
H	4.3286014	2.1654912	2.1576028
H	5.7925694	2.2795522	1.1555828
H	3.3181784	4.0131593	-0.9067792
H	3.2584724	4.0104052	0.8649018
H	4.8251224	4.0995022	0.0368428
H	4.0160884	1.9189672	-2.1303632
H	4.8671484	0.5952192	-1.2735242
H	5.6167774	2.1800862	-1.3931652
P	-3.4650336	-2.2889288	-0.4037322
C	-3.5362926	-3.8838938	-1.2798792
H	-4.4174896	-3.9246888	-1.9305802
H	-2.6299066	-3.9949268	-1.8853122
H	-3.5752006	-4.7076978	-0.5610992
C	-5.0188956	-2.1505448	0.5332508

H	-5.0669906	-1.1473748	0.9715208
H	-5.8770696	-2.3024258	-0.1325652
H	-5.0439026	-2.8905308	1.3382128
C	-3.5727846	-1.0239918	-1.7098292
H	-2.8213076	-1.2294758	-2.4796862
H	-4.5690866	-1.0307178	-2.1699332
H	-3.3810726	-0.0310808	-1.2864142
H	4.3026724	-1.0662308	0.4948438
H	1.1269904	-2.7418658	1.6089078
B	6.7041224	-1.1557488	0.0920338
F	7.1104714	0.1626892	-0.0144762
F	7.7503884	-2.0286648	0.2023408
F	5.8525334	-1.2734518	1.2481528
F	5.8826984	-1.4822398	-1.0146262
E-1			
C	-4.2118459	-1.8086415	2.7116655
C	-5.5059079	-1.4531515	2.2915055
C	-5.7232329	-0.8685035	1.0560225
C	-4.6074769	-0.6405725	0.2514645
C	-3.2950119	-0.9773905	0.6562085
C	-3.1065859	-1.5824035	1.9101375
N	-4.5230099	-0.0656375	-0.9993715
C	-3.2123279	-0.0076585	-1.3812475
C	-2.4198399	-0.5596915	-0.4066575
O	0.2134171	-1.7502155	1.3133985
C	-0.3615289	-1.8591175	0.2371815
C	-0.9280959	-0.6060385	-0.4546755

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C	2.3552201	-1.0057165	-1.4295415
C	2.9017351	-2.1842785	-2.0833255
O	1.6113611	1.8143085	0.4373255
C	-1.1896639	-3.6630245	-1.5182545
C	-0.4732169	-4.9831635	-1.7982825
C	-2.6449449	-3.9497785	-1.1557675
C	-1.1118229	-2.7921855	-2.7664535
C	-2.8541349	3.9936035	-0.7537615
C	-4.1117129	3.9670425	-0.1456395
C	-4.3461079	3.0909045	0.9181035
C	-3.3415289	2.2448115	1.3560775
C	-2.0835389	2.2494825	0.7479585
C	-1.8538089	3.1406345	-0.2958185
C	-1.0028439	1.3197285	1.2256845
O	-5.1592169	4.7412385	-0.5140905
C	-4.9550129	5.6871355	-1.5360395
H	-4.0798309	-2.2694695	3.6873775
H	-6.3507399	-1.6420665	2.9488305
H	-6.7225159	-0.5921585	0.7276835
H	-2.1095299	-1.8544245	2.2529745
H	-5.2956019	0.3332005	-1.5093795
H	-2.9219509	0.4534245	-2.3186685
H	-0.6237059	-0.6222825	-1.5093955

H	-0.0939569	-3.7765385	0.2754305
H	3.5292171	-2.7438245	-1.3807105
H	3.5029261	-1.9232805	-2.9597085
H	2.0798301	-2.8384295	-2.3978755
H	0.5783451	-4.8190975	-2.0654495
H	-0.9591559	-5.5081715	-2.6272165
H	-0.5069989	-5.6461045	-0.9241765
H	-3.2058109	-3.0265155	-0.9794215
H	-3.1324229	-4.4992285	-1.9702435
H	-2.7036019	-4.5622755	-0.2482015
H	-1.4735269	-3.3699295	-3.6244495
H	-0.0792819	-2.4862715	-2.9834225
H	-1.7447909	-1.9024525	-2.6915315
H	-2.6433029	4.6762365	-1.5719035
H	-5.3303669	3.0906055	1.3801375
H	-3.5440719	1.5525085	2.1736675
H	-0.8730889	3.1678185	-0.7709975
H	-0.2200239	1.8698795	1.7582335
H	-1.4098179	0.5742995	1.9194305
H	-5.8995519	6.2199805	-1.6598175
H	-4.6886399	5.2069575	-2.4889335
H	-4.1695129	6.4082655	-1.2696775
Au	3.9791581	0.5823505	-0.6382735
P	5.8023861	1.8801425	-0.0155955
C	5.4311231	2.6594015	1.5846385
H	5.2828231	1.8749135	2.3342915
H	6.2472611	3.3236975	1.8913595

