

Supporting Information

A Quantum Chemical Study: Thoughtful Exploration for Optimal Donors in Y-Type Dual Donor-Based Dye Sensitizers

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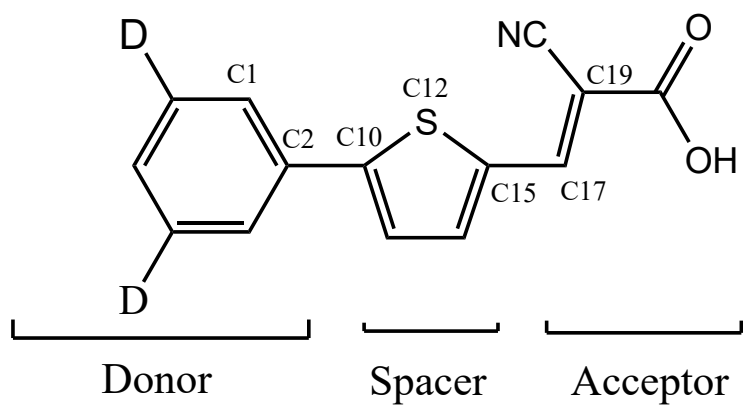


Figure S1. Schematic diagram showing the donor, spacer and acceptor for the dye sensitizer. Here D is the different Donor groups. The numbering given here are followed in the tables below.

Table S1. The specific distances for the dye sensitizers.

Name	Distances	
	C2-C10	C15-C17
P-1	1.46577	1.42632
NS-1	1.46711	1.42507
NS-2	1.46664	1.42613
NS-3	1.46643	1.42566
NS-4	1.4667	1.42636
NS-5	1.46746	1.42672
NS-6	1.46694	1.42671
NS-7	1.46764	1.42938
NS-8	1.46657	1.42596
NS-9	1.46746	1.42842
B-1	1.46725	1.42727
B-2	1.4669	1.42671
B-3	1.4667	1.42638
B-4	1.46694	1.42799
B-5	1.46675	1.42657
B-6	1.46695	1.42662
B-7	1.46736	1.42833
B-8	1.46713	1.42723
B-9	1.46752	1.4273
B-10	1.46736	1.42711
Cb-1	1.46901	1.42647
Cb-2	1.46718	1.42754
Cb-3	1.46806	1.42925
Cb-4	1.4664	1.42626
Cb-5	1.46703	1.42782
Cb-6	1.46737	1.42811
Cb-7	1.46645	1.42577
Cb-8	1.46641	1.42624
H-1	1.46686	1.42691
H-2	1.46787	1.4274
H-3	1.46731	1.42865
H-4	1.46654	1.42594
H-5	1.46748	1.42672
H-6	1.46735	1.42654
H-7	1.46724	1.42638

Table S2. The specific dihedral angles for the dye sensitizers.

Name	C1-C2-C10-C12	C12-C15-C17-C19	C1-C2-C17-C19	C2-C10-C15-C17
P-1	24.27219	-1.23291	20.69062	-0.60706
NS-1	28.6437	-1.28289	24.47771	-1.5986
NS-2	-24.49473	1.20574	-20.90938	0.61238
NS-3	26.30207	-0.46746	23.2184	-0.58331
NS-4	-27.18896	0.85957	-23.4923	1.18566
NS-5	26.28195	-0.63496	23.0819	-0.18054
NS-6	-26.75339	0.56723	-23.29908	1.46911
NS-7	-27.23688	0.6378	-23.7256	1.15833
NS-8	-28.11322	0.65576	-24.48738	1.14583
NS-9	27.37281	-0.82507	23.65676	-1.37536
B-1	-23.85801	1.27385	-20.27334	0.66788
B-2	-28.06644	0.78544	-24.34887	0.99123
B-3	-25.83252	1.238	-21.8973	1.45511
B-4	-27.8682	0.76014	-24.20712	0.99393
B-5	-25.33603	0.82477	-21.88474	0.97683
B-6	-25.66449	1.13928	-22.00349	0.60051
B-7	-27.40879	0.77494	-23.74497	1.26117
B-8	26.97737	-0.87269	23.24919	-1.37639
B-9	26.81716	-0.75017	23.3478	-0.70865
B-10	-26.93588	0.4671	-23.58134	1.31616
Cb-1	-26.97938	1.10964	-23.03983	1.35712
Cb-2	-27.49714	0.65049	-23.90124	1.38953
Cb-3	27.24447	-0.66711	23.69699	-1.24582
Cb-4	-27.64838	0.80184	-23.94348	1.14925
Cb-5	23.87901	-1.41186	20.16894	-0.60475
Cb-6	25.69295	-0.23795	22.78603	-0.82847
Cb-7	-26.32345	0.98324	-22.74414	0.56002
Cb-8	-26.54804	0.80437	-23.2251	0.3482
H-1	-27.33912	0.89178	-23.57854	1.25017
H-2	-26.69869	1.26526	-22.86979	0.46485
H-3	-23.25615	1.7106	-19.35649	0.47072
H-4	-28.63529	1.03486	-24.61375	1.37303
H-5	-28.63529	1.03486	-24.61375	1.37303
H-6	-22.30825	0.93969	-19.11054	0.84471
H-7	-21.20161	1.46498	-17.58318	1.23926

Table S3. ESP charges of the different donor groups.

System	ESP charges	Systems	ESP charges
P-1	0.1424	B-9	0.1060
NS-1	0.0869	B-10	0.1218
NS-2	0.1267	Cb-1	0.0973
NS-3	0.1337	Cb-2	0.1091
NS-4	0.1386	Cb-3	0.0575
NS-5	0.0986	Cb-4	0.1267
NS-6	0.1287	Cb-5	0.1194
NS-7	0.0735	Cb-6	0.1146
NS-8	0.1266	Cb-7	0.1271
NS-9	0.1218	Cb-8	0.1322
B-1	0.1144	H-1	0.1101
B-2	0.1115	H-2	0.1031
B-3	0.1199	H-3	0.1128
B-4	0.0850	H-4	0.1762
B-5	0.1253	H-5	0.1166
B-6	0.1252	H-6	0.1453
B-7	0.1079	H-7	0.1403
B-8	0.0976		

Table S4. The electrostatic charges of spacers and acceptors for the dual donor-based dyes.

System	Spacer	Acceptor
P-1	0.04213	-0.184516
NS-1	0.095541	-0.182447
NS-2	0.050178	-0.176879
NS-3	0.043273	-0.177031
NS-4	0.035606	-0.17427
NS-5	0.073377	-0.172
NS-6	0.050465	-0.17916
NS-7	0.082537	-0.15611
NS-8	0.067477	-0.19408
NS-9	0.046514	-0.16831
B-1	0.054933	-0.16937
B-2	0.064513	-0.176042
B-3	0.058458	-0.178391
B-4	0.072205	-0.157192
B-5	0.050281	-0.175565
B-6	0.057113	-0.182361
B-7	0.060469	-0.168345
B-8	0.066938	-0.164513
B-9	0.057643	-0.163661
B-10	0.05579	-0.17919
Cb-1	0.077017	-0.174324
Cb-2	0.061685	-0.170845
Cb-3	0.086966	-0.144497
Cb-4	0.054667	-0.181402
Cb-5	0.054033	-0.173434
Cb-6	0.060004	-0.174621
Cb-7	0.060371	-0.18745
Cb-8	0.050712	-0.18295
H-1	0.054322	-0.16442
H-2	0.057552	-0.16071
H-3	0.045491	-0.15833
H-4	0.062247	-0.23843
H-5	0.062527	-0.17918
H-6	0.036671	-0.18198
H-7	0.03682	-0.17715

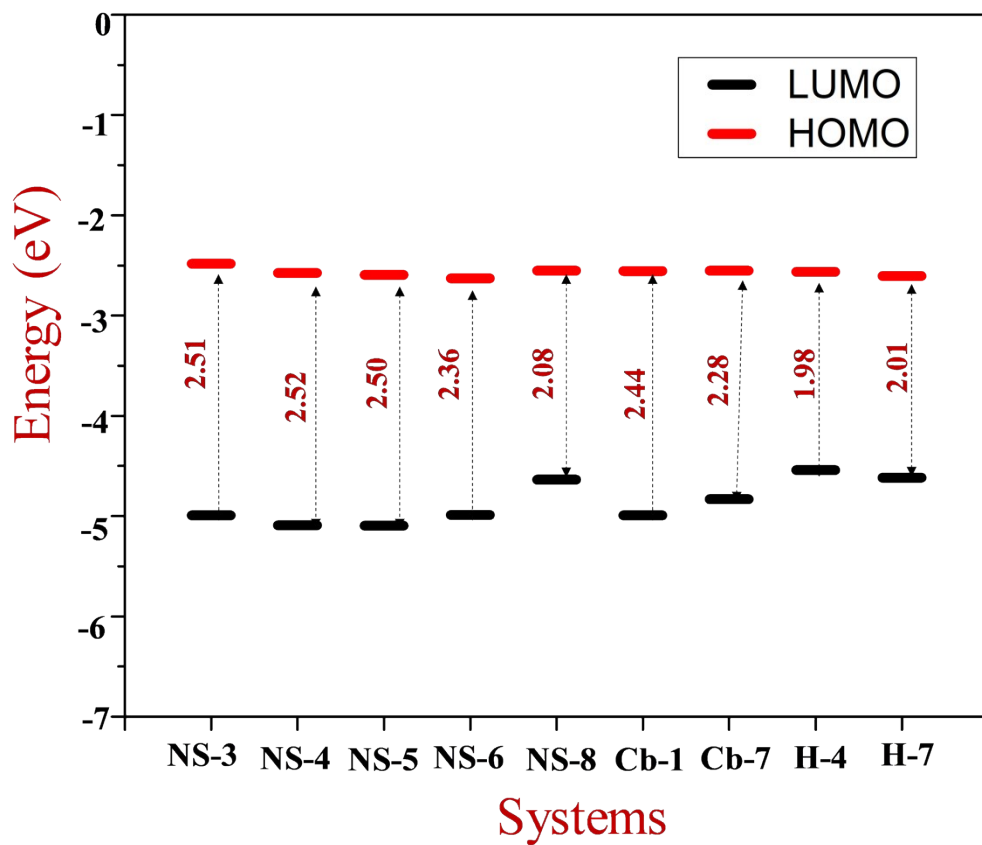
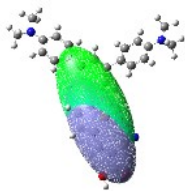
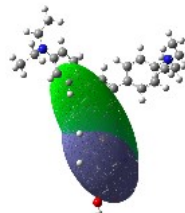
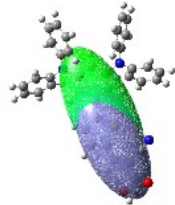
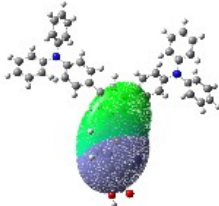
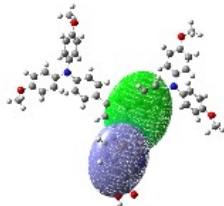
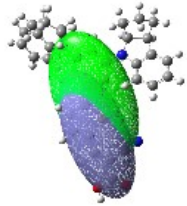
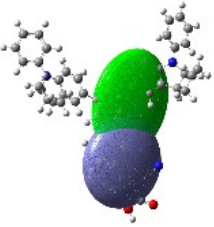
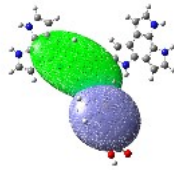
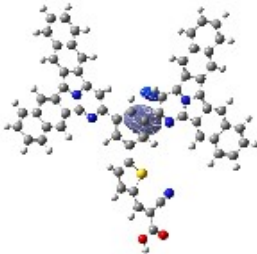


Figure S2. HOMO and LUMO energies and the H-L gap for the selected double donor-based dyes in eV are given here.

Table S5. The Calculated charge transfer length (DCT) and the descriptor for the charge-transfer possibility (Δr) are given here for the efficient dyes.

Systems	D_{CT} in Å	Δr	Centroids
NS-3	3.12	5.91	
NS-4	4.70	8.88	
NS-5	3.85	7.28	
NS-6	2.72	5.14	
NS-8	5.91	11.17	

Cb-1	3.67	6.94	
Cb-7	5.88	11.11	
H-4	5.16	9.78	
H-7	4.34	8.20	

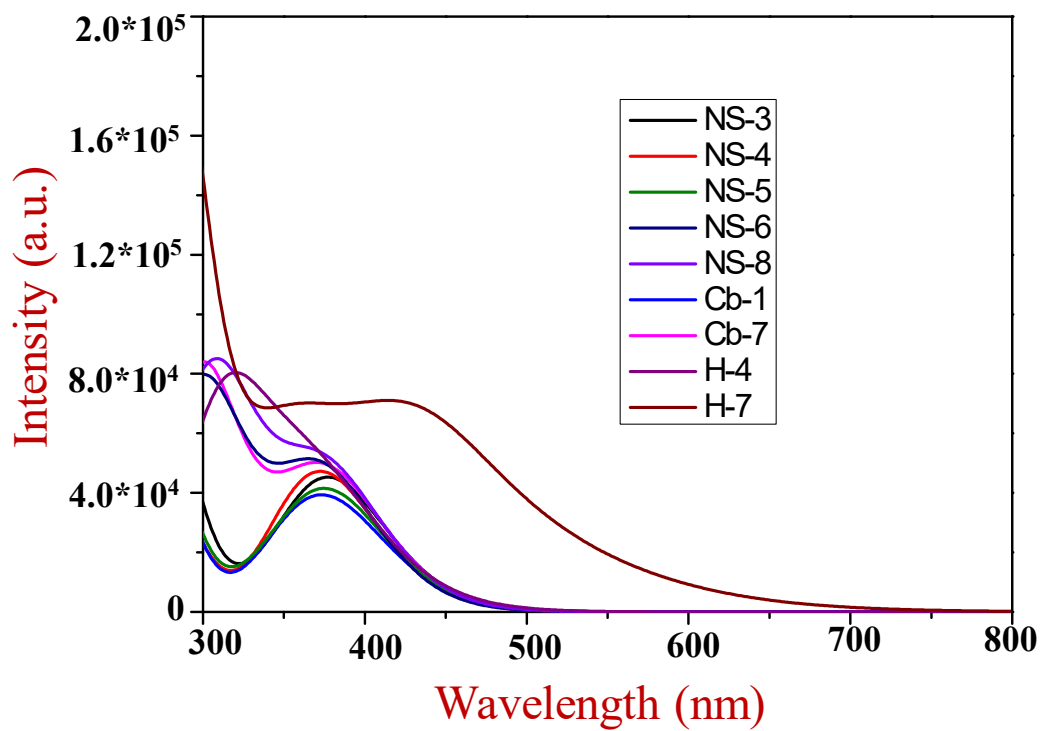


Figure S3. Absorption spectra of the free dyes in DCM solvent.

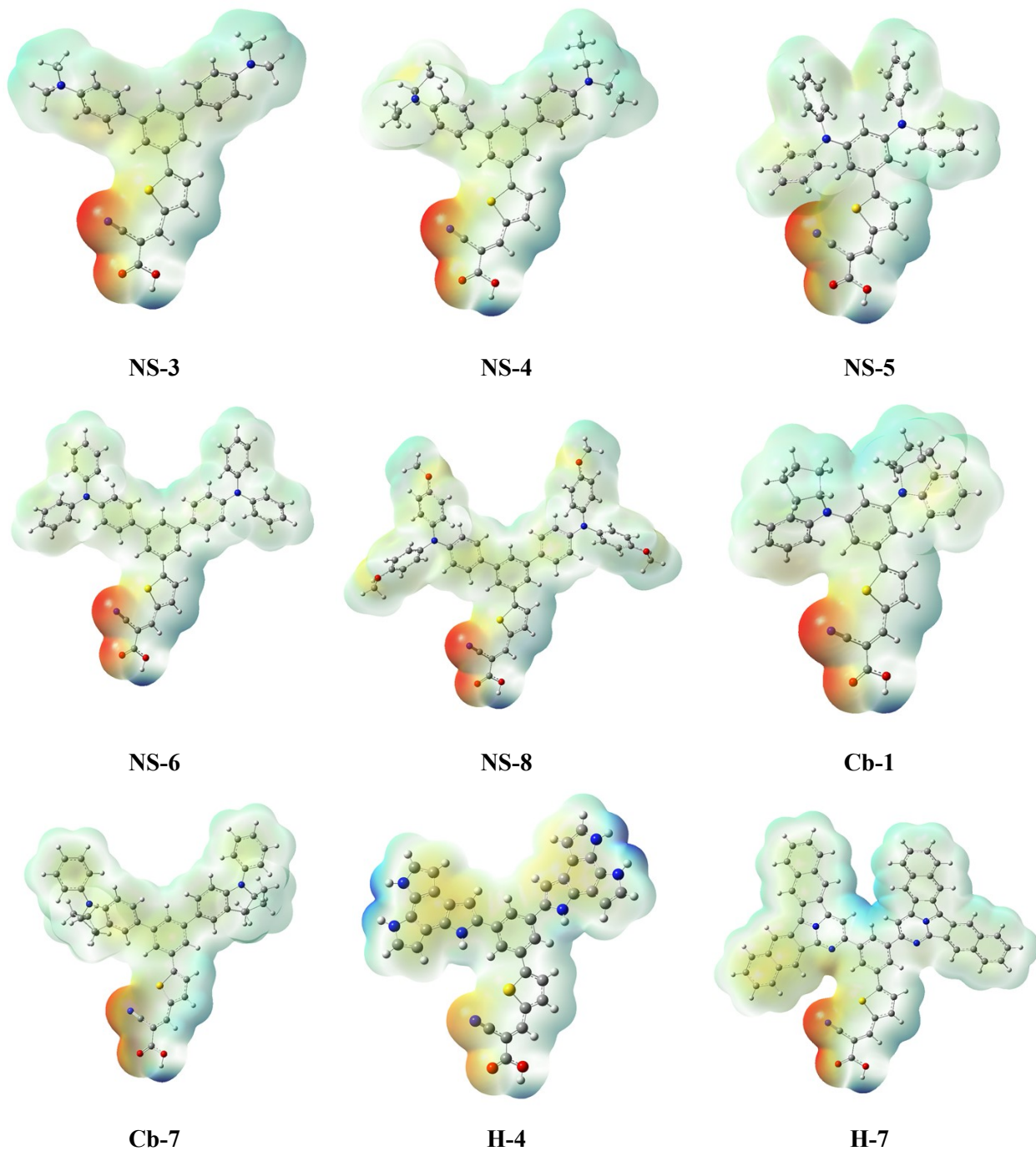
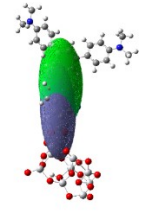
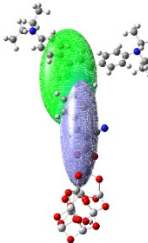
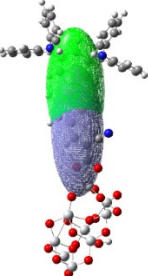
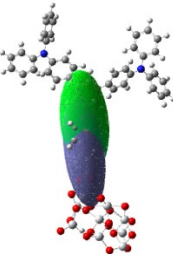
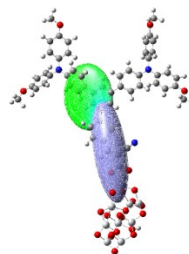


Figure S4. MESP analysis of the selected 9 dye sensitizers. The MESPs are generated at isosurface value of 0.0004 e/au^3 .

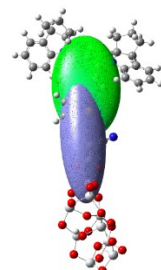
Table S6. The Calculated charge transfer length (D_{CT}) and the descriptor for the charge-transfer possibility (Δr) are given here for the efficient dyes interacted to TiO_2 . The Charge Density Difference plots and the Centroids of the different dyes in DCM solvent are also given here. (isosurface value of 0.0004 a.u.) Charge density transfers from sky blue to purple.

Systems	D_{CT}	Δr	Centroids
NS-3	9.07	17.14	
NS-4	10.67	20.16	
NS-5	8.84	16.71	
NS-6	8.59	16.23	

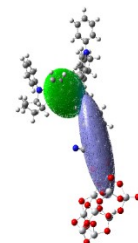
NS-8	10.36	19.59
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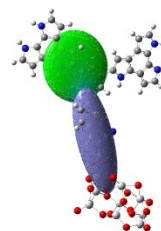
Cb-1	7.70	14.56
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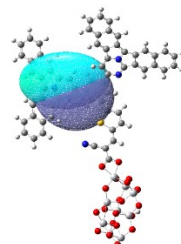
Cb-7	12.36	23.37
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H-4	13.54	25.60
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H-7	3.88	7.34
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Answer to the reviewer for the radiative lifetime calculation and comparing with our previous calculations for selected dye sensitizers with two different solvent model.

Emission rate for a transition between two levels $|i\rangle$ state to $|f\rangle$ State.