H	4.4989121	3.2271545	1.4967945
C	6.1647751	3.2497935	-1.1579285
H	6.9858801	3.8607365	-0.7651065
H	6.4446311	2.8549535	-2.1390065
H	5.2732111	3.8734495	-1.2734255
C	7.3753631	0.9928455	0.1984705
H	8.1432701	1.6747385	0.5816675
H	7.2268811	0.1703045	0.9046265
H	7.7024591	0.5804125	-0.7606215
C	4.8710411	-1.7726365	1.5652655
C	5.2844071	-1.0170445	2.6195905
C	4.0971861	-0.4932115	3.2225835
C	3.0547651	-0.9783285	2.4964115
O	3.5150211	-1.7659925	1.4919175
H	5.3868471	-2.3912895	0.8430745
H	6.3051611	-0.8819815	2.9565245
H	4.0289501	0.1385375	4.0982865
H	1.9766561	-0.8873825	2.5481105
E-ts1			
C	-0.0672112	2.7670137	-3.2816717
C	0.3723208	2.0996947	-4.4360657
C	1.0476708	0.8907757	-4.3581477
C	1.2700088	0.3708097	-3.0859187
C	0.8264288	1.0212007	-1.9158407
C	0.1496408	2.2403197	-2.0183087
N	1.9267748	-0.7872793	-2.6912767
C	1.9162718	-0.8807063	-1.3401437

C	1.2193458	0.1883517	-0.7996157
N	1.5551228	-1.1098283	2.3511123
C	2.1620718	-0.3129623	1.4489323
C	1.2449028	0.6153947	0.6327523
O	3.3604678	-0.3089943	1.2040523
N	-0.1049442	0.7699527	1.1708363
C	-1.1684242	0.1339847	0.6357073
C	-0.8841872	-0.8449003	-0.4312517
O	-2.3307912	0.2771227	1.0133183
C	-1.2429032	-1.8041993	-1.1705737
C	-0.7742592	-2.7617503	-2.1895727
Au	-3.3732942	-1.8284463	-0.6219167
C	0.7534828	5.2265187	0.9732863
C	-0.4096272	5.6721757	0.3354423
C	-1.5561152	4.8714707	0.3470413
C	-1.5222042	3.6344897	0.9839733
C	-0.3648412	3.1756167	1.6117943
C	0.7693348	3.9950167	1.6039883
C	-0.3239762	1.7976407	2.2050553
O	-0.3278202	6.8820367	-0.2529477
C	-1.4716562	7.3861747	-0.9037547
C	2.2444598	-2.1338463	3.1719813
C	1.1679778	-2.7871923	4.0275483
C	3.2895498	-1.4709703	4.0625343
C	2.8853738	-3.1728143	2.2565433
H	-0.5827482	3.7195557	-3.3800027
H	0.1866548	2.5424927	-5.4111607

H	1.3986398	0.3798687	-5.2513577
H	-0.1929002	2.7681447	-1.1289287
H	2.4963718	-1.3906193	-3.2699027
H	2.4386578	-1.6861993	-0.8371307
H	0.5572918	-1.0022473	2.4764433
H	1.7160398	1.6105247	0.6763423
H	-1.2963662	-3.7197183	-2.1234927
H	0.3032298	-2.9302043	-2.0829967
H	-0.9617242	-2.3484853	-3.1881247
H	1.6265878	5.8731707	0.9614163
H	-2.4745922	5.2052007	-0.1264887
H	-2.4120592	3.0055387	0.9872703
H	1.6779388	3.6652107	2.1085573
H	0.4926728	1.7013017	2.9329793
H	-1.2627472	1.5457207	2.7074963
H	-1.1934882	8.3613037	-1.3064517
H	-2.3111832	7.5124537	-0.2063217
H	-1.7861492	6.7330767	-1.7304457
H	0.4011458	-3.2673243	3.4051373
H	0.6827528	-2.0532483	4.6838943
H	1.6133868	-3.5593363	4.6634243
H	4.0541038	-0.9707373	3.4620953
H	2.8209968	-0.7332183	4.7248173
H	3.7765878	-2.2285563	4.6875883
H	3.6569078	-2.7217003	1.6243033
H	2.1268258	-3.6400563	1.6150633
H	3.3525598	-3.9611393	2.8582593