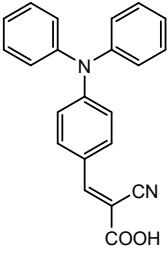
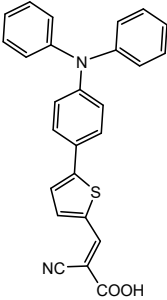
$$A = \frac{\omega^3}{3\epsilon_0\pi\hbar C^3} |\mu_{if}|^2 \dots\dots\dots(1)$$

Systems	Reviewer calculation		Our calculation	
	(Radiative life time τ)		(Excited state life time τ)	
	$A = \frac{4\omega^3}{3C^3} \mu_{if} ^2$ $\tau = 1/A \text{ (in ns)}$		$\tau = \frac{1.499}{fE^2} \text{ (in ns)}$	
	CPCM model	SS-cLR-PCM model	CPCM model	SS-cLR-PCM model
NS-3	7.05	5.18	2.69	3.28
NS-5	6.69	5.85	2.83	3.05
NS-6	6.85	5.62	2.58	2.45
NS-8	6.99	5.21	2.65	3.32

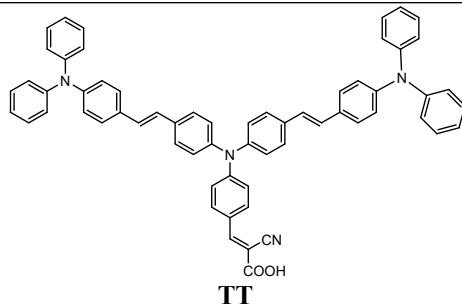
Proof of concept from experimental analysis

From the data presented in the table below, it is evident that the incorporation of a double donor and a thiophene spacer significantly increases the efficiency of the dye. The efficiency of the dye TT with the double donor is almost double (5.12%) that of the dye T with a single donor (2.79%). WR5 with the thiophene spacer shows a higher efficiency of 4.70%.

In our manuscript, we have tried to search for the best donor moieties for such thiophene spacer-based dye sensitizers. So, this definitely have a vision of increasing the efficiency of the dye sensitizers through such design. Thus, our research aims to identify the best donor moieties for such dual donor based dye sensitizers, using carboxylic acid as a reference acceptor. Through molecular modelling, we are looking to design better and more efficient dual donor-based dyes grounded on the experimental results.

Serial number	Structure and Reference	Experimental Efficiency η (%)
1	 <p style="text-align: center;">T</p> <p>Ref: Jia, J., Cao, K., Xue, P., Zhang, Y., Zhou, H., & Lu, R., Tetrahedron 2012, 68, 3626–3632.</p>	2.79
2	 <p style="text-align: center;">WR5</p> <p>Ref: Wang, S., Guo, J., He, L., Wang, H., Zhao, J., Lu, C. Synthetic Metals 2013, 168, 1–8.</p>	4.70

3



Ref: Jia, J., Cao, K., Xue, P., Zhang, Y., Zhou, H., & Lu, R., *Tetrahedron* 2012, 68, 3626–3632.

5.12

Cartesian coordinates of all the free dyes

P-1

C	0.06031500	-0.58846800	-0.30049000
C	0.41521300	0.76894900	-0.22275300
C	1.74716000	1.16583600	-0.08272300
C	2.73462600	0.17291100	-0.02664600
C	2.42018200	-1.19099000	-0.10167100
C	1.07839000	-1.55540400	-0.23512500
H	-0.35695200	1.53099300	-0.29405700
H	3.77529500	0.47070600	0.08024600
H	0.81858900	-2.61000100	-0.26181300
C	-1.33744800	-1.00417300	-0.44857700
C	-1.82283500	-2.18222200	-0.99688200
S	-2.64557400	0.01254500	0.10014100
C	-3.22518800	-2.26313200	-0.98564100
H	-1.17925200	-2.94502400	-1.41917800
C	-3.85173700	-1.15144500	-0.42934200
H	-3.78774300	-3.10252700	-1.38196700
C	-5.26745800	-1.01694500	-0.31960400
H	-5.81932900	-1.87143500	-0.70234000
C	-6.03621300	-0.00100500	0.18283700
C	-5.48350300	1.19784200	0.72558700
N	-5.00744200	2.16690200	1.16178100
C	-7.51635700	-0.07643200	0.19592700
O	-8.24777600	0.79051400	0.62574900
O	-7.99209200	-1.23728500	-0.33245500
H	-8.96232800	-1.16977200	-0.26957200
C	2.10069700	2.63686300	0.01172800
C	2.74968800	3.06847500	1.35134800
C	3.09815500	3.16039300	-1.06404800
H	1.16920000	3.20812500	-0.08846200
C	3.32664900	4.44955700	1.01978500
H	3.55403400	2.37171700	1.62369200
H	2.03425700	3.07778900	2.18040700
C	3.93944800	4.27229500	-0.38682200
H	2.57731900	3.57525700	-1.93200700
H	3.74159700	2.35415500	-1.43056900
H	2.51665700	5.18649900	0.94420000
H	4.04669700	4.81482900	1.76173600
H	4.98425400	3.93582600	-0.28905600
C	3.49435300	-2.25733300	-0.03285000
C	4.55897500	-2.19756000	-1.15511100
C	4.36988900	-2.25168300	1.24073400
H	3.00705500	-3.23883900	-0.08007400
C	5.74555000	-3.04446900	-0.62824900
H	4.87421900	-1.15741900	-1.30423700
H	4.17187200	-2.55081400	-2.11650200
C	5.51660100	-3.21238400	0.90371200
H	3.83496000	-2.56904100	2.14045600
H	4.77063000	-1.24583500	1.42028900
H	5.76688800	-4.03545500	-1.09635400
H	6.70745800	-2.56646200	-0.84429000
H	6.42505000	-2.98281300	1.47998500
O	3.89092900	5.44651800	-1.19386600

O	5.05517700	-4.52611900	1.23475200
H	4.43838200	6.12205200	-0.76376700
H	5.73164300	-5.15743700	0.94431300

NS-1

C	-2.94262400	-1.19341300	-0.21955500
C	-3.26596500	0.17983100	-0.21300700
C	-2.28670500	1.18850800	-0.31876600
C	-0.93757600	0.80149400	-0.42905200
C	-0.59410100	-0.55709900	-0.40070400
C	-1.57744200	-1.54822700	-0.29032300
H	-4.29371600	0.48117900	-0.08012800
H	-0.16113900	1.53436700	-0.60193100
H	-1.26609900	-2.58051300	-0.21682100
C	0.81221100	-0.96221700	-0.50355100
C	1.32883800	-2.14328400	-1.01623700
S	2.08989900	0.08157700	0.06371600
C	2.73107000	-2.20462200	-0.96465700
H	0.70530100	-2.91838400	-1.44601700
C	3.32764000	-1.07339900	-0.41323500
H	3.31596600	-3.04238000	-1.33148000
C	4.73680200	-0.91536000	-0.27142400
H	5.31057000	-1.77083100	-0.61828700
C	5.47991300	0.12488400	0.22268400
C	4.89900400	1.33114200	0.71734900
N	4.40196400	2.30667000	1.11419100
C	6.95905500	0.07026800	0.27390700
O	7.67003100	0.95854300	0.69530300
O	7.46448200	-1.09908800	-0.20805000
H	8.43158700	-1.01438200	-0.12266600
N	-2.67301900	2.53283300	-0.30621100
N	-3.93620300	-2.16621100	-0.15207500
C	-1.64773700	3.57627600	-0.25854000
C	-3.96128400	2.90626400	-0.90234600
C	-5.34482400	-1.80077500	-0.03789400
C	-3.59406200	-3.58447900	-0.09105200
H	-5.93105400	-2.65020400	-0.40514700
H	-2.80147000	-3.79219800	-0.82010700
H	-1.25736200	3.79772700	-1.26823700
H	-4.27555900	2.10718200	-1.58340500
C	-2.11378700	4.87630700	0.40216600
C	-5.08101400	3.19453700	0.10622500
H	-3.80340100	3.79213500	-1.53136400
H	-0.81096500	3.19261600	0.32870100
H	-1.27341400	5.57801100	0.44382200
H	-2.92171100	5.36656000	-0.15046100
H	-2.45730100	4.69251700	1.42551800
H	-4.81971000	4.02719100	0.76574900
H	-6.00726400	3.45437000	-0.42131400
H	-5.28226700	2.32395700	0.73932200
C	-5.81588300	-1.43627100	1.37853700
C	-3.17818500	-4.09970700	1.29530000
H	-6.87062600	-1.13589000	1.36232200
H	-5.71750000	-2.28911100	2.05810000
H	-5.23088000	-0.60944900	1.79347700
H	-2.90091000	-5.15940600	1.23891000

H	-2.32129900	-3.54263600	1.68666100
H	-5.55548500	-0.97377100	-0.72676300
H	-4.46996700	-4.14413800	-0.43665400
H	-3.99809200	-4.00237700	2.01443900

NS-2

C	0.38850700	0.80049200	0.24502000
C	0.17629700	-0.58718800	0.25473900
C	1.28191400	-1.44735700	0.14661200
C	2.58549300	-0.94300900	0.04872400
C	2.76288700	0.44960200	0.05503300
C	1.67931200	1.33790400	0.14339500
H	-0.46089700	1.47354900	0.31328400
H	1.12197700	-2.51883800	0.08549900
H	3.77172100	0.85025700	0.03900600
C	-1.17471800	-1.14885100	0.35637800
C	-1.54014600	-2.40085400	0.82863800
S	-2.57758400	-0.23941200	-0.14522500
C	-2.92648200	-2.62397100	0.79669700
H	-0.82385200	-3.11762300	1.21259600
C	-3.66102500	-1.55033900	0.30138800
H	-3.40180600	-3.53887500	1.13613800
C	-5.08251600	-1.55501800	0.18655500
C	3.74812900	-1.85799700	-0.05707600
C	3.79008300	-3.07491400	0.64417200
C	4.85381400	-1.54563600	-0.86604100
C	4.87530600	-3.93766200	0.54535000
H	2.96667000	-3.34138500	1.30144900
C	5.94401700	-2.40085000	-0.97399300
H	4.84815100	-0.62718000	-1.44666700
C	5.97538500	-3.61579000	-0.26809000
H	4.88322500	-4.86453300	1.11485800
H	6.78033300	-2.13211100	-1.61576600
C	1.89520700	2.80507400	0.15081200
C	1.09599800	3.66145100	0.92728600
C	2.90913500	3.39801200	-0.62068300
C	1.29601900	5.03646600	0.93690100
H	0.31888200	3.24231200	1.56048600
C	3.11769000	4.77183700	-0.62028500
H	3.53252500	2.77409000	-1.25539200
C	2.31246400	5.61915400	0.16048000
H	0.66265600	5.66981200	1.55412500
H	3.90016600	5.20032100	-1.24281700
N	7.09224500	-4.45039100	-0.32605000
N	2.47954900	7.00299200	0.11974700
H	2.12120600	7.50610700	0.92162500
H	3.40474400	7.32065300	-0.14035200
H	6.91422700	-5.42401600	-0.11323100
H	7.66298700	-4.34877100	-1.15602000
C	-5.95197900	-0.59271400	-0.25392400
H	-5.54384400	-2.48551900	0.50684500
C	-7.41583900	-0.82119900	-0.28589300
C	-5.52739400	0.69221300	-0.70776000
N	-5.15697700	1.73444200	-1.07177000
O	-8.23393600	-0.00800100	-0.66108000
O	-7.76927800	-2.05966700	0.15602300
H	-8.74108700	-2.08877800	0.08830100

NS-3

C	-0.35318600	-0.82877800	-0.25499000
C	-0.35133400	0.57483100	-0.23114900
C	0.84539300	1.29902300	-0.13442900
C	2.05051000	0.58162000	-0.06657400
C	2.08443500	-0.82204000	-0.07477900
C	0.86970100	-1.51496000	-0.16656300
H	-1.29255300	1.11373100	-0.28427800
H	2.98787500	1.12902500	-0.05520600
H	0.87290400	-2.59881300	-0.11582500
C	-1.60598100	-1.58493600	-0.35059400
C	-1.78493500	-2.87567400	-0.82683900
S	-3.12503000	-0.89641500	0.16475100
C	-3.12221300	-3.30244700	-0.78717500
H	-0.97272600	-3.47651800	-1.21863500
C	-4.00498800	-2.35193300	-0.28178000
H	-3.45862800	-4.27651400	-1.12817600
C	-5.40873800	-2.56823400	-0.15849200
H	-5.72861200	-3.55587500	-0.48021600
C	-6.40942600	-1.74768300	0.29127800
C	-7.82223700	-2.19206700	0.33040100
O	-8.75076600	-1.51145500	0.71287200
O	-7.98985500	-3.46837100	-0.11404700
H	-8.94607500	-3.64176800	-0.04083100
C	-6.17874700	-0.41529900	0.74811000
C	0.83785800	2.78099800	-0.12496300
C	-0.09318300	3.51990800	-0.87264700
C	1.76390100	3.51599000	0.63245200
C	-0.10816800	4.90879500	-0.86641200
H	-0.80899200	2.99885400	-1.50285300
C	1.76353500	4.90498400	0.65286900
H	2.49165800	2.98974900	1.24460000
C	0.81605300	5.64599400	-0.09067000
H	-0.84062800	5.41985800	-1.47954200
H	2.49946800	5.41342800	1.26429100
N	0.78961000	7.03247000	-0.05368000
C	1.88002800	7.75165100	0.58139300
C	-0.08819600	7.75627700	-0.95675500
H	1.68618900	8.82405400	0.51718500
H	1.95797000	7.49356000	1.64480700
H	2.85545400	7.54926800	0.11069600
H	-0.00219500	8.82622300	-0.75744400
H	0.15234600	7.58325100	-2.01815400
H	-1.13564200	7.47377000	-0.79687300
N	-5.96682800	0.66955900	1.11444100
C	3.37082300	-1.55396000	0.00874100
C	3.58692900	-2.74811000	-0.69713500
C	4.43583000	-1.08485500	0.79415300
C	4.78935800	-3.44075700	-0.62592300
H	2.80569700	-3.13220600	-1.34806100
C	5.64470500	-1.76417300	0.87959100
H	4.31082500	-0.17446500	1.37444900
C	5.85476400	-2.97338100	0.17752900
H	4.90041200	-4.34498300	-1.21235400
H	6.42535600	-1.35255300	1.50809300
N	7.04936700	-3.67366200	0.27995400

C	7.29289200	-4.80114100	-0.60297700
C	8.18871700	-3.04745100	0.92872700
H	7.96517000	-2.81149800	1.97615700
H	9.03024100	-3.74292500	0.92181000
H	8.50609900	-2.11699000	0.43107600
H	7.30312900	-4.51817600	-1.66811900
H	8.26019500	-5.24421700	-0.35797300
H	6.53085000	-5.57775200	-0.46664300

NS-4

C	-0.57690900	-1.13660200	-0.29659600
C	-0.89615700	0.23021000	-0.25920500
C	0.10544300	1.20266600	-0.14359100
C	1.44198900	0.78326900	-0.07378300
C	1.79689400	-0.57570600	-0.10087900
C	0.77033000	-1.52434700	-0.20783600
H	-1.93457700	0.54248900	-0.31637600
H	2.22728200	1.53219600	-0.04485200
H	1.01980400	-2.57967600	-0.16991400
C	-1.62319500	-2.15837300	-0.40832700
C	-1.50283500	-3.44630500	-0.90862600
S	-3.25749200	-1.84537200	0.11841900
C	-2.70711800	-4.16881500	-0.87818100
H	-0.57597400	-3.83786400	-1.31100900
C	-3.78188300	-3.45516900	-0.35579100
H	-2.81271500	-5.18757400	-1.23756000
C	-5.09912700	-3.98919500	-0.23672900
H	-5.18661800	-5.01741900	-0.57779200
C	-6.25765600	-3.42696700	0.22941600
C	-6.33330200	-2.08601800	0.71261300
N	-6.36977600	-0.98857400	1.10015900
C	-7.53274800	-4.18189500	0.26066100
O	-8.58893200	-3.73702800	0.65779700
O	-7.40778200	-5.45346000	-0.20942400
H	-8.29878000	-5.84218600	-0.13949200
C	-0.23977600	2.64775300	-0.11688500
C	-1.27912800	3.16158900	-0.91089500
C	0.46140200	3.54343700	0.70620200
C	-1.60459300	4.51527700	-0.88107200
H	-1.82267000	2.49740000	-1.57735800
C	0.13582800	4.89819000	0.73496500
H	1.25203800	3.17061500	1.35156800
C	-0.90043400	5.40465100	-0.05596200
H	-2.40947100	4.88407400	-1.51153200
H	0.67376400	5.58522200	1.38115200
C	3.21501500	-0.99549600	-0.01781600
C	3.69969600	-2.10808900	-0.72364300
C	4.14567400	-0.30183600	0.77214100
C	5.02668100	-2.51124900	-0.64885400
H	3.02656600	-2.66674900	-1.36901600
C	5.47717400	-0.68733600	0.85645400
H	3.81869900	0.55463300	1.35599500
C	5.96538300	-1.81110000	0.14688500
H	5.32923600	-3.38455700	-1.21422700
H	6.14153800	-0.09981900	1.47874300
N	-1.20553400	6.81387700	0.00645200
N	7.29207100	-2.20474200	0.22680100

C	-2.55299200	7.09519000	0.52933400
C	-2.74252600	6.61403900	1.96658500
C	8.92138300	-0.32396300	0.57485000
H	-3.73389800	6.90479900	2.33178500
H	-2.66348000	5.52505800	2.04290700
H	-1.98582900	7.05773800	2.62242900
H	8.19302600	0.44814800	0.30756400
H	9.61940400	0.09925400	1.30700700
H	9.48882200	-0.57530500	-0.32834400
C	-0.94273500	7.52177600	-1.25697600
C	8.22806200	-1.56731200	1.14820100
C	7.82607100	-3.27783200	-0.60644800
C	0.52979000	7.48540300	-1.66187900
H	0.86802900	6.46468600	-1.86653800
H	0.68425600	8.07948900	-2.56976000
H	1.15691100	7.89851000	-0.86461700
C	7.66335700	-4.67908400	-0.00186300
H	6.60796700	-4.92191500	0.15735800
H	8.09528700	-5.43728300	-0.66596800
H	8.17180700	-4.74751000	0.96647500
H	-2.68153600	8.18392100	0.49548000
H	-3.34662000	6.66777900	-0.11300900
H	-1.56533700	7.13644100	-2.08741500
H	-1.24602000	8.56435200	-1.10211100
H	7.70773800	-1.31992700	2.07973100
H	8.98292900	-2.31455500	1.41976000
H	7.36186500	-3.23246400	-1.59753800
H	8.89044600	-3.07063400	-0.76791000

NS-5

C	-0.63288500	-0.72088800	0.17040700
C	-0.41054700	0.66095300	0.26798200
C	0.89776700	1.16663200	0.29607300
C	1.98167000	0.27792600	0.23275300
C	1.76770600	-1.10176500	0.10770400
C	0.45790500	-1.59871800	0.07180100
H	-1.24733300	1.34615300	0.34412300
H	2.99372700	0.66085200	0.28698000
H	0.29414600	-2.66091400	-0.06426500
C	-1.99514900	-1.26550100	0.13785300
C	-2.41030800	-2.52840700	0.53152000
S	-3.33830300	-0.32001100	-0.44993800
C	-3.79171800	-2.73106800	0.37393500
H	-1.73496500	-3.26663400	0.94818900
C	-4.46894300	-1.63150100	-0.14539100
H	-4.30417400	-3.65049400	0.63883900
C	-5.87529400	-1.61397300	-0.38497400
H	-6.37415600	-2.54477200	-0.12814100
C	-6.69007700	-0.63087700	-0.87956800
C	-6.21036900	0.65515900	-1.27132200
N	-5.79521000	1.69678600	-1.58522400
C	-8.14860900	-0.83750000	-1.04502100
O	-8.91901600	-0.00579000	-1.47602800
O	-8.55545100	-2.07791400	-0.65900300
H	-9.51772700	-2.09263500	-0.81294000
N	1.12439300	2.55723400	0.42094000
N	2.86997400	-1.98914800	0.03059000

C	0.26867400	3.35383200	1.23766200
C	-0.22531600	4.57740400	0.76168600
C	-0.08201300	2.92907900	2.52825400
C	-1.04988300	5.36127800	1.56679900
H	0.03902600	4.90591400	-0.23849900
C	-0.92193800	3.71076000	3.31964500
H	0.30581600	1.98708800	2.90355700
C	-1.40698100	4.93181800	2.84663500
H	-1.42775100	6.30510600	1.18311100
H	-1.18676600	3.36798500	4.31642400
H	-2.05757700	5.54091700	3.46754000
C	2.20634200	3.17715100	-0.26627400
C	3.00750200	4.12732700	0.38570300
C	2.47907200	2.85812800	-1.60573400
C	4.05445600	4.74755700	-0.29362300
H	2.80255300	4.37577500	1.42220900
C	3.54000800	3.46970000	-2.27097000
H	1.85357700	2.13514800	-2.11976900
C	4.33115900	4.42019000	-1.62256700
H	4.66482000	5.48182100	0.22555100
H	3.73744400	3.21208200	-3.30817300
H	5.15218400	4.90075500	-2.14683100
C	4.02527000	-1.63358800	-0.72255200
C	5.30852300	-1.86327900	-0.20291200
C	3.89699200	-1.05659000	-1.99549600
C	6.43760300	-1.52834700	-0.94807800
H	5.41289000	-2.30449200	0.78332000
C	5.03183200	-0.70752800	-2.72542300
H	2.90679100	-0.88781300	-2.40700500
C	6.30769200	-0.94476000	-2.21007300
H	7.42437200	-1.71251100	-0.53147500
H	4.91570400	-0.26172600	-3.70976900
H	7.18996900	-0.67800400	-2.78477200
C	2.82226700	-3.24785100	0.69294900
C	3.28257900	-4.40765600	0.04992700
C	2.32005900	-3.34759900	2.00063000
C	3.24579200	-5.63674200	0.70632500
H	3.66830500	-4.33818200	-0.96219200
C	2.27024900	-4.58392200	2.64195500
H	1.97364900	-2.45291300	2.50829600
C	2.73556400	-5.73513400	2.00242100
H	3.60674800	-6.52450200	0.19363000
H	1.88037500	-4.64273200	3.65488200
H	2.70291200	-6.69574700	2.50844100