P	-5.6550432	-1.9498283	-0.1365327
C	-6.0743112	-0.7065603	1.1266513
H	-7.1446182	-0.7351123	1.3616893
H	-5.4920092	-0.9005663	2.0327193
H	-5.8023472	0.2875647	0.7584913
C	-6.7605982	-1.6027583	-1.5413387
H	-6.6136922	-2.3532953	-2.3235447
H	-7.8064312	-1.6206233	-1.2132517
H	-6.5277512	-0.6178563	-1.9568527
C	-6.2300912	-3.5399453	0.5393033
H	-5.6621162	-3.7829053	1.4422063
H	-7.2965852	-3.4821193	0.7861913
H	-6.0714832	-4.3347503	-0.1954397
C	5.0423438	-3.5546843	-2.7186787
C	6.1795828	-3.7560093	-2.0108757
C	6.2013338	-2.7483213	-0.9970047
C	5.0788218	-2.0077533	-1.1660537
O	4.3514938	-2.4908193	-2.2191787
H	4.5974858	-4.0515763	-3.5687927
H	6.9180088	-4.5258533	-2.1874017
H	6.9601678	-2.5939923	-0.2424757
H	4.6634958	-1.1548813	-0.6410077
E-int4			
C	0.7797605	3.3367876	-2.7583791
C	1.8206635	2.9954866	-3.6231591
C	2.4325995	1.7452106	-3.5544051
C	1.9495165	0.8803066	-2.5891641

C	0.9077115	1.1962326	-1.7187781
C	0.3090285	2.4418316	-1.7961131
N	2.3676455	-0.4419284	-2.2876001
C	1.6916485	-0.9378514	-1.2924381
C	0.6981805	0.0414556	-0.7643731
N	1.5783185	-1.1027174	2.4957459
C	1.9947025	-0.5511194	1.3539219
C	1.0625485	0.4780736	0.7074709
O	3.0542335	-0.8001384	0.7727129
N	-0.1981585	0.6602046	1.3662889
C	-1.2668315	0.1171136	0.6670069
C	-0.7468745	-0.4635994	-0.5968751
O	-2.4179305	0.1709336	1.0663069
C	-1.5002115	-1.1816944	-1.4536091
C	-0.9851475	-1.6678924	-2.7647541
Au	-3.4788405	-1.6239254	-0.9598151
C	0.6606035	5.0633146	0.8420059
C	-0.5261735	5.4840616	0.2319599
C	-1.6839525	4.7107146	0.3621719
C	-1.6363245	3.5198456	1.0821769
C	-0.4545575	3.0817446	1.6794789
C	0.6889795	3.8786336	1.5583039
C	-0.4022485	1.7362426	2.3440599
O	-0.4520485	6.6411676	-0.4596331
C	-1.6306155	7.1385166	-1.0529181
C	2.2914885	-2.1640754	3.2501999
C	1.4216035	-2.4822694	4.4579879

C	3.6511955	-1.6463884	3.7035029
C	2.4380435	-3.4019094	2.3694179
H	0.3282545	4.3238796	-2.8277521
H	2.1634825	3.7151776	-4.3611711
H	3.2464455	1.4714636	-4.2202011
H	-0.4982645	2.7238646	-1.1206451
H	3.1139705	-0.9791514	-2.7402851
H	1.8339465	-1.9654054	-0.9716921
H	0.6434755	-0.8446654	2.7949899
H	1.6316965	1.4197556	0.6674969
H	-1.0653915	-2.7606204	-2.8255341
H	0.0528765	-1.3865994	-2.9964361
H	-1.6183295	-1.2848964	-3.5751631
H	1.5413845	5.6919836	0.7418849
H	-2.6219705	5.0283466	-0.0833401
H	-2.5338055	2.9088766	1.1729979
H	1.6160315	3.5692076	2.0424489
H	0.4078555	1.6876046	3.0846579
H	-1.3444385	1.5038206	2.8522079
H	-1.3602995	8.0783186	-1.5369291
H	-2.4097245	7.3324986	-0.3033091
H	-2.0260365	6.4455806	-1.8098031
H	0.4338195	-2.8508764	4.1525539
H	1.2881095	-1.5986114	5.0942759
H	1.8956065	-3.2617354	5.0632869
H	4.2809485	-1.3865134	2.8480079
H	3.5359635	-0.7600904	4.3380649

H	4.1617005	-2.4197504	4.2888279
H	3.0544955	-3.1941464	1.4881989
H	1.4551005	-3.7604624	2.0394519
H	2.9180255	-4.2061134	2.9388779
P	-5.7153965	-2.0523454	-0.2983441
C	-6.1074375	-1.1138924	1.2185739
H	-7.1376685	-1.2966804	1.5458119
H	-5.4104115	-1.4049464	2.0107619
H	-5.9644325	-0.0458704	1.0263529
C	-7.0287355	-1.5683174	-1.4719641
H	-6.9311355	-2.1477424	-2.3949161
H	-8.0195565	-1.7441544	-1.0367231
H	-6.9251285	-0.5074864	-1.7192621
C	-6.1296795	-3.7794434	0.1291409
H	-5.4490275	-4.1368014	0.9077729
H	-7.1625515	-3.8507884	0.4898749
H	-6.0095105	-4.4169614	-0.7518811
C	4.6439655	-3.5879364	-3.2269601
C	5.4631395	-4.3838794	-2.5016331
C	5.5357665	-3.8064464	-1.1945751
C	4.7582795	-2.6983454	-1.2156621
O	4.1975025	-2.5484694	-2.4589121
H	4.2906635	-3.6087274	-4.2474531
H	5.9614545	-5.2772634	-2.8514421
H	6.1024175	-4.1726984	-0.3496891
H	4.4939985	-1.9439154	-0.4835451