NS-6

C	0.29254600	2.40377300	-0.32251400
C	1.27041600	1.39703300	-0.29127900
C	0.91661700	0.04320200	-0.20503100
C	-0.44674000	-0.28677600	-0.15561900
C	-1.44946400	0.69505400	-0.19285500
C	-1.06289300	2.03930300	-0.27312200
H	2.31837000	1.66522800	-0.38431600
H	-0.73266600	-1.32656000	-0.03160000
H	-1.82511500	2.81125600	-0.29676100
C	0.66311100	3.81910900	-0.42935500

C	-0.08294900	4.85797000	-0.96478600
S	2.20034600	4.39491800	0.16187200
C	0.57477000	6.09850600	-0.90987700
H	-1.06024800	4.71371000	-1.41042300
C	1.83973700	6.04314100	-0.33209700
H	0.15593300	7.02449000	-1.29099800
C	2.68742100	7.18033900	-0.17810200
H	2.25017400	8.10520600	-0.54505100
C	3.94579000	7.29650000	0.34910800
C	4.67437200	6.18780100	0.87590300
N	5.24726400	5.26649400	1.29888000
C	4.64962800	8.59986300	0.40797000
O	5.76313100	8.76270200	0.86017900
O	3.91330200	9.62321100	-0.10509900
H	4.47323000	10.41552800	-0.01216900
C	1.95767600	-1.01166300	-0.16421500
C	3.17797000	-0.80958400	0.50338800
C	1.76438300	-2.25365000	-0.79276300
C	4.15398900	-1.79793900	0.55072700
H	3.35305700	0.12344600	1.03184700
C	2.73998800	-3.24313800	-0.76625400
H	0.84960800	-2.43525900	-1.35041000
C	3.95367300	-3.03395200	-0.08831000
H	5.07557100	-1.61951800	1.09468100
H	2.57119800	-4.18203200	-1.28319300
C	-2.88315800	0.32013700	-0.12602300
C	-3.81449500	1.10471700	0.57546400
C	-3.36468200	-0.83615000	-0.76323000
C	-5.15734600	0.75224900	0.64599100
H	-3.47520600	1.98513000	1.11443100
C	-4.70803600	-1.18992200	-0.71297800
H	-2.68211000	-1.45035200	-1.34415800
C	-5.62956000	-0.40206700	-0.00204700
H	-5.84757500	1.36464700	1.21691000
H	-5.05357000	-2.07599500	-1.23533200
N	4.94777400	-4.04037400	-0.05204000
N	-6.99730900	-0.76246000	0.06063700
C	4.57875300	-5.41176100	0.04416800
C	5.22186500	-6.37686000	-0.74688300
C	3.57378900	-5.82055800	0.93541100
C	4.86934600	-7.72098600	-0.64057600
H	5.99670200	-6.06631100	-1.44061200
C	3.21552600	-7.16461800	1.02159200
H	3.07948000	-5.08074300	1.55712100
C	3.86217500	-8.12367500	0.23898500
H	5.37764500	-8.45505300	-1.26034500
H	2.43600500	-7.46395000	1.71740100
H	3.58553900	-9.17141100	0.31448400
C	6.32718900	-3.68971100	-0.11099500
C	7.25319700	-4.30929800	0.74255500
C	6.78036900	-2.72600700	-1.02552500
C	8.60430500	-3.97420800	0.67442500
H	6.90739700	-5.05113100	1.45547600
C	8.13048800	-2.38366300	-1.07326000
H	6.07035000	-2.24876300	-1.69357300
C	9.05121800	-3.00730500	-0.22853100

H	9.30827700	-4.46280700	1.34297200
H	8.46461700	-1.63380300	-1.78542600
H	10.10364600	-2.74220500	-0.27285900
C	-7.37385500	-2.13122600	0.16854600
C	-6.69431700	-2.99160100	1.04556000
C	-8.43554500	-2.63790300	-0.59741200
C	-7.06498400	-4.33155900	1.14246600
H	-5.87854700	-2.60392500	1.64755800
C	-8.81086700	-3.97495300	-0.48000600
H	-8.96162700	-1.97879400	-1.28073200
C	-8.12669600	-4.83131400	0.38525200
H	-6.52857600	-4.98389400	1.82659800
H	-9.63524900	-4.35091400	-1.08028600
H	-8.41756600	-5.87451800	0.46903500
C	-8.00565100	0.24151500	0.02032800
C	-7.91809800	1.30461400	-0.89256900
C	-9.10608900	0.17852700	0.88968200
C	-8.90631000	2.28682400	-0.92393500
H	-7.07464700	1.35383000	-1.57404100
C	-10.09863500	1.15551200	0.83843600
H	-9.17692000	-0.63821800	1.60100400
C	-10.00405900	2.21753900	-0.06342100
H	-8.82345700	3.10263500	-1.63736400
H	-10.94387900	1.09151400	1.51868300
H	-10.77620700	2.98085100	-0.09581600

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C	1.25066800	2.27341400	-0.15552300
C	1.06959500	0.88400200	-0.16386300
C	-0.23922300	0.37890800	-0.16278700
C	-1.35451700	1.23039600	-0.15080700
C	-1.14226100	2.61468100	-0.13454900
C	0.15529700	3.15116300	-0.13798400
H	2.25694900	2.67723400	-0.20989100
H	-0.39304200	-0.69466600	-0.11480500
H	-1.99570500	3.28476600	-0.11913300
C	0.34788600	4.60610700	-0.13918200
C	-0.50567800	5.58042200	-0.62959400
S	1.78546800	5.31894700	0.54448700
C	-0.00667000	6.88576800	-0.46736000
H	-1.44548800	5.35256800	-1.11926300
C	1.23783700	6.94129000	0.15071600
H	-0.52583000	7.77897000	-0.79964500
C	1.93870300	8.15844700	0.41614500
H	1.40606100	9.05070300	0.09794200
C	3.15647700	8.37685100	0.99872500
C	3.99060600	7.31987700	1.47346500
C	3.70437600	9.74491800	1.17958900
O	4.77595600	9.99241500	1.68878800
O	2.87242300	10.71197600	0.71011300
H	3.33013400	11.55575700	0.87997400
N	4.64678300	6.43472000	1.84976900
C	2.23939400	-0.02992300	-0.17125100
C	3.40913000	0.28265300	0.54280400
C	2.21573900	-1.23502100	-0.89379400
C	4.50641100	-0.57242300	0.54244700
H	3.44995500	1.18962800	1.13866700

C	3.31293300	-2.08986300	-0.91078800
H	1.34080100	-1.48976000	-1.48474800
C	4.46978500	-1.76761500	-0.18827100
H	5.39173000	-0.32094300	1.11800300
H	3.28198700	-3.00484600	-1.49412400
C	-2.73212500	0.67656100	-0.13232000
C	-3.74803600	1.27854500	0.62970600
C	-3.06415400	-0.46721200	-0.87819000
C	-5.03896700	0.76056200	0.65148900
H	-3.51600300	2.14158000	1.24688000
C	-4.35588100	-0.98403400	-0.87412300
H	-2.30996000	-0.93758200	-1.50234600
C	-5.35696000	-0.37499800	-0.10560500
H	-5.80309400	1.22779000	1.26490400
H	-4.59635100	-1.85496400	-1.47590100
N	5.59718200	-2.64660200	-0.19802700
C	6.88160200	-2.12523000	-0.47898800
C	7.03592300	-1.09103300	-1.42180500
C	8.01927200	-2.61808200	0.18926500
C	8.29165700	-0.56549400	-1.69316100
H	6.16715600	-0.70815000	-1.94550000
C	9.27783800	-2.10237400	-0.08702900
H	7.91042700	-3.39972800	0.93297300
C	9.40389900	-1.07892100	-1.02647500
H	8.42528700	0.22399400	-2.42242600
H	10.15968800	-2.46738000	0.42496400
C	5.40537200	-4.02186700	0.06601600
C	4.44867600	-4.43415500	1.01372900
C	6.15006200	-4.99872900	-0.62371900
C	4.24059500	-5.78295600	1.26572000
H	3.87692500	-3.68992000	1.55674200
C	5.95183900	-6.34816600	-0.36711400
H	6.87669400	-4.69480500	-1.36902700
C	4.99620800	-6.73022500	0.57471200
H	3.51470900	-6.11276400	1.99876000
H	6.51189900	-7.10905700	-0.89669000
N	-6.68519600	-0.90429200	-0.09404200
C	-7.77806700	-0.03646800	-0.31872800
C	-8.99024500	-0.20867200	0.37797000
C	-7.66004200	1.02824400	-1.23295500
C	-10.05695100	0.65231000	0.16081900
H	-9.08764500	-1.01327900	1.09837600
C	-8.72102600	1.89726700	-1.44512700
H	-6.73438700	1.16389600	-1.78101600
C	-9.91308200	1.70097300	-0.74793300
H	-10.99100400	0.53586000	0.69661300
H	-8.64614000	2.71446900	-2.15193400
C	-6.87935100	-2.28478300	0.14296500
C	-7.88565500	-2.99724700	-0.53795000
C	-6.05186600	-2.97006600	1.05307300
C	-8.06759200	-4.35386300	-0.30796200
H	-8.51668400	-2.48471500	-1.25562500
C	-6.22409700	-4.32885600	1.27801200
H	-5.27966000	-2.42877700	1.58822400
C	-7.23332400	-5.00974500	0.59742000
H	-8.83230100	-4.91507200	-0.83077000

H	-5.60061500	-4.86598100	1.98215500
N	10.73060100	-0.53266800	-1.31831100
N	4.78025100	-8.15305800	0.84122200
N	-7.41944600	-6.44223600	0.83632800
N	-11.03377800	2.61529300	-0.97223100
O	5.47675500	-8.96302800	0.22707400
O	3.91410600	-8.45665300	1.66357600
O	10.80549700	0.37882300	-2.14388400
O	11.69334300	-1.01831400	-0.72216200
O	-6.65310000	-6.99479200	1.62717000
O	-8.33108100	-7.00947700	0.23207800
O	-12.07897200	2.40238800	-0.35560800
O	-10.86503000	3.54439700	-1.76416900

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C	1.25822000	2.06546900	-0.26907900
C	1.04401400	0.68414000	-0.15902500
C	-0.27940800	0.21925900	-0.10265400
C	-1.37740200	1.09297200	-0.15539600
C	-1.12865000	2.46816400	-0.25806900
C	0.18315600	2.96709700	-0.31532200
H	2.27382100	2.43630300	-0.36846600
H	-0.45832000	-0.84187100	0.03985700
H	-1.96564000	3.15779000	-0.29353000
C	0.40881200	4.41019100	-0.44713200
C	-0.44845600	5.36353700	-0.97657200
S	1.89500000	5.14399000	0.09889600
C	0.08382400	6.66323000	-0.95217800
H	-1.41682200	5.11745000	-1.39616600
C	1.36187000	6.74156600	-0.40588900
H	-0.43363600	7.53786700	-1.33359300
C	2.09620300	7.95827600	-0.28869500
H	1.55840900	8.83059600	-0.65075700
C	3.35269000	8.20603800	0.19741100
C	4.20572500	7.18247900	0.70925800
C	3.92348000	9.57330900	0.22139200
O	5.02938500	9.85303700	0.63392300
O	3.07183700	10.51248700	-0.27502100
H	3.55317500	11.35720800	-0.20724000
N	4.88362200	6.32959900	1.12043900
C	2.18662700	-0.25750000	-0.09921300
C	3.37927800	0.07942100	0.56448700
C	2.12554600	-1.52437600	-0.70393300
C	4.45228800	-0.80028500	0.62940000
H	3.45664300	1.03452300	1.07694100
C	3.19746300	-2.40764600	-0.66004000
H	1.23530800	-1.81099900	-1.25753100
C	4.38522200	-2.06415200	0.01278900
H	5.34771000	-0.51592700	1.17145400
H	3.12476300	-3.36697200	-1.16116000
C	-2.76500200	0.57557100	-0.08141900
C	-3.77477500	1.27323900	0.60365400
C	-3.12673700	-0.63597200	-0.69446200
C	-5.07455400	0.78817300	0.68136500
H	-3.52925900	2.19429200	1.12568700
C	-4.42623800	-1.12523100	-0.63671800
H	-2.38449500	-1.18981800	-1.26304300

C	-5.42855900	-0.42323400	0.05826100
H	-5.82252700	1.33936100	1.24140500
H	-4.67533200	-2.05224700	-1.14212300
N	5.47403800	-2.95776300	0.06816800
C	6.81422600	-2.47029900	0.11519600
C	7.25365400	-1.47965100	-0.76917900
C	7.72812500	-2.98884900	1.04865900
C	8.56312000	-0.99653000	-0.71914200
H	6.56239900	-1.07281300	-1.50086100
C	9.03740600	-2.53126900	1.08877600
H	7.40228200	-3.75782000	1.74224000
C	9.46638000	-1.52534200	0.20978900
H	8.86516700	-0.22236700	-1.41519700
H	9.74662700	-2.92846600	1.80830400
C	5.25957200	-4.36737000	0.06030200
C	4.31525500	-4.95766200	0.91910900
C	6.00195800	-5.19794400	-0.78510700
C	4.11465400	-6.33053500	0.91602200
H	3.73698800	-4.32866500	1.58882400
C	5.82212500	-6.58312600	-0.77768100
H	6.73607800	-4.75765400	-1.45277200
C	4.86962300	-7.15781600	0.07076200
H	3.38634300	-6.79030400	1.57687700
H	6.42000400	-7.19491100	-1.44363200
O	10.76949300	-1.13691900	0.34062400
O	4.60290300	-8.49572100	0.15452900
C	11.24895100	-0.10713500	-0.50854300
C	5.33985400	-9.37694900	-0.67613700
H	4.97516300	-10.38019600	-0.44771100
H	5.17251600	-9.16485400	-1.74080300
H	6.41664200	-9.32642500	-0.46531600
H	10.68879300	0.82677200	-0.36739000
H	12.29157000	0.05220000	-0.22729100
H	11.20029500	-0.39920600	-1.56628500
N	-6.74634700	-0.92017500	0.13198100
C	-7.85822000	-0.02888200	0.18390400
C	-8.88158500	-0.22029800	1.12844700
C	-7.96669300	1.04304700	-0.70838400
C	-9.97652800	0.63084200	1.17057300
H	-8.81201200	-1.04753700	1.82795900
C	-9.05439300	1.91795300	-0.65741000
H	-7.18885900	1.20043100	-1.44933800
C	-10.07135300	1.71206900	0.28156300
H	-10.76953200	0.48594100	1.89764700
H	-9.10208700	2.74004700	-1.36251400
C	-6.99342700	-2.32473500	0.13738500
C	-7.97337400	-2.88099300	-0.69080500
C	-6.27397200	-3.17923300	0.99171600
C	-8.24385700	-4.25124900	-0.67049200
H	-8.53819700	-2.23455200	-1.35541500
C	-6.52085200	-4.54443500	1.00095400
H	-5.51574100	-2.76301300	1.64777100
C	-7.51181700	-5.09381900	0.17314200
H	-9.01460800	-4.64528800	-1.32308300
H	-5.96710900	-5.20793600	1.65793200
O	-11.18333300	2.49533000	0.41373400

O	-7.68331800	-6.44606200	0.26805600
C	-11.33109800	3.60000000	-0.46243500
C	-8.67133600	-7.05349700	-0.54741700
H	-8.64025100	-8.11915400	-0.31293200
H	-9.67409100	-6.66332600	-0.32680200
H	-8.45790100	-6.91156700	-1.61544800
H	-11.38514800	3.28015300	-1.51183400
H	-12.27099200	4.08029000	-0.18402500
H	-10.50925000	4.31979600	-0.34857200

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C	0.29020000	2.39543900	-0.28554700
C	1.26776600	1.38800900	-0.27036200
C	0.91442800	0.03331600	-0.20958500
C	-0.44746200	-0.30166100	-0.17081500
C	-1.44839000	0.68167300	-0.19001300
C	-1.06432400	2.02742700	-0.24360300
H	2.31574900	1.65897300	-0.35432500
H	-0.73320600	-1.34398700	-0.06924800
H	-1.82733700	2.79898900	-0.25273100
C	0.66080500	3.81319100	-0.36346500
C	-0.07763400	4.85992100	-0.89151300
S	2.18864000	4.37763900	0.26096800
C	0.57961700	6.10008400	-0.80492400
H	-1.04819500	4.72442600	-1.35457900
C	1.83476000	6.03364300	-0.20898300
H	0.16634700	7.03259800	-1.17573700
C	2.68212000	7.16784800	-0.01936400
H	2.25356900	8.10037100	-0.37694100
C	3.92994700	7.26873200	0.53243000
C	4.64313500	6.14619600	1.05136800
N	5.19987800	5.21146200	1.46616100
C	4.63913200	8.56854200	0.62998700
O	5.74383900	8.71448600	1.10737200
O	3.91726400	9.60325500	0.12208900
H	4.47656800	10.39289200	0.23959700
C	1.95851100	-1.02135700	-0.18467200
C	3.16926800	-0.82991600	0.50292500
C	1.77022800	-2.24552000	-0.84849400
C	4.14663200	-1.81936500	0.53514100
H	3.33526800	0.09097800	1.05434800
C	2.74843200	-3.23421900	-0.83427000
H	0.86112300	-2.41253700	-1.41906700
C	3.94767200	-3.03311300	-0.13699800
H	5.06523000	-1.65782400	1.09031000
H	2.59129500	-4.16369800	-1.37245400
C	-2.88343900	0.30522400	-0.13229500
C	-3.80682700	1.06485900	0.60594700
C	-3.36480900	-0.82409500	-0.81595200
C	-5.15090000	0.71092100	0.66584100
H	-3.46170800	1.92240500	1.17640200
C	-4.71008300	-1.17622700	-0.77473700
H	-2.68334200	-1.41457400	-1.42162800
C	-5.61862400	-0.41282400	-0.02901800
H	-5.84285500	1.29886400	1.26068300
H	-5.06426700	-2.04004900	-1.32851700
N	4.95026400	-4.04967600	-0.11304400

C	6.29074500	-3.71127300	-0.41380600
C	7.36989800	-4.32894600	0.23767000
C	6.59318000	-2.72723400	-1.36743700
H	7.20390700	-5.08593600	0.99617200
C	7.92870000	-2.42025800	-1.61544800
H	5.80424600	-2.21512900	-1.90708700
H	8.17536400	-1.66069700	-2.35562100
C	4.58279900	-5.37764700	0.20531800
C	3.57486900	-5.64455500	1.14499800
C	5.19236700	-6.48044000	-0.41375000
H	3.06976700	-4.83605300	1.66186800
C	4.77678900	-7.76199300	-0.06182500
H	5.96854500	-6.34275200	-1.15837400
H	5.24007000	-8.62457800	-0.53834100
N	-6.99949800	-0.77421800	0.02246400
C	-7.98350000	0.21106300	-0.22427300
C	-9.20743400	0.21954100	0.46332800
C	-7.76436600	1.23534100	-1.15855000
C	-10.12933800	1.22393000	0.17992300
H	-9.43349700	-0.53549100	1.20812100
H	-6.84134100	1.28087700	-1.72590000
H	-11.08037100	1.24255600	0.70987900
C	-7.35636600	-2.11070300	0.31811700
C	-8.46357000	-2.72833600	-0.28466000
C	-6.60086600	-2.88025200	1.21624300
H	-9.08010400	-2.19335300	-0.99852800
C	-6.98324100	-4.19704300	1.45919100
H	-5.73681100	-2.45911300	1.71825100
H	-6.40709800	-4.80222100	2.15745900
C	-8.75720900	2.19227700	-1.35174700
H	-8.59985000	2.98877100	-2.07751700
C	-8.75509000	-4.05000900	0.04281000
H	-9.60942800	-4.54053800	-0.42105600
C	3.23677100	-6.96905100	1.40990800
H	2.45950700	-7.18780100	2.14057500
C	8.66538600	-3.94629300	-0.10032800
H	9.51031400	-4.41640000	0.40045800
N	-9.93156100	2.20793100	-0.70760200
N	-8.04122000	-4.79578800	0.89664800
N	3.81481600	-8.03003700	0.83136800
N	8.96751900	-3.00869800	-1.00826500

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C	-2.11627000	1.33672100	0.10372600
C	-0.80306600	0.86420400	0.22320900
C	-0.52318600	-0.51161800	0.23662700
C	-1.58708500	-1.42180600	0.12221400
C	-2.91001800	-0.97925800	0.00542900
C	-3.15651700	0.40170300	-0.00066000
H	0.01063900	1.57887600	0.30246300
H	-1.38287100	-2.48750400	0.12507300
H	-4.17875600	0.75563500	-0.09135000
C	0.85061100	-1.00877500	0.37207300
C	1.26521800	-2.23238500	0.87499500
S	2.21646900	-0.04374100	-0.12647300
C	2.66161700	-2.39031100	0.86835200
H	0.57799500	-2.97456100	1.26412400

C	3.35215000	-1.29355600	0.36206300
H	3.17360200	-3.27488900	1.23361800
C	4.77493600	-1.23258500	0.26687000
H	5.27559600	-2.13266100	0.61383300
C	5.60193900	-0.23873000	-0.18269300
C	5.12059000	1.01334900	-0.67072000
N	4.70194900	2.02674600	-1.06262600
C	7.07660500	-0.39465500	-0.19018000
O	7.85709900	0.45094900	-0.57265000
O	7.48349500	-1.60379600	0.28353900
H	8.45658100	-1.58782200	0.23039800
C	-2.40047000	2.79578300	0.08769200
C	-1.68823000	3.67848700	0.91646500
C	-3.38848000	3.32713400	-0.75794500
C	-1.95474900	5.04669600	0.90007500
H	-0.93661500	3.28673200	1.59619500
C	-3.65531300	4.69527400	-0.77410400
H	-3.93162800	2.66624800	-1.42779900
C	-2.93963000	5.56088400	0.05493800
H	-1.39573700	5.71068100	1.55388000
H	-4.41714700	5.08637300	-1.44321600
H	-3.14645200	6.62746200	0.04129500
C	-4.02845900	-1.95209100	-0.10944600
C	-3.89497400	-3.11614600	-0.88445500
C	-5.24641000	-1.73055600	0.55457700
C	-4.94371900	-4.02853600	-0.99129200
H	-2.97159300	-3.29265800	-1.42939500
C	-6.29525600	-2.64282600	0.44786900
H	-5.36200800	-0.84920200	1.17938500
C	-6.14838700	-3.79586800	-0.32531900
H	-4.82216100	-4.91802800	-1.60379000
H	-7.22605200	-2.45584000	0.97677000
H	-6.96597300	-4.50663100	-0.40878200

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C	0.19068600	-0.69348000	0.25590900
C	-0.93415000	-1.52777100	0.14935600
C	-2.22075000	-0.99383000	0.00328100
C	-2.36325400	0.40179200	-0.04279000
C	-1.26087900	1.26368300	0.06446500
C	0.01271500	0.69851500	0.21617100
H	-0.80553200	-2.60494000	0.17818800
H	-3.34760400	0.82463000	-0.21850700
H	0.86917000	1.35194200	0.35204000
C	1.52226900	-1.28416800	0.42845500
C	1.84466100	-2.51347500	0.98287700
S	2.95643600	-0.44132100	-0.09770300
C	3.22595300	-2.77132300	0.99406100
H	1.10274100	-3.18719700	1.39542300
C	3.99690100	-1.74850500	0.44945700
H	3.67108700	-3.67467300	1.39896400
C	5.42023100	-1.79376800	0.36244300
H	5.85386600	-2.71034700	0.75367000
C	6.31848300	-0.88349700	-0.12697100
C	5.92977800	0.37443800	-0.67837000
N	5.58587400	1.39423500	-1.12296100
C	7.77769700	-1.14443700	-0.11643000

O	8.61879700	-0.37693700	-0.53403800
O	8.09559100	-2.35505500	0.41845400
H	9.06748200	-2.41054600	0.37091700
C	-1.43593000	2.73646800	0.01490900
C	-0.48864200	3.56308900	-0.62013800
C	-2.54766700	3.35734600	0.59936900
C	-0.64768600	4.93994000	-0.66759800
H	0.37388600	3.11629200	-1.10647700
C	-2.72297500	4.74158300	0.56075400
H	-3.28455600	2.75359000	1.12204000
C	-1.76832500	5.54277400	-0.07647300
H	0.07971500	5.57249400	-1.16650100
H	-3.59322200	5.17951000	1.03616400
C	-3.40191700	-1.88445900	-0.12247700
C	-3.33521200	-3.09105600	-0.84535900
C	-4.62543800	-1.55669100	0.47619400
C	-4.43657400	-3.92628000	-0.96171700
H	-2.41137400	-3.36390800	-1.34786800
C	-5.74347500	-2.38572300	0.36924100
H	-4.70609600	-0.64551200	1.06262000
C	-5.65295000	-3.58068600	-0.35389100
H	-4.38494300	-4.84974400	-1.53000500
H	-6.66676900	-2.09648500	0.85808400
O	-1.83363100	6.90095200	-0.17667900
C	-2.94793000	7.56538400	0.39766400
H	-3.89174300	7.23989700	-0.05962600
H	-2.99876800	7.40455000	1.48271100
H	-2.79808900	8.62784600	0.19781900
O	-6.67517400	-4.46671100	-0.52594600
C	-7.93396100	-4.16226300	0.05419200
H	-8.59403200	-4.98950800	-0.21259100
H	-7.86772300	-4.08992000	1.14786500
H	-8.34621000	-3.22605100	-0.34477300

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C	0.16911400	2.19706500	0.28951900
C	1.02706400	1.08763600	0.35114700
C	0.53191200	-0.21998300	0.25440000
C	-0.85185000	-0.39761200	0.10169400
C	-1.73829700	0.68958600	0.04822400
C	-1.21106500	1.98406900	0.13923000
H	2.08814900	1.23994300	0.52370100
H	-1.24300300	-1.40167700	-0.03026800
H	-1.88172600	2.83586300	0.09131100
C	0.68841300	3.56415400	0.40183900
C	0.02627200	4.69492400	0.85563300
S	2.32332400	3.94691700	-0.07239000
C	0.82404700	5.85133300	0.83224200
H	-0.99337600	4.67392400	1.22221300
C	2.11630400	5.63809000	0.36090200
H	0.48521200	6.82863300	1.16123500
C	3.09855400	6.66707300	0.25637700
H	2.74309700	7.64528400	0.56941000
C	4.40005100	6.62551200	-0.16800300
C	5.03591900	5.42763800	-0.61332800
N	5.53157500	4.43674900	-0.97173700
C	5.25153100	7.83844100	-0.19250200

O	6.40872200	7.86205200	-0.55517700
O	4.59983200	8.95235700	0.24036900
H	5.25307400	9.67305700	0.17910800
C	1.44967000	-1.38469400	0.30789400
C	2.72427500	-1.33437500	-0.27293200
C	1.07341100	-2.58266300	0.94502100
C	3.59737500	-2.42196700	-0.22780000
H	3.04001700	-0.43651000	-0.79689900
C	1.92914700	-3.67286000	0.99877000
H	0.10328800	-2.65006000	1.42965700
C	3.20227500	-3.60323900	0.41202200
H	4.56973600	-2.33983900	-0.69927900
H	1.63998100	-4.59074800	1.50112900
O	3.96746200	-4.72496800	0.51873900
C	5.28176600	-4.71976300	-0.04022300
C	5.90904800	-6.07915300	0.23623600
C	7.33303800	-6.19478200	-0.32269500
C	7.97656700	-7.56044100	-0.04963400
C	9.40107200	-7.68691100	-0.60458800
C	10.03667100	-9.05311100	-0.32774100
H	5.22682500	-4.52814300	-1.12195600
H	5.87747200	-3.91471800	0.41440000
H	5.91430500	-6.24837000	1.32073100
H	5.26801200	-6.85602600	-0.20009900
H	7.31831000	-6.01217100	-1.40734000
H	7.96349700	-5.40456600	0.11091700
H	7.99174300	-7.74404100	1.03485400
H	7.34664700	-8.35156000	-0.48257200
H	9.38509900	-7.50310900	-1.68831000
H	10.02981300	-6.89588600	-0.17169500
H	10.09873600	-9.25055400	0.74954300
H	9.44909900	-9.86251200	-0.77834400
H	11.05202600	-9.11193500	-0.73586900
C	-3.19724600	0.47457800	-0.12255400
C	-3.85359200	-0.58868700	0.51141900
C	-3.97507900	1.33134200	-0.92481100
C	-5.22502400	-0.80186800	0.36325800
H	-3.28958400	-1.25510500	1.15830900
C	-5.33893900	1.13363300	-1.08297300
H	-3.49609100	2.14935900	-1.45584700
C	-5.97890000	0.06338000	-0.43904400
H	-5.69180600	-1.63156200	0.88140800
H	-5.93288100	1.78922100	-1.71220500
C	-8.03230900	-1.12132200	-0.04659600
H	-7.93547800	-1.06083900	1.04755100
H	-7.60561200	-2.08243400	-0.36946400
C	-9.49169300	-1.00991300	-0.46585800
H	-9.54470700	-1.03956000	-1.56175100
C	-10.36208100	-2.12111800	0.13502300
H	-10.29141100	-2.09052900	1.23240200
H	-9.87020100	-0.02632400	-0.15922100
H	-9.96731400	-3.10194200	-0.16870400
C	-11.83613400	-2.02072100	-0.27837000
H	-11.90825800	-2.05113100	-1.37556000
H	-12.23210300	-1.04026500	0.02477800
O	-7.31942300	-0.04535200	-0.65679900

C	-12.71455500	-3.12798600	0.31782800
H	-12.31813600	-4.10740000	0.01430100
H	-12.64129000	-3.09721500	1.41430200
C	-14.18497800	-3.02101400	-0.09878200
H	-14.29394900	-3.08361400	-1.18851800
H	-14.78508200	-3.82487300	0.34237900
H	-14.61962100	-2.06631800	0.22211500

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C	0.09182300	-0.71885400	0.29399100
C	0.09479500	0.68448700	0.30328800
C	-1.09690000	1.41386000	0.16551300
C	-2.30435600	0.71119600	0.04218400
C	-2.33801800	-0.69077700	0.04297100
C	-1.12993900	-1.39701700	0.15882200
H	1.02792400	1.21179800	0.47766700
H	-3.23282100	1.26341900	-0.05740100
H	-1.13062700	-2.47941500	0.07652300
C	1.34192200	-1.47651800	0.41688400
C	1.52278700	-2.75680300	0.91493200
S	2.85748300	-0.79054600	-0.10696800
C	2.86398300	-3.17842300	0.88654800
H	0.71249700	-3.35473500	1.31560000
C	3.74233700	-2.23286000	0.36698200
H	3.20380800	-4.14465300	1.24548700
C	5.15022900	-2.43917600	0.24691000
H	5.48177400	-3.41664600	0.58713900
C	6.13685100	-1.61434700	-0.22101700
C	5.88212600	-0.29516900	-0.70369700
N	5.64166200	0.77668000	-1.08993200
C	7.55846100	-2.03707000	-0.25702700
O	8.47086600	-1.34693000	-0.65836100
O	7.74614800	-3.29949400	0.21295900
H	8.70430300	-3.46366900	0.14139300
C	-1.09212500	2.87726400	0.17339200
C	-2.08683100	3.76645500	0.52633600
C	-0.22621100	4.95364300	-0.08984600
C	-1.56551500	5.09048600	0.37214200
N	0.04323500	3.60301100	-0.17458700
H	0.85021500	3.20871100	-0.63459900
H	-3.06465000	3.49887400	0.90299300
C	0.58495500	6.05809500	-0.37042100
C	-2.08550700	6.38239400	0.57514900
C	-1.28246900	7.48055800	0.30201300
C	0.03832500	7.31983100	-0.16928000
H	-3.10227200	6.51516100	0.93565500
H	-1.67344900	8.48327100	0.45103400
H	0.64121500	8.19974100	-0.37579000
H	1.60391400	5.93585700	-0.72786400
C	-3.61370100	-1.39440600	-0.10498400
C	-4.78038700	-0.99925400	-0.72521500
C	-5.08014600	-3.10715900	0.12445100
C	-5.72727800	-2.06623500	-0.59866900
N	-3.79042900	-2.68669900	0.38287000
H	-3.16741600	-3.12718700	1.04271700
C	-5.72625500	-4.30307300	0.45282200
C	-7.05639400	-2.25656000	-1.01922400

H	-5.21974900	-5.08576100	1.01166400
H	-7.57107900	-1.48171200	-1.58133700
C	-7.69974400	-3.44405500	-0.69917500
C	-7.04259200	-4.45563400	0.03287700
H	-7.57413000	-5.37303200	0.27005200
H	-8.72748500	-3.60091500	-1.01470900
H	-4.92445800	-0.06918100	-1.25788100

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C	-0.36159000	0.63030700	-0.29560300
C	-0.06973900	-0.73168200	-0.46996600
C	1.27347100	-1.14016900	-0.51115600
C	2.31578600	-0.21491100	-0.37844900
C	1.99067500	1.14058700	-0.21047600
C	0.65899400	1.57957300	-0.15226400
H	-1.39233800	0.96992800	-0.32306200
H	1.51396800	-2.18913400	-0.65012800
H	2.79125600	1.86030200	-0.06917100
C	-1.13921700	-1.72185400	-0.63467300
C	-1.08166600	-2.93904200	-1.29634700
S	-2.72172600	-1.45813900	0.05076800
C	-2.29550100	-3.64605900	-1.26255300
H	-0.19576000	-3.28703900	-1.81460600
C	-3.31282500	-2.99115900	-0.57434800
H	-2.44908900	-4.61059600	-1.73608900
C	-4.62811900	-3.52092900	-0.41801400
H	-4.76596300	-4.49453000	-0.88097000
C	-5.73186300	-3.01079400	0.21194100
C	-5.73578600	-1.74582400	0.87330400
N	-5.71257500	-0.71066000	1.40608300
C	-7.01791100	-3.74691000	0.25032200
O	-8.02685700	-3.34533700	0.79051300
O	-6.96184800	-4.94541600	-0.39248200
H	-7.85305600	-5.32907300	-0.30046900
C	0.32949300	3.01178300	0.06289400
C	-0.69644000	3.39716600	0.85218200
C	1.14669000	4.05408900	-0.58214200
C	-0.97254500	4.85384000	1.13714500
H	-1.28783600	2.65462100	1.38493400
C	0.74514400	5.33353500	-0.62977000
H	2.07404000	3.75694800	-1.06553100
C	-0.59611200	5.74898800	-0.06306800
H	1.33894900	6.07911400	-1.15509700
C	3.73314100	-0.66297900	-0.38919800
C	4.12564200	-1.79428200	0.23055000
C	4.74428600	0.16883800	-1.06964000
C	5.55576100	-2.26891000	0.30003800
H	3.40056300	-2.37585800	0.79791600
C	6.01602000	-0.22642800	-1.20583300
H	4.42244300	1.11529100	-1.49599700
C	6.52910300	-1.55434900	-0.70936700
C	-2.41725100	5.13192500	1.60113800
H	-2.44819500	6.12724500	2.06657500
H	-1.32604100	6.16844200	-1.93106000
C	-3.41503300	5.09656600	0.43594900
C	-2.94949000	6.03463400	-0.68004100
H	-0.29602600	5.14093600	1.96256100

H	-0.53217200	6.78927000	0.31363500
H	-2.70133700	4.41374400	2.38106600
H	-3.48735800	4.07926500	0.03173000
H	-4.41472400	5.38604400	0.78206200
H	-2.97606000	7.08006200	-0.30811300
H	-3.62763600	5.97761400	-1.53923000
N	-1.61513100	5.62478700	-1.12036800
H	6.74199400	0.39467900	-1.72655900
H	6.63592400	-2.21228600	-1.58801000
H	5.55781500	-3.34240700	0.05846300
C	6.10445200	-2.14384300	1.74170200
H	5.40589800	-2.60017200	2.45298500
H	7.90766700	-0.53381700	0.40763100
C	8.34928000	-2.51740000	0.59100000
C	7.49765200	-2.79050200	1.86369100
H	8.31299800	-3.38499900	-0.08073600
H	7.39740600	-3.87324800	2.01645900
H	6.15325800	-1.07898800	2.00400700
H	8.00283800	-2.39777600	2.75502100
H	9.40348700	-2.37154400	0.85125500
N	7.89675200	-1.36250200	-0.18738400

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C	0.54613800	1.57059800	0.78985000
C	1.23040100	0.35604500	0.61425200
C	0.54642100	-0.86659300	0.59905000
C	-0.84936400	-0.85082500	0.74845000
C	-1.56329300	0.34487700	0.91942400
C	-0.84855100	1.54994100	0.94458200
H	2.31376700	0.35837600	0.54002200
H	-1.39379300	-1.78750300	0.68163700
H	-1.38899800	2.48181100	1.07417400
C	1.26530300	2.84848300	0.83159800
C	0.88586100	4.01950200	1.46980500
S	2.79005300	3.05226600	0.00826300
C	1.81180200	5.06395100	1.30826400
H	-0.01921300	4.10252100	2.06010300
C	2.92288400	4.72179200	0.54302900
H	1.69494700	6.05105400	1.74428800
C	3.98998400	5.62357600	0.25436000
H	3.85406200	6.61356700	0.68175000
C	5.14280800	5.44931100	-0.46378600
C	5.48770300	4.21659300	-1.09540400
N	5.74558300	3.19994100	-1.60121000
C	6.12709100	6.54416200	-0.63640400
O	7.16352700	6.44845000	-1.25898300
O	5.75210000	7.69650800	-0.01638600
H	6.46827600	8.33189700	-0.19880400
C	1.28996900	-2.14261500	0.43538700
C	2.48517400	-2.16809200	-0.42993700
C	0.91494500	-3.27712400	1.06825000
C	3.33281800	-3.20751000	-0.40924500
H	2.66557600	-1.32081800	-1.08637300
C	1.63088700	-4.59420000	0.86172000
H	0.04862600	-3.26766700	1.72523600
C	3.13855300	-4.34968200	0.56771800
H	4.23293900	-3.21832200	-1.01661900

C	-3.04311400	0.33109800	1.04089100
C	-3.82839300	1.30322300	0.52795600
C	-3.70244000	-0.80213300	1.72130900
C	-5.33323000	1.29178900	0.74225800
H	-3.41837400	2.14170100	-0.02883500
C	-5.01750500	-1.03344700	1.57568200
H	-3.09139400	-1.45816200	2.33655900
C	-5.87306800	-0.15252900	0.68674500
H	-5.47846300	-1.89498000	2.05357500
C	-6.82892700	1.72806500	-1.26698400
C	-6.12765700	0.45306500	-1.78742800
C	-6.61135500	3.36370400	0.60882700
H	-5.83278300	3.84917300	1.20844400
H	-7.00269100	4.11948300	-0.07774600
H	-7.42983800	3.07688600	1.29593500
H	-5.49405100	1.62177900	1.78355700
H	-6.89237000	-0.13494100	1.09057700
C	-6.97649500	-1.82058400	-0.90868400
H	-6.78278600	-2.63212200	-0.19681500
H	-7.99406300	-1.45509700	-0.72858800
H	-6.95308100	-2.25352300	-1.91584900
C	0.95286500	-5.45743000	-0.24014400
C	1.80039200	-6.71401900	-0.49467300
C	3.28443800	-6.41828100	-0.83063400
H	1.56932900	-5.17313100	1.79472400
H	3.57738100	-3.98468900	1.51017700
C	-0.48747100	-5.83701800	0.12799500
H	-0.93667500	-6.46103400	-0.65389800
H	-0.51864000	-6.40814000	1.06556900
H	-1.12203900	-4.95257000	0.25080800
H	1.35388600	-7.29991100	-1.31018800
H	1.75800700	-7.35324700	0.40017500
C	3.39799000	-5.71882800	-2.20313500
C	4.04287700	-7.75283600	-0.95612700
H	2.98300700	-6.36625100	-2.98467300
H	2.86455000	-4.76704800	-2.24622800
H	4.44978200	-5.52526800	-2.43783900
H	5.11363600	-7.58113500	-1.11411500
H	3.91819900	-8.39466000	-0.07854000
H	3.65976100	-8.30517500	-1.82078900
H	0.91679200	-4.85792400	-1.15945100
N	3.91262900	-5.55877500	0.22172100
C	4.35158500	-6.26750100	1.42538200
H	5.11980700	-7.00303800	1.17835800
H	4.80994500	-5.54420100	2.10737600
H	3.55219000	-6.78940500	1.98356100
N	-6.02959400	2.25403500	-0.13146900
C	-5.93343500	-0.70147600	-0.77140300
H	-4.95451600	-1.14672300	-0.98515900
H	-5.13967800	0.76393800	-2.14873600
H	-6.67892100	0.08968900	-2.66381700
C	-8.31459600	1.45895700	-0.91384300
C	-6.79241700	2.76363000	-2.41302400
H	-8.82736800	2.38776600	-0.64028200
H	-8.84243000	1.03854500	-1.77782400
H	-8.43040800	0.76172700	-0.07958900

H	-5.75725600	3.00561700	-2.67301800
H	-7.29385900	2.36636200	-3.30356100
H	-7.30243900	3.69465500	-2.14340300

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C	-0.91918300	0.39903300	-0.07752500
C	-1.09878300	-0.99039700	-0.16579200
C	0.01986700	-1.82938400	-0.03632100
C	1.29959600	-1.30214100	0.17643700
C	1.44560200	0.09074500	0.26610700
C	0.34762400	0.95553300	0.14312300
H	-1.76789500	1.05905800	-0.22806300
H	-0.10795800	-2.90500800	-0.10130000
H	2.42321200	0.50551100	0.49260400
C	-2.42473500	-1.57010900	-0.40854200
C	-2.73078600	-2.77739000	-1.01574400
S	-3.87295600	-0.73684900	0.09259800
C	-4.11296000	-3.02649800	-1.08696400
H	-1.97782400	-3.44164500	-1.42390000
C	-4.89767500	-2.01832100	-0.53654700
H	-4.54686800	-3.91279000	-1.53873900
C	-6.32511300	-2.05511600	-0.50205900
H	-6.75170100	-2.95405200	-0.93916600
C	-7.23067200	-1.15287500	-0.01429700
C	-6.84845400	0.08195500	0.59167200
N	-6.50624900	1.08174400	1.08064700
C	-8.69270700	-1.39680600	-0.08359200
O	-9.53731500	-0.63213800	0.33064600
O	-9.00265900	-2.58483400	-0.66846100
H	-9.97614500	-2.63362700	-0.65829300
C	0.51850000	2.42776800	0.24817700
C	-0.45093700	3.21033200	0.90843100
C	1.65056400	3.05085500	-0.30984600
C	-0.33308900	4.59581500	1.03126600
H	-1.30633200	2.71867300	1.36033400
C	1.76917500	4.42820000	-0.18688100
H	2.39424200	2.47151600	-0.84763800
C	0.79003900	5.19684700	0.47450700
H	-1.08957200	5.17568800	1.55046600
C	2.47340700	-2.20146700	0.32779500
C	2.36309500	-3.40126100	1.05959400
C	3.70562700	-1.85756900	-0.25883300
C	3.43976100	-4.27447400	1.22664200
H	1.41741500	-3.64130800	1.53501400
C	4.77667400	-2.72483500	-0.09312700
H	3.80456000	-0.95164100	-0.84827700
C	4.64977700	-3.92218000	0.63992100
H	3.33359000	-5.18805700	1.80321800
H	3.57558700	5.11945700	-1.13769900
H	0.75351900	7.32885200	0.77446600
C	2.41796600	6.62380800	-0.27074200
N	2.73272400	5.32894600	-0.62360200
N	1.22067500	6.51442400	0.40360700
S	3.28807800	8.00652900	-0.58798800
C	6.80264400	-3.79398300	-0.12911400
N	5.89410200	-4.53560400	0.59576700
N	6.09090700	-2.68787600	-0.54199600