E-int1

C	0.7812031	-2.3400113	2.6412071
C	-0.2937589	-1.7675283	3.3523701
C	-1.0594389	-0.7200643	2.7932501
C	-0.7026409	-0.2897133	1.5137131
C	0.3696171	-0.8464353	0.7890721
C	1.1235791	-1.8808843	1.3486911
N	-1.2982559	0.7409717	0.7118951
C	-0.5712119	0.9751497	-0.3982579
C	0.4897771	-0.1398703	-0.5624389
N	0.7511841	2.4866807	-0.0707459
C	1.7153871	1.9950037	-1.0288339
C	1.9154511	0.4840607	-0.8185459
O	2.1897021	2.6703347	-1.9458949
N	2.4403751	-0.1940903	-1.9784419
C	1.5167981	-1.0173093	-2.6205199
C	0.2363171	-1.0090633	-1.8267449
O	1.7939351	-1.6686233	-3.6562679
C	-0.9109679	-1.6836013	-2.1375189
C	-1.0445049	-2.4710303	-3.4372649
Au	-2.5942069	-1.9265563	-0.9585609
C	6.5085951	-0.0356163	0.3771011
C	6.6427331	-1.4116023	0.6618241
C	5.8718241	-2.3570883	-0.0508799
C	4.9735951	-1.9134153	-1.0385369
C	4.8251961	-0.5426133	-1.3330879
C	5.6095531	0.3870067	-0.6118869
C	3.8522221	-0.0778163	-2.4071769

O	7.5635111	-1.7305083	1.6551491
C	7.8344461	-3.1344223	1.9464571
C	0.3203231	3.9593877	-0.0607979
C	-0.6896679	4.1195347	1.0988311
C	-0.3458839	4.3226037	-1.4065599
C	1.5656061	4.8441947	0.2025481
H	1.3547091	-3.1433533	3.0946551
H	-0.5327579	-2.1315513	4.3479341
H	-1.8804149	-0.2702093	3.3449861
H	1.9503411	-2.3315753	0.8059741
H	-2.2077379	1.1731437	0.8980471
H	-1.0273039	1.4620917	-1.2503979
H	2.5733901	0.3433247	0.0530541
H	-1.1617449	-3.5407783	-3.2072699
H	-0.1871349	-2.3565803	-4.1023349
H	-1.9617159	-2.1669163	-3.9603589
H	7.1256381	0.6693107	0.9257771
H	5.9773411	-3.4205983	0.1388221
H	4.3978921	-2.6463313	-1.6013219
H	5.5347521	1.4485927	-0.8431969
H	4.0549301	0.9610097	-2.6900569
H	3.9252391	-0.6957073	-3.3086719
H	8.6028921	-3.1224643	2.7210711
H	8.2125191	-3.6569843	1.0576051
H	6.9366211	-3.6430003	2.3243111
H	-0.2641799	3.7951347	2.0592111
H	-1.6159439	3.5648067	0.9146301

H	-0.9516469	5.1783367	1.1987801
H	0.3446621	4.2122097	-2.2457299
H	-1.2410299	3.7163517	-1.5955629
H	-0.6666939	5.3698407	-1.3677319
H	2.3007311	4.7518447	-0.6007769
H	2.0445831	4.5856977	1.1567811
H	1.2560711	5.8943017	0.2612471
P	-4.6449679	-2.5590793	0.2715641
C	-4.9645359	-1.6991853	1.9156751
H	-5.8832619	-2.0810183	2.3747251
H	-4.1223399	-1.8827153	2.5897991
H	-5.0632709	-0.6213463	1.7540751
C	-6.2487309	-2.3093083	-0.6812089
H	-6.1924809	-2.8402853	-1.6362349
H	-7.1004069	-2.6899883	-0.1063989
H	-6.3966519	-1.2435573	-0.8805919
C	-4.6687109	-4.3880423	0.7142491
H	-3.8108769	-4.6228543	1.3514871
H	-5.5945439	-4.6455963	1.2407041
H	-4.5951739	-4.9853153	-0.1996059
H	0.9757941	2.1734747	0.8813451
C	-4.7127269	2.8946677	1.2683271
C	-5.7630699	3.2368367	0.4572741
C	-5.6647669	2.4233337	-0.7418689
C	-4.5605549	1.6233717	-0.6033009
O	-3.9414419	1.8919997	0.6403041
H	-4.3761769	3.2146927	2.2414141