H	6.52469200	-1.96776800	-1.10058800
H	6.15679600	-5.41324300	1.01965900
S	8.39777800	-4.15354200	-0.43692300

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C	-0.57807000	-0.78299300	0.02960000
C	-0.95695900	0.55888300	-0.11315000
C	0.00042300	1.58379400	-0.17487700
C	1.36153100	1.24750000	-0.08651600
C	1.77228600	-0.08496600	0.04956800
C	0.79011600	-1.08597500	0.10435400
H	-2.01246800	0.80684100	-0.17080000
H	2.10714800	2.03550300	-0.07247300
H	1.09875400	-2.12518100	0.15670400
C	-0.39610200	2.98928700	-0.31565600
C	0.35468500	4.03514800	-0.83029400
S	-1.97262200	3.54288900	0.18840100
C	-0.32854700	5.26294000	-0.82763100
H	1.35641900	3.90589100	-1.22295200
C	-1.61956200	5.19001900	-0.31374800
H	0.09140000	6.19160900	-1.20076400
C	-2.49629900	6.31249400	-0.22226100
H	-2.05567500	7.24145300	-0.57446400
C	-3.78516100	6.40974900	0.22854100
C	-4.52418700	5.29233800	0.72124700
N	-5.10599700	4.36431200	1.11631300
C	-4.51532000	7.70039600	0.23086700
O	-5.65711400	7.84572900	0.61260600
O	-3.76780600	8.73241100	-0.24694800
H	-4.34632200	9.51519000	-0.19652400
C	-1.59870400	-1.85872200	0.08226700
C	-2.77466800	-1.78392900	-0.69169800
C	-1.42220800	-2.98284200	0.90674600
C	-3.73467000	-2.78360300	-0.64619900
H	-2.92127900	-0.93847100	-1.35824100
C	-2.37975400	-3.98928100	0.95624400
H	-0.53960100	-3.05433100	1.53580100
C	-3.54748400	-3.90415900	0.18385200
H	-4.63268300	-2.72210500	-1.25043700
H	-2.25221700	-4.85475000	1.59926500
C	3.21313900	-0.42879300	0.13449600
C	4.17099800	0.26626800	-0.63168800
C	3.66495700	-1.45585100	0.98023200
C	5.52029800	-0.04597200	-0.55984700
H	3.84097300	1.04454400	-1.31464300
C	5.01602400	-1.77399600	1.05796600
H	2.95305100	-1.99055500	1.60236500
C	5.96101700	-1.07588800	0.29161000
H	6.24962600	0.48613600	-1.16027200
H	5.37076800	-2.56016800	1.71740900
N	-4.44786800	-4.98214600	0.31641900
N	7.30117600	-1.48571300	0.45260800
N	8.13733000	-0.84154700	-0.25812300
C	9.44500000	-1.23003800	-0.11039400
C	10.12531200	-2.18593500	0.64929700
C	11.49310300	-2.07352300	0.33427300
H	9.65507100	-2.86875600	1.34112300

C	11.62872100	-1.05741000	-0.60728000
H	10.15444700	0.18646200	-1.50511500
H	12.30352200	-2.66263600	0.74163100
H	12.50758600	-0.66613000	-1.09897800
N	10.38991300	-0.55854600	-0.86572600
C	-6.43401500	-7.11554600	0.44521600
C	-7.64978400	-7.74810900	0.12208700
H	-5.65746400	-7.46448500	1.10945900
C	-8.32963100	-6.92688000	-0.77294700
H	-7.78078100	-5.04227200	-1.59400300
H	-8.00532200	-8.69957700	0.49371800
H	-9.28905200	-7.05195900	-1.25370700
C	-6.39231900	-5.91127300	-0.26317800
N	-7.56215000	-5.82660600	-0.99692500
N	-5.50662600	-4.87009500	-0.38033500

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C	-1.08114900	1.21405200	-0.22039200
C	-0.05254100	2.16766600	-0.16516600
C	1.28027300	1.72906200	-0.09736400
C	1.59422600	0.36397100	-0.09704500
C	0.54376900	-0.56417600	-0.16173400
C	-0.79851900	-0.15878700	-0.21819100
H	-2.11539800	1.54238900	-0.26278700
H	2.07747300	2.45771700	0.00779100
H	0.77788200	-1.62264700	-0.21912800
C	-0.34561700	3.60530700	-0.16017100
C	0.46679100	4.63659000	-0.60538600
S	-1.85599000	4.22214200	0.45857300
C	-0.11959200	5.90551400	-0.46200100
H	1.44125700	4.46984400	-1.04940500
C	-1.39358900	5.87938300	0.09727200
H	0.35728800	6.83202100	-0.76565000
C	-2.17522400	7.05031600	0.33104200
H	-1.68087800	7.97206000	0.03575000
C	-3.42875600	7.20193100	0.85993600
C	-4.22544900	6.10341200	1.30268500
C	-4.05471700	8.53742400	1.01141500
O	-5.15950700	8.73316600	1.47172500
O	-3.25574600	9.54946100	0.57552000
H	-3.76837600	10.36492800	0.72431600
N	-4.85548700	5.19063700	1.65724300
C	-1.89021500	-1.15960700	-0.29456700
C	-3.03622700	-0.93176200	-1.07320800
C	-1.82486400	-2.37195400	0.40138100
C	-4.05590000	-1.87365800	-1.16871000
H	-3.11636600	-0.02348700	-1.66361900
C	-2.86298600	-3.29910100	0.34884700
H	-0.96964200	-2.58510500	1.03609800
C	-4.01203000	-3.07787200	-0.43172500
H	-2.76786000	-4.20093300	0.93841700
C	3.00619200	-0.08916400	-0.03107300
C	4.02105100	0.60288900	-0.71176200
C	3.37723800	-1.22215000	0.70705200
C	5.35197100	0.20350800	-0.62582300
H	3.77106100	1.46062000	-1.32912000
C	4.70176000	-1.64901500	0.76604700

H	2.62217800	-1.77540300	1.25783800
C	5.72025300	-0.93703100	0.11417500
H	4.94244900	-2.53898600	1.33699400
C	7.69595800	-0.17678900	-1.89469800
C	7.82835900	-1.28546000	-1.03580700
S	6.63281000	1.16896500	-1.40424700
N	7.07792600	-1.32696600	0.16663500
C	8.41956100	-0.10415600	-3.08496300
C	8.69635500	-2.31985500	-1.41860600
C	9.31550900	-1.11757300	-3.42819600
C	9.44710800	-2.22416500	-2.59132700
H	8.28606500	0.75698900	-3.73361700
H	9.89221900	-1.04571400	-4.34550600
H	10.12270400	-3.03298500	-2.85562000
H	8.78263900	-3.21068800	-0.80591800
C	7.54573100	-2.15712100	1.28039200
C	7.40335300	-1.46653900	2.64428300
C	7.93334400	-2.33899700	3.78995600
C	7.81730400	-1.65861500	5.15778300
H	7.05092500	-3.14198600	1.29238100
H	8.60711800	-2.34655400	1.10800600
H	7.95365100	-0.51761700	2.60798600
H	6.35519800	-1.20947000	2.83611600
H	7.38496800	-3.29187800	3.80855600
H	8.98477200	-2.59685800	3.59833600
H	8.20164800	-2.30268300	5.95653900
H	8.38493800	-0.72071800	5.18251300
H	6.77338700	-1.41971900	5.39426300
C	-6.66223500	-2.48789200	-1.57551700
C	-6.39114300	-3.63084000	-0.79383500
C	-7.97313500	-2.08947200	-1.83637700
C	-7.49350300	-4.37473000	-0.33752900
H	-8.13978100	-1.19017600	-2.42282800
H	-7.34303500	-5.26276800	0.26155300
C	-9.05351900	-2.84501200	-1.38058800
C	-8.80245700	-3.99561800	-0.64007400
H	-10.06983600	-2.53559900	-1.60452600
H	-9.62431000	-4.60491100	-0.27447200
S	-5.33855100	-1.60497300	-2.36992000
N	-5.06016900	-4.01860200	-0.50084900
C	-4.81712800	-5.37941300	-0.00870000
C	-4.98562700	-5.61969400	1.50554600
C	-4.70475000	-7.08137700	1.88014600
C	-4.86185000	-7.35644100	3.37909900
H	-5.48811700	-6.04581800	-0.56125100
H	-3.80098900	-5.65517800	-0.31134200
H	-4.31643300	-4.96029000	2.07030800
H	-5.99924300	-5.34710600	1.82109200
H	-5.38041600	-7.73915600	1.31469100
H	-3.68660900	-7.35008900	1.56342500
H	-4.65529300	-8.40637900	3.61458700
H	-4.17347500	-6.74000100	3.96979000
H	-5.88022300	-7.13224900	3.71865600

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C	-0.36396400	2.91050300	0.11028700
C	-1.26105500	1.84381900	-0.05786900

C	-0.80316600	0.53051600	-0.23005700
C	0.58088100	0.30054900	-0.22959800
C	1.50393800	1.34502100	-0.06799800
C	1.01564400	2.64705000	0.09933400
H	-2.32961200	2.03641800	-0.05923600
H	0.94792900	-0.71258700	-0.36007100
H	1.71723100	3.46525600	0.22402800
C	-0.84153400	4.28479000	0.30107400
C	-0.19487600	5.32600800	0.94902100
S	-2.38982600	4.79996100	-0.31735900
C	-0.93619000	6.51979100	0.95695100
H	0.77039600	5.21397100	1.42884600
C	-2.16815300	6.42455300	0.31703200
H	-0.60056400	7.43903000	1.42643400
C	-3.08692600	7.51127900	0.20969200
H	-2.73088800	8.43167200	0.66499700
C	-4.32756900	7.58396900	-0.36442800
C	-4.95537500	6.47359200	-1.00509000
N	-5.44600800	5.55216600	-1.52092500
C	-5.11783100	8.83854500	-0.35752300
O	-6.22073300	8.96142200	-0.84655600
O	-4.47591100	9.86538900	0.26371100
H	-5.08539000	10.62371100	0.20515500
C	-4.50457500	-3.87127100	-0.99879800
C	-5.46807800	-4.42570100	-0.21854400
C	-6.35278900	-5.47986400	-0.78747900
C	-6.77706700	-5.43025300	-2.12828000
C	-6.78323700	-6.56299100	0.00101900
C	-7.57740200	-6.43637900	-2.66645200
H	-6.49747100	-4.57945400	-2.74279900
C	-7.58144900	-7.57001600	-0.53807700
H	-6.47589800	-6.61911300	1.04080800
C	-7.98101400	-7.51336200	-1.87491300
H	-7.89854700	-6.37058400	-3.70279700
H	-7.89137800	-8.40244600	0.08840900
H	-8.60954400	-8.29518400	-2.29277900
H	-4.36614000	-4.32244100	-1.98039800
C	-5.67090500	-4.08104400	1.22012800
C	-6.93084200	-3.67317900	1.68930800
C	-4.61835200	-4.19585200	2.14287000
C	-7.12426600	-3.36044900	3.03471100
H	-7.75893700	-3.59539200	0.99017800
C	-4.81454300	-3.89414600	3.49018000
H	-3.64381500	-4.52548400	1.79490200
C	-6.06664600	-3.47016700	3.94007000
H	-8.10315000	-3.03445200	3.37641300
H	-3.98861000	-3.99316500	4.18974600
H	-6.21894300	-3.23280300	4.98957400
C	-1.75878200	-0.59110900	-0.40867600
C	-2.98015100	-0.62646100	0.28691600
C	-1.47925200	-1.65016600	-1.28789500
C	-3.87606100	-1.67666400	0.12720000
H	-3.22571100	0.17381200	0.97953600
C	-2.37954300	-2.69594900	-1.45530700
H	-0.56324000	-1.63697600	-1.87201600
C	-3.59199100	-2.74899000	-0.74077700

H	-4.81102300	-1.66103700	0.67501800
H	-2.14523000	-3.49289600	-2.15736200
C	2.96376800	1.07598500	-0.07429600
C	3.86761300	1.97119500	-0.66934600
C	3.49249200	-0.08077300	0.52572000
C	5.23400600	1.71467900	-0.66733900
H	3.49425900	2.86598200	-1.15989000
C	4.85735900	-0.34177000	0.52085100
H	2.82512300	-0.77071400	1.03481700
C	5.76547000	0.54533500	-0.08986700
H	5.90978900	2.42505300	-1.13812300
H	5.22705400	-1.23144200	1.01750100
C	7.22334900	0.36274400	-0.09953200
H	7.77521900	1.29880800	-0.17369200
C	7.97311400	-0.76811900	-0.03905300
C	7.40533800	-2.14572400	-0.13699200
C	6.61582800	-2.52181400	-1.23601300
C	7.68358300	-3.10828100	0.84791400
C	6.10471200	-3.81530700	-1.33789900
H	6.40770800	-1.79134000	-2.01221200
C	7.16289800	-4.39865300	0.75187300
H	8.30749000	-2.83706500	1.69517400
C	6.37167400	-4.75679200	-0.34174900
H	5.50009500	-4.08882900	-2.19867400
H	7.37959800	-5.12619600	1.52970800
H	5.97194700	-5.76426300	-0.42039800
C	9.45382000	-0.65860200	0.07565000
C	10.29767700	-1.57585500	-0.57763300
C	10.05288800	0.36697400	0.83030200
C	11.68383400	-1.45445100	-0.50240300
H	9.85928200	-2.38055500	-1.15984800
C	11.43931600	0.48667300	0.90732200
H	9.42223600	1.05828100	1.38177400
C	12.26207600	-0.42166700	0.23852500
H	12.31430100	-2.16854600	-1.02583600
H	11.87755700	1.28314000	1.50321600
H	13.34312800	-0.33171100	0.30248800

Cb-1

C	-0.40634900	-0.74335600	-0.24669400
C	-0.34790200	0.65304400	-0.13930600
C	0.88830600	1.30247600	0.02812100
C	2.05398700	0.51970000	0.12581000
C	2.00343900	-0.88128800	0.04166000
C	0.76631000	-1.50967800	-0.16877200
H	-1.26042300	1.23283300	-0.17564200
H	3.01040200	1.00439200	0.26689400
H	0.72023100	-2.58521700	-0.27464800
C	-1.69209100	-1.42480700	-0.44786300
C	-1.91625800	-2.65224900	-1.05272900
S	-3.19042900	-0.71632300	0.09822700
C	-3.27310400	-3.01507800	-1.08639600
H	-1.12256200	-3.25146900	-1.48320300
C	-4.12386300	-2.07728300	-0.50875300
H	-3.64443200	-3.93369300	-1.52960200
C	-5.53935100	-2.23826300	-0.43592600
H	-5.89579900	-3.16996300	-0.86735800

C	-6.51140200	-1.42361700	0.08059900
C	-6.23040600	-0.16150900	0.68511600
N	-5.97689500	0.86475400	1.17339200
C	-7.94427400	-1.80109800	0.04505500
O	-8.84840100	-1.12164600	0.48330400
O	-8.15946300	-3.01152200	-0.53981900
H	-9.12397900	-3.14667100	-0.50379600
C	-0.64361100	5.91109400	0.39209400
C	-1.87204100	4.67227200	-1.28156400
C	0.20232400	4.82338800	0.55933800
H	-0.48752100	6.81938100	0.96981400
C	-1.02695700	3.56868400	-1.12438500
H	-2.67603700	4.61781400	-2.01052900
C	-0.00170300	3.64344800	-0.17551900
H	-1.15983700	2.69009000	-1.74478400
C	2.87772800	-4.88162600	1.96666900
C	5.08872600	-4.55714400	1.04832800
C	2.44864900	-3.65483700	1.44719300
H	2.17655700	-5.47734900	2.54555400
C	4.67926500	-3.33893500	0.52705300
H	6.11284200	-4.89480500	0.90562900
C	3.35751500	-2.88833900	0.70894700
H	1.44305100	-3.30380600	1.64530400
N	3.18769600	-1.62575900	0.12040400
C	5.45560900	-2.31708600	-0.26380800
C	4.48908100	-1.08929500	-0.33495600
C	4.50241400	-0.60470800	-1.81015300
C	5.76397000	-2.66780300	-1.74148100
C	5.71990700	-1.30432600	-2.44744500
C	1.42078200	4.68433600	1.44820500
C	2.03328300	3.32023600	0.97780400
C	2.52094700	5.73861800	1.19249200
C	3.33821300	3.69029500	0.20912700
H	4.20363900	3.46261600	0.84564500
C	3.26213800	5.20796400	-0.04383000
N	0.98426900	2.69184100	0.14405200
H	2.24977200	2.64870500	1.81355200
H	1.12945900	4.66030800	2.50572200
H	3.44441900	3.10974300	-0.71209600
H	4.24800100	5.66434400	-0.18173500
H	2.67449600	5.41291900	-0.94657800
H	3.20209200	5.77806000	2.05293500
H	2.11006100	6.74408700	1.05395900
H	4.82075500	-0.29446400	0.34710800
H	6.38849100	-2.03625500	0.23907100
H	4.54594100	0.48540000	-1.89809800
H	3.58031800	-0.93323200	-2.30218300
H	6.63779600	-0.74167100	-2.22968000
H	5.63822000	-1.38257100	-3.53691900
H	6.71902400	-3.19101800	-1.85712000
H	4.97802100	-3.32333400	-2.13723500
C	-1.69652300	5.83366100	-0.52840800
C	4.17949800	-5.34265800	1.76995000
H	-2.36713500	6.67736400	-0.66150100
H	4.49089400	-6.29728100	2.18363300

Cb-2

C	0.54249700	-1.39107400	-1.14360500
C	-0.77773700	-0.94292600	-1.01466000
C	-1.08451800	0.42791400	-1.01214300
C	-0.03729100	1.35670500	-1.13510000
C	1.29032600	0.93715100	-1.27071500
C	1.56308300	-0.43891800	-1.27849100
H	-1.57423500	-1.67589400	-0.92337300
H	-0.26049400	2.41826400	-1.12874700
H	2.58955500	-0.76977100	-1.40082100
C	-2.46830800	0.90032500	-0.89138700
C	-3.00200500	2.09254000	-1.35569900
S	-3.68392700	-0.05554800	-0.08295300
C	-4.37180600	2.23335200	-1.07435600
H	-2.42353500	2.82251100	-1.90993900
C	-4.92165200	1.15499100	-0.38826900
H	-4.96633500	3.09217100	-1.36927400
C	-6.29440600	1.08222700	-0.00339500
H	-6.87542700	1.95555500	-0.28781600
C	-6.98990400	0.10542600	0.65648100
C	-6.39006100	-1.11021900	1.10368700
N	-5.87614800	-2.09328600	1.45760200
C	-8.43602900	0.24343500	0.95521000
O	-9.10238200	-0.58820200	1.53372500
O	-8.95875100	1.41799500	0.50929200
H	-9.90038000	1.39348600	0.75976600
C	0.83520700	-2.85190900	-1.17004800
C	0.11675900	-3.68854900	-2.04489800
C	1.79120400	-3.44724100	-0.33698500
C	0.34755000	-5.06453400	-2.09307800
H	-0.62047200	-3.24518800	-2.70864300
C	2.01173700	-4.84089500	-0.37843500
C	1.29757100	-5.65448800	-1.25945100
H	-0.22097900	-5.67803000	-2.78666300
H	1.46882900	-6.72715700	-1.29165800
C	3.71127900	4.82011100	0.40080500
C	4.34773900	6.64784000	1.82728600
C	2.64534400	4.51535500	1.27028700
C	3.28838500	6.34484100	2.69032100
H	5.00561300	7.48221500	2.05537900
C	2.42959200	5.27502000	2.41476000
H	3.13167100	6.94535900	3.58232300
H	1.60843500	5.04453700	3.08958900
C	2.66539000	-2.82462400	0.73874200
H	3.35745000	-2.07114100	0.34203200
C	3.02275500	-5.19112900	0.62806200
C	3.41259900	-4.01616500	1.30051500
C	3.58346700	-6.42350500	0.97112600
C	4.36320000	-4.06613900	2.31402000
H	3.28630600	-7.33427100	0.45741800
H	4.66843500	-3.16232900	2.83630800
C	4.53681000	-6.46898200	1.98998300
C	4.92431200	-5.30121200	2.65703500
H	4.98194300	-7.42050000	2.26838900
H	5.66701400	-5.35420500	3.44854400
C	3.69975400	3.85792200	-0.70924200
C	1.87052000	3.32520300	0.74402500

C	2.61627300	2.97054400	-0.53153700
C	4.56944900	3.71997200	-1.79223300
C	2.39996300	1.91935100	-1.43154900
H	5.40218100	4.40452600	-1.92999500
C	4.35524300	2.67607600	-2.69246400
C	3.29291900	1.78820700	-2.51177100
H	5.01910800	2.54940000	-3.54338300
H	3.13556000	0.98656500	-3.22824300
H	0.81862000	3.58166600	0.56518500
H	1.85952800	2.48622200	1.45367400
H	2.06371100	-2.31159500	1.50191600
C	4.56781800	5.88837000	0.67670300
H	5.39266100	6.12884000	0.01070700