H	-6.5209439	3.9750717	0.6744551
H	-6.3335839	2.4450337	-1.5899109
H	-4.0909759	0.8627997	-1.2089029
E-ts2			
C	1.7733068	-2.2366688	2.1212073
C	0.6821868	-2.0886078	2.9759433
C	-0.3652162	-1.2152278	2.6711273
C	-0.2707242	-0.5178368	1.4794933
C	0.8085088	-0.6615458	0.6130713
C	1.8470348	-1.5209368	0.9246793
N	-1.1711102	0.4259792	0.9215763
C	-0.6566482	0.9866162	-0.1885687
C	0.6146338	0.2328732	-0.5870807
N	0.1653318	2.6662322	0.2327023
C	1.2064798	2.6202902	-0.7825747
C	1.7923668	1.2234482	-0.7830017
O	1.4578728	3.5170072	-1.5330377
N	2.4216018	0.8727222	-2.0097357
C	1.7586488	-0.1388448	-2.6953227
C	0.5213148	-0.4783228	-1.9363127
O	2.2026718	-0.6491428	-3.7056757
C	-0.4474602	-1.3398898	-2.3149537
C	-0.4420652	-1.9831258	-3.6698577
Au	-2.0147322	-2.0056598	-1.1157397
C	5.7355458	-0.0990048	0.8964183
C	5.8735678	-1.4647728	0.6297803
C	5.4022278	-1.9842628	-0.5805697

C	4.7889098	-1.1380838	-1.5002197
C	4.6385718	0.2254072	-1.2427617
C	5.1287358	0.7302552	-0.0335577
C	3.8575218	1.0886892	-2.1947917
O	6.4736388	-2.1948348	1.5945843
C	6.6982168	-3.5642388	1.3482233
C	-0.6677532	3.9138612	0.4261693
C	-1.6439102	3.6175022	1.5573013
C	-1.4303102	4.2312712	-0.8520407
C	0.2538268	5.0605612	0.8285703
H	2.5809258	-2.9126598	2.3899883
H	0.6490998	-2.6510338	3.9053963
H	-1.2046712	-1.0794678	3.3497383
H	2.6988428	-1.6346428	0.2519263
H	-2.1472032	0.5275042	1.1845013
H	-1.3415662	1.3710062	-0.9445387
H	2.5014878	1.1499552	0.0651013
H	0.3387908	-1.6094178	-4.3358997
H	-1.4239502	-1.8633058	-4.1449827
H	-0.3029372	-3.0670548	-3.5537437
H	6.1269248	0.2837682	1.8353603
H	5.5180978	-3.0373588	-0.8195497
H	4.4141998	-1.5437918	-2.4395567
H	5.0451078	1.7980702	0.1744443
H	4.0741598	2.1549422	-2.0531497
H	4.0633488	0.8354312	-3.2397527
H	7.2110478	-3.9569108	2.2277663

H	7.3329288	-3.7175208	0.4648353
H	5.7546498	-4.1116878	1.2090503
H	-1.1262412	3.3022532	2.4734143
H	-2.3772332	2.8514712	1.2804023
H	-2.2033322	4.5295442	1.7919883
H	-0.7622092	4.4378612	-1.6913527
H	-2.1237552	3.4249222	-1.1244937
H	-2.0383902	5.1256962	-0.6758607
H	0.9622708	5.3105012	0.0353633
H	0.8102748	4.8185012	1.7434033
H	-0.3512432	5.9495132	1.0390523
P	-3.8330352	-2.9333588	0.1499253
C	-3.8351782	-2.5135468	1.9295003
H	-4.6625712	-3.0122548	2.4478633
H	-2.8849262	-2.8227178	2.3776543
H	-3.9460522	-1.4286078	2.0383783
C	-5.5075002	-2.4514248	-0.4013717
H	-5.6425232	-2.7222948	-1.4529957
H	-6.2718342	-2.9550618	0.2020483
H	-5.6290302	-1.3671208	-0.3037157
C	-3.8719162	-4.7592868	0.1325953
H	-2.9364522	-5.1497738	0.5448973
H	-4.7151672	-5.1355578	0.7235103
H	-3.9663952	-5.1145638	-0.8981387
H	0.5649868	2.3817522	1.1337113
C	-4.8494322	1.9369602	1.1709963
C	-5.2686952	2.7468402	0.1691303

C	-4.7908692	2.1644402	-1.0470087
C	-4.1116272	1.0442622	-0.6959707
O	-4.1333922	0.8874222	0.6659083
H	-4.9720012	1.9513582	2.2444903
H	-5.8611542	3.6451242	0.2756753
H	-4.9480602	2.5287302	-2.0532737
H	-3.5993932	0.2608812	-1.2477027

E-int2

C	-0.0807733	-2.8388037	2.5078740
C	-1.1190713	-2.2740507	3.2495150
C	-1.5982683	-0.9958427	2.9621930
C	-1.0144043	-0.3093317	1.9062150
C	0.0300697	-0.8584107	1.1679730
C	0.5062137	-2.1275047	1.4625340
N	-1.3487163	0.9948173	1.4518240
C	-0.4341813	1.3394973	0.4009220
C	0.4751587	0.1018243	0.0991700
N	0.4796917	2.4578173	0.9205790
C	1.8943627	1.8623823	1.0329120
C	1.9257857	0.5713093	0.2695890
O	2.7370477	2.4247973	1.6528160
N	2.3788607	0.8632273	-1.0671250
C	1.6111867	0.1886843	-2.0327590
C	0.4013177	-0.3372017	-1.3555380
O	1.9625797	0.1155313	-3.1937290
C	-0.6198483	-1.0226267	-1.9180480
C	-0.6333633	-1.3686737	-3.3758010

Au	-2.2950923	-1.6642097	-0.8532410
C	6.1689567	-0.8680047	0.8394070
C	6.3428037	-2.0131567	0.0542630
C	5.6923427	-2.1135257	-1.1788570
C	4.8812157	-1.0707007	-1.6134770
C	4.7070397	0.0782733	-0.8429090
C	5.3603387	0.1625753	0.3916830
C	3.7911877	1.1705313	-1.3143060
O	7.1527607	-2.9604417	0.5715780
C	7.3982967	-4.1171617	-0.1956140
C	0.3468257	3.8561443	0.2316890
C	-1.1214833	4.2462093	0.3410200
C	0.8060037	3.7455773	-1.2082930
C	1.1991987	4.8466523	1.0100270
H	0.2805667	-3.8330627	2.7554010
H	-1.5501333	-2.8299697	4.0792980
H	-2.3836023	-0.5395027	3.5617030
H	1.3110867	-2.5628197	0.8717130
H	-2.3223823	1.1197043	1.1837800
H	-0.9408643	1.7064983	-0.4938340
H	2.5806737	-0.1453597	0.7932480
H	-0.6762613	-2.4604357	-3.4871580
H	0.2242487	-0.9877677	-3.9354460
H	-1.5605693	-1.0001117	-3.8365890
H	6.6899027	-0.8137917	1.7916830
H	5.8194547	-2.9895567	-1.8077890
H	4.3775087	-1.1453957	-2.5768510

H	5.2345367	1.0548533	1.0064350
H	4.0359897	2.1237203	-0.8232820
H	3.8635357	1.3199943	-2.3972240
H	8.0822807	-4.7354667	0.3880160
H	7.8689917	-3.8713107	-1.1574060
H	6.4747327	-4.6829277	-0.3825530
H	-1.4580433	4.2529803	1.3862950
H	-1.7886113	3.6029853	-0.2420190
H	-1.2329653	5.2648123	-0.0452650
H	1.8643897	3.4718173	-1.2824260
H	0.2236727	3.0239063	-1.7922370
H	0.6805577	4.7259433	-1.6802580
H	2.2690527	4.6444483	0.9276250
H	0.9313847	4.8693043	2.0735490
H	1.0114897	5.8451153	0.6011530
P	-4.2678783	-2.4178057	0.2687290
C	-5.0098783	-1.2035197	1.4166260
H	-5.9079703	-1.6167797	1.8911060
H	-4.2798213	-0.9496847	2.1930580
H	-5.2780923	-0.2928057	0.8672260
C	-5.6552983	-2.8490737	-0.8383140
H	-5.3459043	-3.6369307	-1.5317230
H	-6.5225183	-3.1928997	-0.2624590
H	-5.9344613	-1.9650867	-1.4210400
C	-4.0341123	-3.9055497	1.3022980
H	-3.2616283	-3.7006267	2.0520090
H	-4.9683473	-4.1872697	1.8021940

H	-3.6928493	-4.7363947	0.6770870
H	0.1778627	2.6080683	1.8938020
C	-4.6112943	2.3661823	0.1127850
C	-5.7707063	2.0480363	-0.5141070
C	-5.4059013	1.2667263	-1.6562140
C	-4.0524263	1.1691943	-1.6371610
O	-3.5478483	1.8344693	-0.5592020
H	-4.3691173	2.9470043	0.9931630
H	-6.7665283	2.3426133	-0.2124240
H	-6.0677723	0.8560803	-2.4068140
H	-3.3221753	0.7012433	-2.2842720