Cb-3

C	0.38854700	5.85381100	-2.13931500
C	0.72049400	4.57367300	-2.61320300
C	0.33716300	3.42283200	-1.92691800
C	-0.38584800	3.58282600	-0.74211400
C	-0.74311300	4.86610600	-0.25828900
C	-0.34547700	6.00570000	-0.96661200
H	0.70544700	6.73092500	-2.69602700
H	1.28721300	4.47424000	-3.53484300
H	0.59052100	2.43908700	-2.30789100
H	-0.61073100	6.99608800	-0.60621900
C	-1.59874000	3.26335000	1.15767300
C	-2.25165200	2.72589800	2.26991300
C	-2.84078000	3.61428500	3.16768200
C	-2.77824700	5.00391100	2.97081700
C	-2.11269000	5.53318200	1.86901500
C	-1.51241500	4.66286800	0.95204500
H	-2.29514300	1.65520400	2.43956000
H	-3.35558400	3.21947300	4.03920600
H	-3.24893900	5.66926600	3.68878600
H	-2.05399800	6.60868000	1.72416000
N	-0.90976200	2.61057200	0.12379900
C	-0.77618400	1.20927700	-0.02689800
C	0.49197800	0.63986900	-0.17852000
C	-1.91464600	0.39478200	-0.01735800
C	0.63465100	-0.74803300	-0.33991500
H	1.36275000	1.28692400	-0.17640400
C	-1.77964200	-0.99028600	-0.16581000
H	-2.89725400	0.83522200	0.10607500
C	-0.51376300	-1.55749400	-0.33298200
H	-0.42815700	-2.63224000	-0.44477800
C	-4.05518400	-1.67245000	-0.97823500
C	-3.12956400	-2.93148600	0.67560000
C	-4.30399000	-0.73752900	-1.98646700
C	-4.98238200	-2.70023300	-0.67298300
C	-2.30999300	-3.44939800	1.68204700
C	-4.39427700	-3.50036200	0.38150800
C	-5.51174300	-0.83320400	-2.67513800
H	-3.58352000	0.03525600	-2.23310900
C	-6.18818200	-2.77349000	-1.37989300
C	-2.76706600	-4.56582300	2.37997900
H	-1.35362600	-2.99669300	1.92224500
C	-4.82914000	-4.62163700	1.09742900

C	-6.44868200	-1.83651000	-2.37548600
H	-5.72884500	-0.11546400	-3.46138100
H	-6.90907400	-3.55540500	-1.15599700
C	-4.01096300	-5.15173600	2.09087800
H	-2.14686700	-4.98674400	3.16659300
H	-5.79634100	-5.06852500	0.88292000
H	-7.38185900	-1.88182200	-2.92943600
H	-4.33756200	-6.02217700	2.65250400
N	-2.92914000	-1.81913700	-0.15462600
C	1.95541600	-1.36339700	-0.51909100
C	2.25248600	-2.55579900	-1.15863600
S	3.39954200	-0.60901400	0.10449200
C	3.62590400	-2.85729900	-1.15618000
H	1.50252400	-3.17347800	-1.63898700
C	4.41121400	-1.90512900	-0.51532900
H	4.05319900	-3.74179400	-1.61745600
C	5.83184100	-2.00533000	-0.39480500
H	6.24714700	-2.90225800	-0.84656500
C	6.74105800	-1.16713100	0.18890200
C	6.37367200	0.05478600	0.82908800
N	6.04488700	1.04566100	1.34445800
C	8.19357000	-1.47341800	0.19667000
O	9.04186000	-0.76694400	0.69713700
O	8.48883600	-2.64667100	-0.42432100
H	9.45678200	-2.74019400	-0.35719400

Cb-4

C	0.01850700	1.38224500	0.19333900
C	-0.89250800	0.31919000	0.29731300
C	-0.47372800	-1.01237300	0.16978000
C	0.88979000	-1.26102300	-0.05095800
C	1.82828700	-0.22220900	-0.15077000
C	1.37548900	1.09836900	-0.03347100
H	-1.93336200	0.52620100	0.52680300
H	1.22922100	-2.28753900	-0.14937800
H	2.07724100	1.91412500	-0.17403900
C	-0.42486800	2.77470000	0.31508800
C	0.31469700	3.87285800	0.72761700
S	-2.05668600	3.23915200	-0.09187400
C	-0.42189200	5.06921500	0.72787000
H	1.34771100	3.80077200	1.04721800
C	-1.74303400	4.92038800	0.31511600
H	-0.01844600	6.03008200	1.03142800
C	-2.67352800	5.99887300	0.24247400
H	-2.25515800	6.95864300	0.53410100
C	-3.99117300	6.02389000	-0.13055000
C	-4.70540600	4.85951200	-0.54481800
N	-5.26534200	3.89494900	-0.87960600
C	-4.77805100	7.27977100	-0.12975200
O	-5.94539000	7.36331300	-0.44850800
O	-4.05280400	8.35960500	0.27186200
H	-4.66942300	9.11323700	0.23090400
C	-1.44748300	-2.12827000	0.28186200
C	-2.74202400	-2.00145500	-0.24030600
C	-1.08492200	-3.33734400	0.91983000
C	-3.64865900	-3.05667900	-0.12847300
H	-3.03254800	-1.08939700	-0.75439800

C	-1.96764000	-4.40499300	1.04416700
H	-0.09422600	-3.42585800	1.35609500
C	-3.25242200	-4.26182900	0.51112900
H	-1.65994700	-5.31200300	1.55592600
C	3.26448700	-0.51229800	-0.39737700
C	4.26411700	0.23066900	0.24403100
C	3.64617600	-1.54605100	-1.28389700
C	5.61042700	-0.05263900	0.00555000
H	3.98876600	1.00979900	0.94982800
C	4.97897600	-1.84889200	-1.54140000
H	2.87297000	-2.10631900	-1.80138600
C	5.96202200	-1.09383200	-0.89441400
H	5.23479300	-2.64617400	-2.23282100
C	6.85324400	0.50222700	0.50061300
C	7.89938600	-0.22575200	-0.12682600
N	7.34573900	-1.17775700	-0.97880300
C	7.16878900	1.52945200	1.39679400
C	9.24378900	0.05528000	0.13582000
H	10.04544200	-0.50552600	-0.33545300
C	8.50602100	1.81509600	1.65853600
C	9.52952200	1.08307000	1.03239400
H	6.37932000	2.09571100	1.88439200
H	8.76310100	2.60895000	2.35389200
H	10.56705200	1.31957600	1.25244900
C	8.09097000	-2.16239600	-1.74743900
C	8.37611200	-3.45408300	-0.97317500
H	7.52092600	-2.37776300	-2.65740400
H	9.02652100	-1.69481300	-2.07244200
H	8.96422500	-3.24779200	-0.07308000
H	7.44368200	-3.93849400	-0.66559200
H	8.93882000	-4.15609300	-1.59899000
C	-5.02111100	-3.24499000	-0.55144300
C	-5.39263300	-4.55429700	-0.14608400
N	-4.30777500	-5.16314200	0.48171900
C	-5.94937400	-2.43849000	-1.21928100
C	-6.67271000	-5.05955800	-0.39286400
H	-6.96286800	-6.05670300	-0.07524100
H	-5.68108600	-1.43333000	-1.53367400
C	-7.22379700	-2.93926100	-1.47098600
C	-7.57732800	-4.23617900	-1.06072900
H	-7.95384000	-2.32176900	-1.98601500
H	-8.57867700	-4.60630700	-1.26378300
C	-4.31431000	-6.48271300	1.09256200
C	-4.77744100	-6.47768400	2.55373900
H	-4.95981200	-7.12835700	0.48748300
H	-3.30242600	-6.89406300	1.01177300
H	-4.12195300	-5.85236000	3.16857200
H	-5.79635500	-6.08635100	2.63846700
H	-4.76410300	-7.49528300	2.96064500
<u>Cb-5</u>			
C	0.17576900	2.40110100	-0.40854000
C	-1.16351100	1.98348900	-0.34015500
C	-1.49335200	0.62867800	-0.20657200
C	-0.45346700	-0.31017300	-0.13095100
C	0.89401100	0.07495300	-0.19086300
C	1.19295300	1.43629700	-0.33500900

H	-0.69883200	-1.36201900	-0.02211300
H	2.22936400	1.74300800	-0.43822500
C	1.97947900	-0.93631300	-0.12096900
C	3.18011500	-0.66436700	0.55581000
C	1.84136200	-2.19537800	-0.72858100
C	4.20444500	-1.60418100	0.61620800
H	3.31421000	0.29334500	1.05034300
C	2.85186600	-3.14918600	-0.65548500
H	0.93377900	-2.43073800	-1.27705700
C	4.04781500	-2.86024800	0.01576700
H	5.13451200	-1.36330800	1.12033000
H	2.71623800	-4.12437300	-1.11132600
C	-2.91212600	0.19852400	-0.12426700
C	-3.90312500	0.81500100	-0.90599500
C	-3.30953600	-0.83887400	0.73590700
C	-5.23234700	0.40862900	-0.84200000
H	-3.62290000	1.59611000	-1.60710900
C	-4.63933900	-1.23936200	0.82125300
H	-2.57416200	-1.31209500	1.38027900
C	-5.61535800	-0.62082400	0.02789900
H	-5.97465400	0.86666700	-1.48749300
H	-4.93249900	-2.01372500	1.52244300
H	-1.95471900	2.72618300	-0.33698600
C	0.49084100	3.82663100	-0.55268300
C	-0.28858900	4.81808700	-1.12729100
S	1.99493100	4.48009500	0.04204500
C	0.31880300	6.08563600	-1.10039300
H	-1.25362600	4.62217400	-1.58004700
C	1.57603600	6.09702100	-0.50446400
H	-0.13104400	6.98281100	-1.51352700
C	2.37728800	7.27124000	-0.37074400
H	1.91216100	8.16755200	-0.77253000
C	3.61979800	7.44929700	0.17457500
C	4.37734600	6.38386500	0.74804500
C	4.27521800	8.77958400	0.20765600
N	4.97250100	5.49571500	1.20933200
O	5.37247300	8.99463900	0.67655400
O	3.51282100	9.75860500	-0.35004900
H	4.04041400	10.57439800	-0.27135200
C	-8.07122600	-0.17975500	0.25283900
C	-9.22741200	-0.89862600	0.31302400
C	-8.88528800	-2.28705400	0.19371000
N	-6.97076100	-1.01909100	0.11261200
C	-8.25008500	1.28710600	0.50675100
C	-10.40867400	-0.01182700	0.59284500
C	-9.80328600	1.41517700	0.38211400
H	-11.26673700	-0.18550500	-0.06841500
H	-10.77628300	-0.14267900	1.62124500
H	-7.89516700	1.56246300	1.51109300
H	-7.72900100	1.94490300	-0.19821600
H	-10.21118000	2.14972600	1.08315000
H	-10.04767200	1.76114100	-0.62807100
C	-7.46371200	-2.33417400	0.06174100
C	5.60733300	-4.58349000	-0.96068400
C	6.61432000	-5.45031600	-0.43584100
C	6.67825300	-5.17869000	0.97152600

N	5.07800500	-3.82766700	0.09916300
C	5.76182200	-4.20891600	1.24904200
C	6.87365900	-4.63187700	3.28517900
C	5.61018000	-3.91197700	2.71094100
C	7.33337300	-5.68690100	2.22554500
H	6.97931700	-6.69551300	2.48510600
H	8.42732400	-5.74687000	2.16738700
H	6.67977000	-5.08030000	4.26433100
H	7.66911100	-3.89111000	3.42010900
H	5.59706100	-2.84656900	2.96702600
H	4.67790200	-4.34006700	3.10864900
C	7.29974700	-6.30673000	-1.31228000
C	5.31694200	-4.53751300	-2.32679600
C	6.01619200	-5.39825100	-3.16936100
C	6.99229700	-6.27905300	-2.66765400
H	8.06686700	-6.97688500	-0.93307900
H	4.57616100	-3.85132500	-2.72439700
H	5.80375500	-5.38473200	-4.23488900
H	7.51727000	-6.93957200	-3.35248600
C	-6.78369200	-3.53888200	-0.13523200
C	-7.53398900	-4.71195100	-0.16119600
C	-8.93243900	-4.68873300	-0.00592800
C	-9.61192500	-3.48811500	0.16474300
H	-5.70703800	-3.56481500	-0.26888600
H	-7.02696900	-5.66187400	-0.30675500
H	-9.48704600	-5.62293300	-0.02778000
H	-10.69385700	-3.47511400	0.26761600

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C	1.19882300	1.62602200	-0.39376700
C	0.14966800	2.55661000	-0.45714900
C	-1.17399700	2.09442200	-0.37771200
C	-1.45757600	0.73003400	-0.23950200
C	-0.38698200	-0.17468000	-0.17356600
C	0.94639700	0.25540100	-0.24825000
H	2.22344700	1.96727200	-0.50568500
H	-1.99172200	2.80645600	-0.42295300
H	-0.59492800	-1.22718500	-0.00748000
C	0.41469000	3.99041400	-0.62190600
C	-0.40044600	4.94712600	-1.20535300
S	1.89840600	4.70147600	-0.04252500
C	0.16392700	6.23497300	-1.19669900
H	-1.35963300	4.71316300	-1.65257100
C	1.42229200	6.29641100	-0.60664500
H	-0.31785200	7.11101000	-1.61904200
C	2.18399400	7.49881100	-0.49023500
H	1.68734600	8.37411200	-0.90051300
C	3.42185400	7.72455300	0.04745100
C	4.21664600	6.69143800	0.62962200
N	4.84210300	5.82819100	1.09801300
C	4.03298700	9.07635800	0.06242200
O	5.12433900	9.33258200	0.52411000
O	3.23620900	10.02269300	-0.50307200
H	3.73624500	10.85672900	-0.43631300
C	2.06588500	-0.71717000	-0.17187100
C	1.96839300	-1.98581000	-0.76692600
C	3.25952100	-0.40009800	0.49785600

C	3.00967600	-2.90514100	-0.68964900
H	1.06630600	-2.25708600	-1.30777700
C	4.31518100	-1.30386800	0.56426800
H	3.36412900	0.56609400	0.98275500
C	4.19683300	-2.56925900	-0.02550700
H	2.90158300	-3.89013400	-1.13171300
H	5.23876100	-1.02595500	1.06118000
C	-2.86125800	0.25405400	-0.14222100
C	-3.82768200	0.97774000	0.57561100
C	-3.26803700	-0.93648500	-0.76669500
C	-5.14633300	0.54146900	0.65882000
H	-3.54220300	1.89250900	1.08708700
C	-4.57926200	-1.39273000	-0.67428900
H	-2.54871700	-1.51255500	-1.34167600
C	-5.53317600	-0.65277700	0.03666800
H	-5.88275600	1.13045800	1.19563600
H	-4.86501300	-2.32980200	-1.14079000
C	6.05759400	-3.76397900	1.16525500
C	5.71589600	-4.32770500	-0.97807200
C	6.99881500	-4.74700100	0.84206300
C	6.77970300	-5.10671200	-0.51100000
C	-7.68187600	-1.08868100	1.26194400
C	-7.63366500	-1.65500900	-0.90715100
C	-8.93780700	-1.61716100	0.94550000
C	-8.90572200	-1.97958800	-0.42412200
N	5.26150800	-3.49662100	0.04875400
N	-6.86975700	-1.10582400	0.12545600
C	-7.52861200	-0.73712600	2.63456000
C	-8.60251400	-2.41994200	-2.84815300
C	-7.46234200	-1.89757800	-2.30102400
C	-8.67843400	-0.98774500	3.33253700
S	-9.96299600	-1.66773700	2.34877800
S	-9.90986300	-2.61449200	-1.69352800
C	5.41517500	-4.52273800	-2.35744000
C	6.10255700	-3.34164300	2.52570100
C	7.09030300	-3.99896100	3.20698000
C	6.24422700	-5.46121900	-2.90886400
S	7.41464600	-6.11569800	-1.77652900
S	7.97511500	-5.15151300	2.22255700
H	7.36801800	-3.87411100	4.24471900
H	5.45076100	-2.60488600	2.97871200
H	6.24196900	-5.82307700	-3.92802100
H	4.64373500	-4.00407800	-2.91316800
H	-8.76283800	-2.71572600	-3.87599000
H	-6.56200800	-1.69813100	-2.86901400
H	-8.86178400	-0.80922900	4.38332400
H	-6.63103200	-0.33098900	3.08442900

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C	0.39321900	2.18833200	0.64341900
C	1.30601400	1.12423300	0.57431100
C	0.86921900	-0.19978600	0.42313700
C	-0.51272900	-0.43677100	0.34736500
C	-1.45345000	0.60303600	0.42617000
C	-0.98251400	1.91515300	0.57069600
H	2.36731400	1.32197400	0.68919200
H	-0.86344100	-1.44868100	0.17024800

H	-1.69364900	2.73301600	0.62555000
C	0.85421300	3.57004400	0.81319100
C	0.17627600	4.63307400	1.39136200
S	2.42912200	4.06746900	0.25044000
C	0.91539000	5.82774900	1.39201600
H	-0.81048400	4.53435500	1.82843200
C	2.17741100	5.71342800	0.81527500
H	0.55762400	6.76219700	1.81283900
C	3.09991700	6.79576600	0.71349200
H	2.72421000	7.73118600	1.11982400
C	4.36662200	6.85046100	0.19446800
C	5.02273200	5.72006100	-0.37925200
N	5.53673200	4.78302800	-0.84170800
C	5.15570500	8.10456900	0.19483100
O	6.28001700	8.21343100	-0.24749700
O	4.48710300	9.15183300	0.75157500
H	5.10000300	9.90745300	0.69462000
C	1.84209200	-1.31495600	0.33973300
C	3.08993000	-1.14655200	-0.29826900
C	1.56196000	-2.56896100	0.90618400
C	3.98960600	-2.19433600	-0.36972600
H	3.34010200	-0.19119200	-0.75327000
C	2.45871600	-3.63674900	0.84305100
H	0.62908800	-2.70991600	1.44522700
C	3.67965700	-3.45028100	0.18314300
H	2.21574600	-4.57506200	1.32722400
C	-2.90688100	0.32193000	0.33364800
C	-3.46214400	-0.82274400	0.92771100
C	-3.78023900	1.20043600	-0.34214000
C	-4.82499200	-1.11747900	0.85914500
H	-2.81719700	-1.48976900	1.49320400
C	-5.13331600	0.92369300	-0.42025300
H	-3.38324300	2.09099200	-0.82343400
C	-5.66800700	-0.24095000	0.16555800
H	-5.21367400	-1.99161600	1.36760400
N	-7.05094700	-0.29324400	-0.02080600
C	-6.23951900	1.70115400	-1.08804700
C	-7.54061600	0.96510300	-0.62591700
C	-8.40982500	0.76822700	-1.89685900
C	-6.28446900	1.65648400	-2.63669700
C	-7.78739100	1.70541400	-2.95114400
C	-7.92329600	-1.31766800	0.38209500
C	-9.21945500	-1.00894600	0.83430900
C	-7.54643800	-2.67187800	0.30444300
C	-10.09753100	-2.02189500	1.21474200
H	-9.53751800	0.02647000	0.89792300
C	-8.42808000	-3.67508700	0.70076800
H	-6.57390300	-2.93561600	-0.09563800
C	-9.70839500	-3.36106000	1.16068700
H	-11.09225300	-1.75712500	1.56408600
H	-8.11399100	-4.71337000	0.63038200
H	-10.39414200	-4.14719600	1.46274700
C	5.37246200	-2.22389600	-0.97972600
C	5.91376100	-3.64324500	-0.58814100
C	5.41238500	-2.17406300	-2.53649700
C	6.37979800	-4.28967700	-1.90838500

H	7.42865500	-4.01529900	-2.08397600
C	5.48418800	-3.64574300	-2.97837900
N	4.74317900	-4.33503600	0.00763900
C	4.78259800	-5.68863100	0.38393500
C	3.65484500	-6.51872700	0.23967600
C	5.97106900	-6.25599600	0.87981200
C	3.70999900	-7.85953000	0.61421200
H	2.74560900	-6.11590500	-0.19245300
C	6.01898700	-7.60221300	1.23665900
H	6.85659500	-5.63994800	0.99631500
C	4.88920400	-8.41288700	1.11659500
H	2.82553300	-8.47981100	0.49298400
H	6.94811500	-8.01561100	1.62060500
H	4.92936300	-9.46019500	1.40142600
H	6.72264000	-3.58339700	0.14991500
H	5.99577900	-1.42853300	-0.55800700
H	6.32659300	-5.38200400	-1.88192300
H	5.87575800	-3.76852400	-3.99366900
H	4.48599700	-4.10038600	-2.95325000
H	6.31658300	-1.64471800	-2.86211600
H	4.55251900	-1.63770200	-2.95013500
H	-8.07352300	1.55542300	0.13139800
H	-6.25772500	2.74678500	-0.75901500
H	-9.47055000	0.97131700	-1.72024600
H	-8.32922100	-0.27367900	-2.22596100
H	-8.16341700	2.72891600	-2.81838500
H	-8.02480300	1.40297800	-3.97671500
H	-5.71348800	2.47039300	-3.09569700
H	-5.85540100	0.71112500	-2.99182300

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C	-1.26409800	1.42631800	0.32964700
C	-0.27468900	2.42215600	0.34730600
C	1.07577000	2.04384400	0.26734300
C	1.44495600	0.69545000	0.17647900
C	0.43059200	-0.27421100	0.15227800
C	-0.92817200	0.06959100	0.22484200
H	-2.30701800	1.70516800	0.44570500
H	1.84431900	2.80856800	0.22064800
H	0.70621100	-1.32123600	0.07278700
C	-0.62983100	3.84154900	0.44503700
C	0.13303900	4.87843200	0.96074100
S	-2.16705600	4.42751100	-0.13607300
C	-0.51246300	6.12485200	0.90081400
H	1.11471200	4.72799600	1.39450900
C	-1.78444000	6.07683000	0.33716500
H	-0.07988700	7.05043100	1.26737200
C	-2.62155300	7.22078800	0.17977900
H	-2.17327300	8.14398500	0.53753200
C	-3.88143400	7.34613500	-0.34266400
C	-4.57199300	8.65585200	-0.40703500
O	-5.68494400	8.82819800	-0.85749000
O	-3.82423300	9.67491000	0.09867200
H	-4.37680500	10.47189400	0.00204700
C	-4.62278700	6.24202700	-0.86119000
N	-5.20639000	5.32496800	-1.27880800
C	-8.05021800	-2.61562100	-1.87401300

C	-6.28607100	-0.94479200	-1.81440700
C	-7.29317800	-3.51050700	-1.12076300
H	-9.04679500	-2.90632700	-2.19539900
C	-5.50416400	-1.82526300	-1.05730000
H	-5.91013100	0.04087900	-2.07557800
C	-6.01668800	-3.10473500	-0.72347100
H	-7.68387700	-4.48546900	-0.84777700
C	2.87561200	0.30484800	0.08490200
C	3.84773200	0.96934700	0.84312200
C	3.27955100	-0.74426700	-0.77412300
C	5.18922100	0.59101200	0.74942000
H	3.55300900	1.76420700	1.52301700
C	4.60727800	-1.14124800	-0.88745600
H	2.53183200	-1.23693100	-1.38877800
C	5.55913500	-0.47136600	-0.11454500
H	4.89334900	-1.93737500	-1.56715400
N	-5.06598500	-3.79210700	0.04073100
C	-4.18497900	-1.73721700	-0.46505600
C	-3.95208200	-2.96799500	0.20080200
C	-5.20957200	-5.10827000	0.56248000
C	-5.17007800	-5.33079500	1.94586900
C	-5.39248000	-6.19417800	-0.29952800
C	-5.29894000	-6.61643000	2.45985200
H	-5.04350300	-4.48676200	2.61695300
C	-5.54410400	-7.48215000	0.21118600
H	-5.41139200	-6.02806500	-1.37219000
C	-5.49204100	-7.69817500	1.59251000
H	-5.26757800	-6.79918900	3.52907900
H	-5.68961800	-8.32075600	-0.46718800
O	-5.62301100	-8.93655300	2.15354700
H	-5.75458500	-9.59198300	1.45089600
C	-2.74596200	-3.21680600	0.86080000
C	-3.19871200	-0.74881000	-0.45570000
H	-3.36197800	0.18473100	-0.98702600
H	-2.56611800	-4.15810600	1.36994100
C	-1.78152600	-2.21507900	0.85527100
C	-1.98475500	-0.97428400	0.20676000
H	-0.85170300	-2.38341700	1.39072700
C	6.40721800	1.06311700	1.37551000
C	7.46475900	0.26986400	0.86085700
N	6.93963700	-0.65945700	-0.04321400
C	7.68654500	-1.63292400	-0.76532900
C	7.44167000	-2.99626200	-0.57406100
C	8.67484200	-1.23480700	-1.67605100
C	8.16463500	-3.94944900	-1.28926400
H	6.68654900	-3.30905700	0.14050800
C	9.41380900	-2.18163600	-2.37651900
H	8.85652600	-0.17626500	-1.83491400
C	9.15709000	-3.54513500	-2.18881100
H	7.96511100	-5.00839000	-1.13650900
H	10.18274100	-1.88403300	-3.08203000
O	9.90625500	-4.42902200	-2.91097300
H	9.63250600	-5.33323400	-2.69157800
C	8.78703500	0.45123600	1.27448200
C	6.69055400	2.06329900	2.31308600
H	9.58785100	-0.16896700	0.88498800

H	5.89191600	2.67951300	2.71812400
C	9.04073100	1.45318800	2.20857200
C	8.00667900	2.25477200	2.72334000
H	10.06075300	1.61489600	2.54657300
H	8.23893200	3.02806500	3.44998400
C	-7.55496600	-1.34656600	-2.22137700
H	-8.17139400	-0.67220900	-2.80863700
H-1			
C	0.92345800	-0.20943800	0.20641600
C	1.05285000	-1.59938300	0.32873100
C	-0.06872700	-2.44178200	0.27519900
C	-1.34042000	-1.87116000	0.10320200
C	-1.50240200	-0.48501500	-0.01526600
C	-0.36044300	0.32969700	0.03471100
H	2.03424000	-2.02475100	0.51489200
H	-2.21382100	-2.51375100	0.05987700
H	-0.46865400	1.39915500	-0.11692100
C	-2.84982900	0.10479300	-0.21441200
C	-4.47440900	1.86504400	0.23369000
C	-3.81230300	-0.52153200	-1.01881900
C	-5.43855000	1.23567100	-0.57964500
C	-5.07345700	0.03717800	-1.21221200
H	-3.56133600	-1.44078800	-1.54022800
H	-5.77255900	-0.46526900	-1.87055400
C	-6.76917300	3.23258100	-0.92510200
C	-5.96636000	4.07003800	-0.12622600
S	-4.93786100	3.33435300	1.13118900
N	-6.71597100	1.82487600	-0.73166100
C	-7.58166100	3.83244600	-1.89999000
C	-5.99725300	5.45562600	-0.28390000
H	-5.35591900	6.07297300	0.33870400
H	-8.17034000	3.21807400	-2.57191500
C	-7.63675500	5.22119000	-2.02892800
C	-6.85070800	6.03971800	-1.22047200
H	-8.28708200	5.65747600	-2.78203000
H	-6.88646700	7.12001600	-1.32468900
C	-7.82477400	0.99726000	-1.21546400
C	-8.25296100	-0.14985400	-0.26886100
C	-8.69371200	0.38624700	1.12184000
C	-9.37341000	-0.95620800	-0.97739200
C	-7.62166800	0.32168100	2.21561000
C	-9.40641500	-2.46498500	-0.67095500
C	-9.70797000	-2.86728800	0.77927900
C	-9.80265200	-4.38667200	0.95827200
H	-8.68698600	1.65801400	-1.32714300
H	-7.60853300	0.59563100	-2.21803300
H	-7.39659500	-0.82246900	-0.12610000
H	-9.03697100	1.42442200	1.01337600
H	-9.56850000	-0.18042000	1.46001300
H	-8.02116000	0.68259000	3.17064800
H	-7.27809500	-0.70942200	2.36977100
H	-10.34859100	-0.50804000	-0.73711500
H	-9.26050900	-0.85398500	-2.06626600
H	-10.16158200	-2.92777800	-1.32285400
H	-8.44332100	-2.90648600	-0.96925500
H	-10.01683100	-4.65431300	1.99914800

H	-10.59864800	-4.81100500	0.33393600
H	-8.86374400	-4.87840000	0.67460400
H	-6.75054900	0.93410100	1.96880000
H	-8.93152900	-2.47443600	1.44805000
H	-10.65204800	-2.40312000	1.09825800
C	2.12180200	0.66482500	0.25235300
C	2.07265700	1.93022600	0.85576200
C	3.33817300	0.26374400	-0.32049800
C	3.20278600	2.74386400	0.92509000
H	1.15139500	2.27547100	1.31632900
C	4.45603800	1.09197300	-0.28816400
H	3.40167100	-0.68570700	-0.84387200
C	4.42695200	2.33648300	0.35994900
H	5.35976500	0.77902800	-0.79570900
C	5.42870900	4.56403900	0.33170300
C	4.30773300	5.21615600	0.87733800
C	6.39836000	5.34711000	-0.31260600
C	4.15916700	6.60082300	0.76278500
H	7.25742100	4.85783200	-0.75754900
H	3.27421700	7.07528400	1.17798000
C	6.27104400	6.73366600	-0.38700500
C	5.14707700	7.36603300	0.14443100
H	5.03346600	8.44388400	0.07377300
H	7.04468700	7.31510000	-0.88088900
N	5.58422300	3.15360100	0.41846500
S	3.10772700	4.28581800	1.81293600
C	6.79939700	2.62658100	1.08450200
C	7.72658900	1.67370500	0.28975600
C	8.10239300	2.24537100	-1.09228200
C	8.98040700	1.35920600	1.13810600
C	8.72137600	0.58400700	2.43753200
C	8.80076600	1.28023400	-2.06863300
C	7.94007900	0.09782000	-2.53693100
C	8.64160700	-0.76968200	-3.58760900
H	9.66757200	0.31442400	2.92023200
H	8.14050400	1.16282600	3.16346600
H	8.17448900	-0.34629100	2.24026900
H	9.67634000	0.77460700	0.52476900
H	7.19031000	2.62281900	-1.57309300
H	8.75396400	3.11950000	-0.94075100
H	9.10653100	1.85860600	-2.95210500
H	9.73297400	0.89725000	-1.63091100
H	7.66586300	-0.53241400	-1.68025000
H	6.99626500	0.48143700	-2.95130100
H	8.00803300	-1.60591100	-3.90340400
H	8.89322500	-0.18407700	-4.48047700
H	9.57526200	-1.19020200	-3.19417800
H	9.50104500	2.30124700	1.36751200
H	7.19295100	0.72578800	0.14574400
H	7.38189800	3.50331400	1.38689900
H	6.48355100	2.12392500	2.00707400
C	0.06714200	-3.89551900	0.41617800
C	-0.87252200	-4.79943800	0.88732900
S	1.54138900	-4.70866400	-0.04114700
C	-0.41123700	-6.12700900	0.89061600
H	-1.84973500	-4.50042700	1.24822400

C	0.89116300	-6.27450600	0.42276100
H	-0.99805700	-6.97210500	1.23636900
C	1.56484300	-7.52984000	0.34290400
H	0.96214900	-8.37231400	0.67184500
C	2.83067000	-7.84285500	-0.07469600
C	3.76172600	-6.86489400	-0.53777500
N	4.50199700	-6.04701300	-0.91060700
C	3.33038700	-9.23874500	-0.07268200
O	4.44033400	-9.57403500	-0.42816100
O	2.40621700	-10.13131500	0.37586800
H	2.84444000	-11.00080100	0.33208300
C	-3.20361800	1.32005000	0.39348400
H	-2.49209100	1.83262100	1.03422900

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C	-1.26885400	1.68026300	-0.27706500
C	-1.31897800	3.06802100	-0.07210300
C	-0.14787000	3.83976700	-0.05061100
C	1.09023800	3.21007100	-0.25250100
C	1.16918100	1.82779200	-0.47631500
C	-0.01734800	1.07768800	-0.47870500
H	-2.28088300	3.54805400	0.07562900
H	2.00060700	3.79929700	-0.24205000
H	0.03554000	0.00573200	-0.64545700
C	-0.19682300	5.28777400	0.18504600
C	0.79315100	6.09336300	0.72545300
S	-1.61108200	6.22418500	-0.22340100
C	0.41826800	7.44473300	0.81887200
H	1.74501800	5.70753100	1.07131800
C	-0.86654400	7.70815800	0.35440400
H	1.05456100	8.22384700	1.22644900
C	-1.45616200	9.00808100	0.35964300
H	-0.80105500	9.78410200	0.74667300
C	-2.69600400	9.43188100	-0.03622800
C	-3.68799400	8.55126100	-0.56356100
N	-4.47984800	7.81107200	-0.98886300
C	-3.10207800	10.85482900	0.06110800
O	-4.18590100	11.28636500	-0.26989300
O	-2.12237100	11.65134200	0.56870900
H	-2.50158600	12.54907400	0.58429700
C	-2.50798600	0.89290700	-0.27649700
C	-3.70869200	1.18906000	0.33072900
S	-2.62482900	-0.64365400	-1.11070900
C	-4.70988100	0.20104400	0.13444200
H	-3.86874300	2.08621700	0.91905400
C	-4.29229100	-0.86800200	-0.62415700
H	-5.71817700	0.28081300	0.52520500
C	2.47456700	1.19632300	-0.70688000
C	3.60907200	1.75554700	-1.25267200
S	2.78160300	-0.47218000	-0.27099800
C	4.70910400	0.86021300	-1.33054100
H	3.64151500	2.77267100	-1.62886300
C	4.43566000	-0.39721900	-0.84314500
C	-5.07032200	-2.33560000	-2.46641800
C	-6.62505800	-4.17839000	-2.15672100
C	-5.06129900	-2.03378900	-1.09671800
H	-4.49497100	-1.71124900	-3.14305300

C	-6.59819100	-3.90647000	-0.78708000
H	-7.23500400	-4.98054800	-2.55792000
C	-5.82590300	-2.84997900	-0.22938900
C	-6.02964000	-2.90864000	1.21053500
C	-6.93719100	-3.97443500	1.45112300
N	-7.27916500	-4.56857200	0.23497200
C	-5.51033500	-2.20886200	2.31153400
C	-7.33478800	-4.33850600	2.74064100
H	-4.79978600	-1.40440300	2.16420800
H	-8.01994600	-5.16404500	2.90267600
C	-5.90449000	-2.56459600	3.59738000
C	-6.81059300	-3.61724100	3.80879200
H	-5.50302600	-2.02297100	4.44919800
H	-7.10327800	-3.87988900	4.82181700
C	-8.14923400	-5.68277400	0.07152700
C	-9.48072300	-5.59787700	0.49633600
C	-7.67654900	-6.86609000	-0.50910100
C	-10.32943800	-6.69463900	0.34698800
H	-9.84230700	-4.67165400	0.93226800
C	-8.53675800	-7.95188300	-0.67249400
H	-6.63816600	-6.92980200	-0.81938900
C	-9.86249900	-7.87154700	-0.24165800
H	-11.36110100	-6.62324400	0.68027300
H	-8.16484700	-8.86666400	-1.12571100
H	-10.52795400	-8.72149600	-0.36366400
C	5.28912900	-1.59855600	-0.82653400
C	4.79242800	-2.79478300	-1.36522200
C	6.61073900	-1.59494000	-0.31903600
C	5.57858400	-3.95066700	-1.44504700
C	7.38509800	-2.78417300	-0.41784800
C	6.89113200	-3.96066100	-0.98582200
H	7.50829400	-4.84932200	-1.06211200
C	7.44924100	-0.61476500	0.35530500
C	8.69744200	-1.24636900	0.60216900
N	8.64989000	-2.55729800	0.12547300
C	9.74112300	-0.60036700	1.27076200
C	7.26180500	0.69959700	0.81252900
C	9.52654200	0.70557600	1.69993400
C	8.29767700	1.34882400	1.47643400
H	5.15973000	-4.84943400	-1.88880700
H	3.78312100	-2.80842200	-1.76492100
H	10.68234400	-1.10608100	1.45927900
H	6.31432900	1.20245900	0.66053800
H	8.15247200	2.36567600	1.83024900
H	10.32149800	1.23047800	2.22278700
C	9.70244100	-3.51125200	0.21477400
C	10.93391200	-3.25217500	-0.39900800
C	9.51164700	-4.70637100	0.91902100
C	11.96907200	-4.18182800	-0.30031100
H	11.06795200	-2.32918900	-0.95474000
C	10.54548500	-5.63951200	0.99688100
H	8.55978100	-4.89147100	1.40715200
C	11.77687600	-5.37885600	0.39237800
H	12.92312900	-3.97434900	-0.77699000
H	10.39097300	-6.56605900	1.54289300
H	12.58244000	-6.10442000	0.46115000

H	5.66772800	1.12100900	-1.76513400
C	-5.83883700	-3.38490800	-2.98512700
H	-5.83279500	-3.57024900	-4.05554500

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C	-0.76401900	-0.37124900	0.13886300
C	-1.24707500	0.94299700	0.17124200
C	-0.37348100	2.04200900	0.16597600
C	1.01027500	1.80323300	0.12887600
C	1.52130600	0.49982200	0.10392900
C	0.62298000	-0.57755100	0.10597500
H	-2.31948700	1.11226100	0.19073800
H	1.69523000	2.64250600	0.06639300
H	1.01012500	-1.59124900	0.12562900
C	2.98845900	0.26251000	0.07681300
C	3.53476900	-0.76425900	-0.70686300
C	3.84812300	1.07236400	0.84019400
C	4.91294300	-0.97549600	-0.73020700
C	5.22825000	0.86847700	0.82321800
H	3.43247600	1.85037800	1.47507100
C	5.77523900	-0.16449700	0.03167200
C	5.47613200	-2.05910900	-1.57255100
C	7.19661400	-0.36799800	0.02244900
C	7.48740100	1.52583200	1.63021700
H	5.72822700	2.39007500	2.15382900
C	7.73819100	-1.40042900	-0.77432200
C	8.05461100	0.44288600	0.79248500
H	7.23302500	-2.92465500	-2.09914900
C	9.12076400	-1.60688900	-0.79082600
C	9.43444600	0.22930300	0.77008700
H	9.54041300	-2.40091200	-1.40334600
C	9.95626900	-0.79348100	-0.02133000
H	10.07196900	0.86711900	1.37197400
H	11.02828300	-0.96576500	-0.04414200
O	8.14900100	2.27928000	2.33259700
H	2.90745100	-1.39455000	-1.32730400
O	4.80888000	-2.80967300	-2.27174000
N	6.10056900	1.64708400	1.57372200
N	6.86210600	-2.17964200	-1.52041400
C	-1.70127300	-1.52495300	0.15933800
C	-1.43393000	-2.67571700	-0.59630800
C	-2.87099400	-1.47311900	0.93825100
C	-2.31830800	-3.75343700	-0.57546700
H	-0.55630900	-2.74439700	-1.22932900
C	-3.76275400	-2.54600700	0.96403900
H	-3.07458800	-0.59882600	1.55053900
C	-3.49026400	-3.70330100	0.20261800
C	-2.02501800	-4.96005600	-1.38681300
C	-4.41110700	-4.80424900	0.23931900
C	-5.86826900	-3.54281100	1.83401000
H	-5.13763400	-1.70292000	2.28047900
C	-4.13620700	-5.95680400	-0.52876600
C	-5.57887700	-4.75174100	1.02648300
H	-2.76220400	-6.79115900	-1.85164500
C	-5.02678500	-7.03394800	-0.50088200
C	-6.46269200	-5.83257200	1.04883300
H	-4.81795300	-7.92223700	-1.09176200

C	-6.17993300	-6.96442600	0.28479900
H	-7.35398500	-5.76605100	1.66258200
H	-6.86301000	-7.80865700	0.29629000
N	-4.92079900	-2.52649900	1.73072300
N	-2.97451100	-5.97328300	-1.29175500
O	-6.85173900	-3.40671300	2.54976000
O	-1.03617300	-5.09386900	-2.09576500
C	-0.88025300	3.41889400	0.18528100
C	-0.22282400	4.56079200	0.61465500
S	-2.48874600	3.79908200	-0.37492300
C	-1.00207900	5.72557800	0.50253000
H	0.78063100	4.54827300	1.02379100
C	-2.27522500	5.50507600	-0.01195100
H	-0.66241200	6.71316900	0.79763300
C	-3.24023200	6.54048600	-0.20617500
H	-2.88166300	7.53021600	0.06393300
C	-4.52655200	6.48795200	-0.66853700
C	-5.36387000	7.70718800	-0.79071700
C	-5.16268100	5.27137600	-1.05994500
N	-5.65569400	4.26278100	-1.36873300
O	-6.50872800	7.71729200	-1.18892600
O	-4.71139400	8.83639000	-0.40514500
H	-5.35152500	9.56126800	-0.52743300

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C	-0.99039900	-2.81957000	-0.62880000
C	-0.49087200	-3.96815100	-1.22385700
S	-2.61312500	-3.07568900	-0.04251300
C	-1.40382800	-5.03646900	-1.21905900
H	0.49174600	-4.01624600	-1.67862400
C	-2.62481900	-4.73583200	-0.62153300
H	-1.19937200	-6.01080900	-1.65162700
C	-3.70152300	-5.66414800	-0.51084800
H	-3.48031300	-6.64404100	-0.92575000
C	-4.95429600	-5.52455400	0.02560100
C	-5.41872500	-4.30817900	0.61068900
N	-5.77211600	-3.30331300	1.08129500
C	-5.92883300	-6.64079100	0.03306300
O	-7.05034200	-6.57506300	0.49057500
O	-5.43834700	-7.77656500	-0.53492700
H	-6.16030900	-8.42824600	-0.47209600
C	-1.20888200	2.14493400	-0.15614300
C	-0.84001800	3.45306500	-0.42387500
C	-3.03231000	3.43950600	0.19815000
C	-1.97599300	4.28620300	-0.20921500
N	-2.55391100	2.14864100	0.19773900
H	-3.03534600	1.36147400	0.60480300
H	0.13109700	3.76645700	-0.78214900
C	-4.32466300	3.93015400	0.52133200
C	-2.21941600	5.69127600	-0.32166500
C	-3.50193500	6.19150900	-0.00465100
C	-4.53849300	5.32410100	0.41446800
C	-1.42007000	6.81591900	-0.70245800
C	-5.56001400	3.34735600	0.95756500
C	-6.46450700	4.36869600	1.10104300
C	-2.20994700	7.93556800	-0.61110100
H	-1.98336500	8.97308900	-0.81132000

H	-7.49991900	4.34910900	1.40917200
H	-0.38283200	6.79922500	-1.00774000
H	-5.76210700	2.30061500	1.14024400
N	-3.47137200	7.56188200	-0.18723100
N	-5.85024400	5.56438900	0.77288500
H	-6.30094400	6.46450300	0.80115200
H	-4.24031900	8.19730600	-0.05001400
C	3.19106600	-0.16146600	-0.13232100
C	4.06264900	0.86426700	-0.45344800
C	5.39083400	0.41484300	-0.19194400
C	5.28633400	-0.90575100	0.29920900
N	3.95046300	-1.24572900	0.29672300
H	3.56510800	-2.04242700	0.78025000
C	6.68736400	1.00330600	-0.32521800
C	6.41847500	-1.66782100	0.69012600
C	7.68959100	-1.06048100	0.56266400
C	7.82251400	0.25447600	0.05797900
C	6.63380800	-2.98350700	1.21837800
C	7.16522700	2.27251900	-0.78301200
H	9.89356100	0.78388900	0.00983700
H	6.56735000	3.09471300	-1.15148400
C	8.53376000	2.26461700	-0.67103000
H	9.26219800	3.02599500	-0.91090800
C	7.98585800	-3.13790700	1.39386400
H	8.55273800	-3.97814200	1.76820700
H	5.88371800	-3.73040100	1.44091900
N	8.93609700	1.04451200	-0.16109600
N	8.62636800	-1.97795100	0.99710500
H	9.62240100	-1.83411200	1.03469200
C	-0.32563900	-1.52356200	-0.45788700
C	1.07429700	-1.46219800	-0.37966800
C	1.73474200	-0.23109100	-0.22819600
C	0.96414200	0.93905200	-0.14398800
C	-0.43663200	0.90918000	-0.23530000
C	-1.06968400	-0.33580100	-0.39460200
H	1.65128300	-2.37929400	-0.44525400
H	1.46208500	1.88560000	0.03741100
H	-2.14579400	-0.37698500	-0.53392700
H	3.77487400	1.81615300	-0.87857700