E-ts3

C	0.0201438	-2.6839843	2.5376339
C	-0.9764202	-2.0588783	3.2906509
C	-1.4516812	-0.7960983	2.9406999
C	-0.9021662	-0.2004923	1.8159659
C	0.0919388	-0.8043683	1.0581959
C	0.5662548	-2.0582543	1.4199669
N	-1.2346992	1.0994087	1.2900459
C	-0.4100612	1.2951357	0.0575149
C	0.5243078	0.0697167	-0.0861971
N	0.3777258	2.4555847	0.5641339
C	1.7834458	2.0296007	0.6899209
C	1.9360208	0.6447527	0.0998429
O	2.6419088	2.7217767	1.1523009
N	2.4397888	0.7939917	-1.2453481
C	1.7593068	-0.0234203	-2.1567171

C	0.5248808	-0.5095223	-1.4883011
O	2.1724168	-0.2336873	-3.2803101
C	-0.4691672	-1.2527743	-2.0211401
C	-0.4198042	-1.7539353	-3.4311791
Au	-2.1693022	-1.7973603	-0.9431111
C	6.2115178	-0.5578473	0.9756329
C	6.4646268	-1.7683423	0.3213789
C	5.8704608	-2.0245683	-0.9172681
C	5.0360728	-1.0691803	-1.4884881
C	4.7838738	0.1442337	-0.8495771
C	5.3807058	0.3842437	0.3929979
C	3.8468468	1.1424417	-1.4671031
O	7.2911748	-2.6208273	0.9651319
C	7.6185708	-3.8350653	0.3300519
C	0.0919658	3.8528647	-0.0061441
C	-1.4189192	4.0551177	-0.0318001
C	0.6818568	3.9232047	-1.4052611
C	0.7068838	4.8938857	0.9197599
H	0.3790748	-3.6658913	2.8339199
H	-1.3773012	-2.5550093	4.1710609
H	-2.2085152	-0.2914113	3.5377839
H	1.3384428	-2.5416983	0.8240289
H	-2.2374342	1.2627117	1.1418849
H	-1.0034772	1.5082267	-0.8336531
H	2.6017968	0.0324657	0.7305219
H	-0.4605652	-2.8514663	-3.4289561
H	0.4680448	-1.4329353	-3.9815321

H	-1.3199302	-1.4332943	-3.9722331
H	6.6901418	-0.3825213	1.9355709
H	6.0595378	-2.9541483	-1.4458401
H	4.5749898	-1.2643613	-2.4564211
H	5.1899448	1.3284247	0.9044779
H	4.0261838	2.1481497	-1.0646821
H	3.9628388	1.1839917	-2.5553381
H	8.3053418	-4.3581453	0.9977099
H	8.1160328	-3.6654273	-0.6348451
H	6.7296158	-4.4613163	0.1687119
H	-1.8545942	3.9844337	0.9738139
H	-1.9498322	3.3648517	-0.6967081
H	-1.6206002	5.0664377	-0.3996241
H	1.7707198	3.7993927	-1.3897581
H	0.2574758	3.1625597	-2.0727551
H	0.4649038	4.9049547	-1.8402751
H	1.7964208	4.8549607	0.9324559
H	0.3439088	4.7711147	1.9471519
H	0.4000718	5.8859657	0.5707449
P	-4.1301642	-2.5322423	0.2320929
C	-4.8968852	-1.3445743	1.3933559
H	-5.7033052	-1.8287333	1.9567859
H	-4.1402732	-0.9743343	2.0942649
H	-5.3100272	-0.4978873	0.8337169
C	-5.5277442	-3.0223633	-0.8366981
H	-5.2080502	-3.8050243	-1.5312631
H	-6.3674512	-3.3912963	-0.2361411

H	-5.8543972	-2.1546583	-1.4194741
C	-3.8132422	-4.0022213	1.2702299
H	-3.0450782	-3.7560113	2.0118169
H	-4.7266442	-4.3276783	1.7818119
H	-3.4368242	-4.8184743	0.6459199
H	-0.3972092	2.1335547	1.5583819
C	-5.0187782	2.2542027	0.5896949
C	-6.0505452	2.1204867	-0.2778641
C	-5.5453382	1.3831347	-1.3947831
C	-4.2423682	1.1225017	-1.1258251
O	-3.9000582	1.6468297	0.0912529
H	-4.9093372	2.7323547	1.5526209
H	-7.0520382	2.5066477	-0.1475731
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H	-3.4547742	0.5969677	-1.6538991

E-int3

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C	-0.9493100	-1.9665140	3.3255007
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C	-0.9119600	-0.1621180	1.7991727
C	0.1198890	-0.7253720	1.0744877
C	0.6281420	-1.9553620	1.4787917
N	-1.3393910	1.0994920	1.1833037
C	-0.2798340	1.4293840	0.0768777
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N	0.5784940	2.4609270	0.5293147
C	1.9154810	2.0362600	0.5640347

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O	2.8657480	2.7194410	0.8614177
N	2.4521860	0.6783810	-1.3350943
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O	2.0006170	-0.3143170	-3.3533083
C	-0.5889770	-1.2174330	-1.9332793
C	-0.6268020	-1.7342600	-3.3408423
Au	-2.2600970	-1.7561090	-0.8065963
C	6.2766320	-0.6538140	0.7860617
C	6.4718100	-1.9018630	0.1853887
C	5.8203830	-2.2040150	-1.0131293
C	4.9866480	-1.2554160	-1.5975263
C	4.7913750	-0.0054530	-1.0124213
C	5.4456110	0.2805240	0.1907887
C	3.8512470	0.9847370	-1.6399823
O	7.3033200	-2.7442450	0.8388797
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H	-0.8654040	1.6747240	-0.8170253
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H	0.2427000	-1.4449610	-3.9359253
H	-1.5400770	-1.3821600	-3.8409753
H	6.7994570	-0.4435290	1.7155367
H	5.9647110	-3.1632810	-1.5014033
H	4.4830010	-1.4867420	-2.5359833
H	5.2962730	1.2528680	0.6607317
H	4.0678930	2.0037920	-1.2969403
H	3.9173840	0.9645910	-2.7329963
H	8.2771380	-4.5029570	0.9150857
H	8.0387860	-3.8829190	-0.7401243
H	6.6677210	-4.6051200	0.1533067
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H	-1.4852740	5.1705600	0.1781137
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H	-4.3553030	-0.8003860	2.1208857

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H	-5.2345990	-3.8537220	-1.3709353
H	-6.4611330	-3.3391560	-0.1782973
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C	-3.9996730	-3.8482790	1.5052327
H	-3.2625350	-3.5615440	2.2630917
H	-4.9411090	-4.1235060	1.9949947
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C	-4.0797560	1.0345210	-1.6262383
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H	-3.2886240	0.5303090	-2.1671323
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C	-2.1206308	-0.4350338	3.1628866
C	-2.4131238	0.4675202	2.1337026
C	-1.4672388	0.5914822	1.1379496
C	-0.2802768	-0.1363478	1.1074326
C	-0.0031568	-1.0333508	2.1232516
N	-1.5066368	1.3802572	-0.0619494

C	-0.0943058	1.6980802	-0.3759854
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C	-1.2790928	-0.9173978	-3.3391854
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C	5.6634062	-2.6122338	-0.9675374
C	4.8782122	-1.6524278	-1.5987644
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C	5.3274092	-0.0899838	0.1707246
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O	7.0699542	-3.1529518	0.9417756
C	7.3225172	-4.4246918	0.3915296
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H	2.5360112	-0.0948068	0.6815936
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H	-0.5317618	-0.4504318	-3.9898824
H	-2.2822148	-0.5713998	-3.6154204
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H	4.3969062	-1.8912568	-2.5471854
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H	7.9874792	-4.9373318	1.0887706
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H	2.0524592	4.3150962	2.0722556
H	0.4439832	3.9440372	2.7355886
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H	-5.2456428	-4.0671908	-1.3737624
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C	-4.6200918	0.9552802	-1.6351854
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H	-3.2779918	1.9108512	-3.1626364
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C	2.0825651	-3.5191024	-2.1094418
C	2.8936401	-2.9643364	-1.1218748

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N	2.9451301	-1.2874024	0.7395882
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N	2.4646591	1.1183556	0.3730382
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N	-0.5409419	1.3244596	1.2582382
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O	-1.5223699	0.5283736	3.1899542
C	-0.2098739	-2.1203514	2.3437642
C	-0.8094949	-2.4271244	3.6752582
Au	-2.1040379	-1.8787274	0.8359822
C	-3.5907719	2.7433086	-1.7628838
C	-4.8040579	2.3358416	-1.1955258
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C	-3.7044149	2.1015106	0.9394922
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C	-2.4533319	2.8363646	-0.9769968
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O	-5.8531179	2.2582106	-2.0446918
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H	-1.4335659	-1.6104734	4.0430292
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H	-7.1147739	0.9191466	-1.0690368
H	5.1639321	0.4773376	0.7697772
H	4.3448541	0.6197946	2.3592842
H	5.4776891	1.8528976	1.8210362
H	2.2953161	3.6574856	1.3519422
H	2.5924921	2.5025956	2.6778732
H	3.8539581	3.6503106	2.1935752

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H	4.5743471	1.9556726	-1.1187138
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C	-4.2916659	-3.7185334	-1.1841228
H	-5.1616839	-3.7141164	-1.8509838
H	-3.4031919	-4.0182544	-1.7497268
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H	-5.4898039	-0.5825544	0.7218272
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H	-3.1595909	-1.3143754	-2.6137658
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H	0.3772591	-2.9112034	1.8645682
C	5.4948821	-0.7363464	-1.6011158
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