H-5

C	-0.74515300	1.33562300	0.11842100
C	0.41660600	0.56319200	0.23970700
C	0.35331200	-0.83776200	0.27890100
C	-0.89951600	-1.46585500	0.19631600
C	-2.07618000	-0.71685500	0.08302700
C	-1.98268600	0.68204200	0.03252300
H	1.36781600	1.07925500	0.30799400
H	-0.97819500	-2.54614900	0.18631000
H	-2.87967400	1.26745800	-0.13709100
C	1.56755900	-1.65122800	0.41076000
C	1.66994500	-2.95399600	0.87482900
S	3.13223400	-1.02447100	-0.04122500
C	2.98750200	-3.44076700	0.87378400
H	0.81843500	-3.52428500	1.22668900
C	3.92789800	-2.52484200	0.41107700
H	3.26746800	-4.43390200	1.21049500

C	5.32451400	-2.80467500	0.32924200
H	5.58834100	-3.80872800	0.65088500
C	6.37461300	-2.02771800	-0.08144200
C	6.22041100	-0.68287500	-0.53437500
N	6.07207700	0.41289300	-0.89925100
C	7.76681900	-2.53688300	-0.08094800
O	8.73624600	-1.89665700	-0.42941900
O	7.86131300	-3.82211800	0.35794600
H	8.81015700	-4.04010300	0.31289800
C	-0.63290000	2.81945700	0.06936300
C	-1.73616000	3.63710600	0.42875300
C	0.73084800	4.60539900	-0.37410900
C	-1.59291100	5.02409600	0.35976300
H	-2.65726100	3.19149500	0.78240400
C	-3.38542000	-1.42029700	-0.00988200
C	-4.46634200	-3.37164200	-0.53253300
C	-5.79447500	-1.43809100	0.24685800
H	-4.55173400	0.25847000	0.74172200
N	-0.34785700	5.39517400	-0.07418900
N	0.58798500	3.29220100	-0.30966600
C	1.77431900	5.54559400	-0.68407300
C	-0.12101200	6.72904500	-0.12861800
C	-2.25570700	6.26946800	0.59363000
C	-1.35418500	7.30382400	0.29459200
C	-7.20493500	-1.33892600	0.46381400
C	-6.75700900	-3.45340800	-0.32217100
C	-4.90380100	-4.69312700	-0.89361500
C	-7.78524500	-2.56865300	0.11560200
C	1.25298200	6.83069700	-0.53125700
C	-6.29287700	-4.73722700	-0.76191300
H	2.77965000	5.28318400	-0.98076700
H	1.79893600	7.75188400	-0.68746700
H	-1.56750200	8.36159900	0.37880200
H	-3.27428800	6.38997000	0.93522200
H	-7.72934000	-0.46595400	0.82652700
H	-8.84072800	-2.80036900	0.17647500
H	-6.91481700	-5.60099100	-0.95739500
H	-4.25711700	-5.49833100	-1.21140000
C	-4.58409800	-0.75212800	0.35512700
N	-5.62728700	-2.71243000	-0.22644900
N	-3.32158300	-2.71559300	-0.43013900

H-6

C	1.20677800	0.75869700	-0.24722700
C	0.36595700	1.88113100	-0.25246700
C	-1.02322900	1.69411300	-0.17892800
C	-1.57269700	0.40889500	-0.09313200
C	-0.70895900	-0.69683300	-0.10207400
C	0.68228100	-0.53901600	-0.18278000
H	2.28294000	0.87099400	-0.31460700
H	-1.69554700	2.54310900	-0.15845200
H	-1.12837300	-1.69516600	-0.04543500
C	0.91756900	3.23847600	-0.33281200
C	0.28340600	4.39121300	-0.77083000
S	2.55761300	3.57530800	0.15786700
C	1.10605600	5.52898600	-0.72036200
H	-0.73511000	4.40010000	-1.14080600

C	2.38971800	5.27767000	-0.24407400
H	0.79079100	6.51977200	-1.03191700
C	3.39419400	6.28219500	-0.11380300
H	3.06151300	7.27458200	-0.40653600
C	4.69317000	6.20289700	0.31286600
C	5.30399900	4.98237100	0.73135000
N	5.78175300	3.97478800	1.06673300
C	5.56994400	7.39684200	0.36664200
O	6.72663600	7.38789500	0.73160000
O	4.94278700	8.53398600	-0.04149400
H	5.61114000	9.23894200	0.03728200
C	1.61093500	-1.69838300	-0.20602800
C	1.16584300	-2.99225300	-0.57962900
C	2.07576800	-4.04522200	-0.57694300
H	0.14189400	-3.15501900	-0.89180800
C	3.76503700	-2.40929400	0.13219300
C	-3.04568800	0.25010000	0.01563000
C	-5.09960500	1.18427200	-0.39170800
C	-4.99533700	-1.02047200	0.68515400
H	-2.97407100	-1.67762900	1.02718900
N	2.90143600	-1.41591000	0.13164600
N	3.34067100	-3.67462000	-0.19736100
N	-5.66083700	0.05390300	0.15188800
C	5.49774300	-3.97346400	0.20123700
C	5.17611900	-2.57764900	0.40391300
C	4.28660200	-4.64872700	-0.18940200
C	3.58728300	-5.82711400	-0.60424000
C	2.20436700	-5.45554500	-0.84908300
C	-6.24157300	1.99552600	-0.75299600
C	-7.01772800	0.02002800	0.20767300
C	-6.05664200	-1.88040000	1.14871200
C	-7.31741500	-1.22627700	0.84672500
C	-7.43418100	1.26748400	-0.37603100
C	-3.61114000	-0.90812400	0.60966600
N	-3.78760000	1.28825500	-0.46457500
C	6.81938700	-4.40585700	0.39762600
C	6.15965000	-1.66016300	0.79162200
C	3.98345200	-7.16418100	-0.79860700
C	1.27445200	-6.41805300	-1.27205500
H	0.23963800	-6.14072100	-1.45549800
H	5.90451300	-0.61493900	0.93963000
H	5.01204600	-7.46508000	-0.62233200
C	3.04191400	-8.08970000	-1.21804800
C	1.69644000	-7.72514400	-1.45432000
H	3.34281000	-9.12288200	-1.36989500
H	0.98887700	-8.48073600	-1.78278000
C	7.77778300	-3.47702600	0.78182300
C	7.45717500	-2.11708700	0.97838200
H	7.08905100	-5.44792300	0.25194300
H	8.80239400	-3.80544400	0.93518300
H	8.23556900	-1.42198600	1.27845200
C	-6.03930300	-3.13213900	1.78305200
C	-8.52255200	-1.86211600	1.19993000
C	-6.33027900	3.25692000	-1.35350800
C	-8.69258700	1.84406800	-0.61745400
H	-9.47763200	-1.39193700	0.98463900

H	-5.09589000	-3.62198400	2.00944800
C	-7.24291700	-3.73152600	2.11813400
C	-8.47185100	-3.09684700	1.82656100
H	-7.24597700	-4.69928400	2.61083400
H	-9.39935500	-3.59182500	2.10173700
C	-8.75342000	3.09652000	-1.21296000
C	-7.58671300	3.80092500	-1.58024300
H	-5.42679400	3.79083100	-1.63318000
H	-7.67732800	4.77823600	-2.04514600
H	-9.72406600	3.54721000	-1.40222800
H	-9.60344800	1.31957900	-0.34363700

H-7

C	1.24997200	1.68233900	-0.21749600
C	0.21492700	2.62736300	-0.18127300
C	-1.11428700	2.18183000	-0.11334100
C	-1.41252900	0.81345300	-0.07313700
C	-0.35705800	-0.11057900	-0.12061800
C	0.97996900	0.30725800	-0.19556600
H	2.28550000	1.99575200	-0.28256800
H	-1.93377500	2.88820100	-0.06192700
H	-0.58333100	-1.17080600	-0.10030500
C	0.50888300	4.06458700	-0.20882900
C	-0.33342000	5.10413000	-0.57347300
S	2.07843200	4.66735700	0.25761800
C	0.27582900	6.36724800	-0.48652200
H	-1.34937500	4.94821400	-0.91673800
C	1.59898300	6.32807900	-0.05542700
H	-0.22029800	7.29865600	-0.74043600
C	2.41617800	7.48692700	0.09888100
H	1.90466000	8.41795400	-0.13074900
C	3.72478900	7.61752700	0.48205500
C	4.55660000	6.50567100	0.81407200
N	5.21829500	5.58453700	1.07815600
C	4.38105100	8.94340300	0.57430600
O	5.53498000	9.12086500	0.90332700
O	3.54957100	9.97040900	0.24773500
H	4.08705500	10.77765100	0.34444000
C	2.11232400	-0.65001700	-0.25325200
C	1.92497200	-2.00868200	-0.61527200
C	3.02531600	-2.85842300	-0.64230100
H	0.94578900	-2.37760500	-0.89381500
C	4.37485400	-0.92463900	0.01753600
C	-2.82727200	0.37804800	0.03098000
C	-5.02543100	0.92728200	-0.32785500
C	-4.50325800	-1.25832300	0.64526200
H	-2.39541300	-1.54823800	0.95373300
N	3.33459300	-0.12261000	0.04622000
N	4.20657800	-2.25049600	-0.30401300
N	-5.36792900	-0.30837300	0.16621300
C	6.39681300	-2.12165400	0.03459500
C	5.80147900	-0.80363600	0.25046600
C	5.32700100	-3.01948200	-0.32335400
C	4.86665600	-4.31889200	-0.71694500
C	3.41674400	-4.22375900	-0.92132300
C	-6.30308400	1.53268400	-0.65417600
C	-6.69540900	-0.59771100	0.22194200

C	-5.37906400	-2.32803800	1.07485500
C	-6.75756900	-1.90694100	0.80407500
C	-7.34910800	0.57156400	-0.30487400
C	-3.16575400	-0.88973400	0.57254600
N	-3.75836600	1.27717800	-0.39918100
C	7.76499700	-2.28128100	0.19127300
C	6.57465300	0.28338100	0.60665200
C	5.50461000	-5.53715300	-0.92001300
C	2.68422500	-5.33203900	-1.31175800
H	1.60951200	-5.26383200	-1.46455500
H	6.11914000	1.25773300	0.76305100
H	6.57740200	-5.63292300	-0.77507600
C	4.76198200	-6.66607900	-1.31845600
C	3.33207300	-6.56625400	-1.51834800
C	8.56700000	-1.17610900	0.55554700
C	7.96837400	0.12294000	0.76622800
H	8.23620400	-3.24853800	0.03734000
C	-5.11563400	-3.56231400	1.64391200
C	-7.80605500	-2.76029000	1.12593200
C	-6.61685700	2.76523100	-1.19200600
C	-8.67821500	0.90821500	-0.51557300
H	-8.83619800	-2.47125200	0.93536100
H	-4.09406900	-3.87609700	1.84590000
C	-6.17942000	-4.42695900	1.97100700
C	-7.54171900	-4.01673100	1.70683200
C	-9.00931900	2.16683400	-1.06356000
C	-7.96853300	3.10964100	-1.40831000
H	-5.82979900	3.46920200	-1.44936900
H	-9.47614800	0.21431500	-0.26460000
C	-10.36521400	2.54590900	-1.29364100
C	-8.33834000	4.37027100	-1.96092700
C	-5.94838200	-5.70529200	2.56042600
C	-8.59541400	-4.91705300	2.05045300
C	2.61192600	-7.72954000	-1.92267500
C	5.38626700	-7.93200000	-1.53619800
C	9.97716900	-1.30308100	0.72523400
C	8.80496200	1.21735700	1.13145500
C	4.65698900	-9.02711400	-1.92456500
H	5.15250700	-9.98086000	-2.08490000
C	3.25119400	-8.92694200	-2.12119000
H	2.68821200	-9.80345600	-2.42937800
C	-6.99040300	-6.54016100	2.87544800
H	-6.79778400	-7.51049300	3.32427200
C	-8.33050100	-6.13865400	2.61602500
H	-9.14771000	-6.80836000	2.86996800
C	-10.68038400	3.77087700	-1.82792500
H	-11.72014800	4.03907800	-1.99486000
C	-9.65600700	4.69625600	-2.16673000
H	-9.92159200	5.66135200	-2.58887400
C	10.15960600	1.05205900	1.28439000
H	10.78492500	1.89554700	1.56278000
C	10.75007400	-0.22402300	1.07858500
H	11.82321800	-0.34303200	1.20249800
H	1.53769800	-7.64673200	-2.07191300
H	6.46049800	-8.01086900	-1.38693400
H	10.43261000	-2.27806900	0.56812800

H	8.34547800	2.19058000	1.28621100
H	-9.62053600	-4.61243900	1.85355600
H	-4.92188300	-6.00634900	2.75692300
H	-11.15113300	1.83999800	-1.03565500
H	-7.54953800	5.07344700	-2.21805400

Cartesian coordinates of the best dyes interacted to the TiO₂ cluster

NS-3-TiO₂

C	7.33806700	-0.49132700	-0.32889900
C	7.51240900	0.89943500	-0.24144000
C	8.78964400	1.46563600	-0.12183300
C	9.89727500	0.60224000	-0.09570600
C	9.75855700	-0.79361400	-0.16752100
C	8.46727700	-1.32691600	-0.28172000
H	6.64488900	1.55214600	-0.26336100
H	10.89494600	1.02909500	-0.06658300
H	8.33730000	-2.40404500	-0.28069100
C	6.00196400	-1.08197200	-0.44742000
C	5.66592900	-2.32467700	-0.97178000
S	4.58107800	-0.23149500	0.09798200
C	4.28834300	-2.58452500	-0.94432600
H	6.39888800	-3.00544800	-1.38779500
C	3.52839600	-1.54920700	-0.39963700
H	3.83333900	-3.49553500	-1.32005300
C	2.11385200	-1.59156700	-0.27987800
H	1.66059800	-2.51395700	-0.63633000
C	1.22117500	-0.66749500	0.20800800
C	-0.21274200	-0.97534000	0.21474100
O	-1.08338100	-0.19237000	0.64982600
O	-0.60878200	-2.14563300	-0.26466800
C	1.60064100	0.60873700	0.72089000
C	8.96508500	2.93519800	-0.04600600
C	8.13246400	3.81603900	-0.75573000
C	9.97425000	3.51549900	0.73959600
C	8.28867300	5.19473400	-0.68702500
H	7.35877200	3.41594900	-1.40563500
C	10.14470800	4.89190500	0.82258500
H	10.63106300	2.87653800	1.32404800
C	9.29618100	5.77685900	0.11711300
H	7.62548700	5.81925300	-1.27333500
H	10.93701400	5.27788400	1.45285000
N	9.44085600	7.15278200	0.21616700
C	10.60716700	7.70336600	0.88424400
C	8.65719500	8.01982600	-0.64657000
H	10.54744400	8.79332300	0.86768500
H	10.64608100	7.39077600	1.93525200
H	11.55325000	7.40333900	0.40589800
H	8.87571200	9.06087600	-0.40065500
H	8.87227700	7.86647900	-1.71637600
H	7.58296500	7.86221600	-0.49157700
N	1.92433200	1.64825900	1.13430600
C	10.94508700	-1.68105400	-0.12730200
C	11.00986300	-2.86014400	-0.88730900
C	12.06221700	-1.38214200	0.66948300
C	12.11785200	-3.69830200	-0.85673500
H	10.18550100	-3.11555500	-1.54816100
C	13.17832300	-2.20858900	0.71480700
H	12.05208200	-0.49041500	1.29069500
C	13.23548900	-3.40199000	-0.04219700
H	12.11470900	-4.58224900	-1.48319400

H	14.00550600	-1.92531700	1.35465100
N	14.33477100	-4.24723500	0.01820500
C	14.43069700	-5.36177700	-0.90856600
C	15.54221100	-3.80063300	0.69181200
H	15.34952500	-3.59317300	1.75154900
H	16.29198400	-4.59276400	0.64366900
H	15.97163600	-2.89185900	0.24043100
H	14.46763500	-5.04124800	-1.96233500
H	15.33815700	-5.92911400	-0.69247700
H	13.57983200	-6.04388500	-0.79220300
Ti	-6.13647800	2.15322200	-1.07727200
Ti	-8.22584700	2.72172200	0.82750300
Ti	-6.33568500	0.64273500	1.82957200
Ti	-8.88907600	1.30037100	-1.50985400
Ti	-4.29966400	-1.71040600	2.18480300
Ti	-4.09468900	0.35454900	-0.90427100
Ti	-2.50648800	-1.96232600	-0.00359700
Ti	-7.20404000	-1.10569700	-0.88562600
Ti	-5.25676600	-3.76135500	-0.11293100
O	-6.95232900	3.56433300	-0.05441000
O	-4.47088400	2.10733000	-1.64260600
O	-7.55422100	1.94842800	2.34829100
O	-8.77129000	-0.51520200	-1.69195400
O	-9.68075400	2.46672800	-0.28994500
O	-7.59041300	2.10407100	-2.37505900
O	-2.65476000	-2.28905300	1.92002500
O	-5.26042800	1.43278800	0.61769600
O	-2.81643000	-0.62254500	-1.50700700
O	-4.12191600	-0.87237300	0.55235900
O	-3.44344300	-3.31934700	-0.59446100
O	-5.28974000	-0.23908800	2.96016700
O	-7.15648100	-1.02321300	1.07949700
O	-5.42363200	-2.99576300	1.67872800
O	-5.83028500	-0.05147000	-1.52561900
O	-5.54693100	-5.35157100	-0.14395500
O	-6.67849300	-2.74271600	-1.03306500
O	-7.64189900	1.13209800	-0.07238500
H	-6.81898400	-1.87061100	1.47663000

NS-4-TiO₂

Ti	-7.93377400	-1.33455900	-2.33699300
Ti	-10.28214900	0.09168900	-1.61025900
Ti	-7.89993900	1.39847600	-0.36773900
Ti	-9.64033800	-2.28250400	-0.19259900
Ti	-5.48028200	2.18279900	1.00942500
Ti	-5.55060000	-0.67111200	-1.12725300
Ti	-2.88478400	0.54055900	0.39202800
Ti	-7.26722100	-1.07772400	1.39463000
Ti	-4.82584700	0.11937800	3.22320400
O	-9.46191400	-0.47038700	-3.08705100
O	-6.23489700	-1.64299400	-2.67010100
O	-9.62456900	1.67690100	-1.06170600
O	-8.75336800	-2.27826700	1.35499100
O	-11.12844100	-1.27938300	-0.71145700
O	-8.77811100	-2.88925800	-1.64353700
O	-3.85739700	2.15153000	0.28984100

O	-7.01852700	0.49307800	-1.80130200
O	-3.81137800	-0.33314600	-0.98620800
O	-6.12475100	0.50152700	0.46337700
O	-3.42517300	-0.11740400	1.91017400
O	-7.03821400	2.86005900	0.14024200
O	-8.42103300	0.63079500	1.44321900
O	-5.47280000	1.88107500	2.73785200
O	-6.28726500	-1.87228000	0.01700200
O	-4.30381200	0.01300200	4.75054100
O	-6.35209000	-1.06027200	2.85357000
O	-8.75655300	-0.66540100	-0.65820200
H	-8.28759500	1.20165300	2.22067900
C	6.99415000	-0.52879800	-0.36496400
C	7.45566400	0.79773200	-0.39593900
C	8.82436400	1.08676300	-0.32459000
C	9.73003800	0.01941900	-0.22853600
C	9.30344300	-1.31902500	-0.18709400
C	7.92642800	-1.57449400	-0.25269800
H	6.74494500	1.61505600	-0.47298800
H	10.79446900	0.23224800	-0.23236300
H	7.57453100	-2.59680100	-0.16258200
C	5.56248700	-0.83465900	-0.42722200
C	4.96416600	-2.02084000	-0.83969300
S	4.36362400	0.33727700	0.04725400
C	3.56484900	-1.98396700	-0.78388700
H	5.53029200	-2.87257800	-1.19694900
C	3.04901200	-0.76906000	-0.32855400
H	2.92200300	-2.80836800	-1.07559600
C	1.66257500	-0.50456400	-0.19669900
H	1.01516300	-1.33697000	-0.46583900
C	0.99446900	0.62644000	0.21428700
C	1.64182500	1.83542600	0.60631200
N	2.18925400	2.81492500	0.91741700
C	-0.46403200	0.59982300	0.25282400
O	-1.15691700	1.61218000	0.63159000
O	-1.14046500	-0.43843800	-0.09241000
C	9.30681700	2.49144700	-0.37019200
C	8.68842200	3.44564600	-1.19633600
C	10.39401200	2.90771900	0.41518700
C	9.13850800	4.76326100	-1.23371200
H	7.86176000	3.14654800	-1.83510600
C	10.84384700	4.22644900	0.37712300
H	10.87444000	2.19878900	1.08392700
C	10.22445600	5.17342200	-0.44556700
H	8.64457400	5.47702100	-1.88774800
H	11.67730000	4.54716300	0.99463000
C	10.27888900	-2.42786800	-0.07723000
C	10.07746700	-3.65727900	-0.72538400
C	11.45395500	-2.30510000	0.68212700
C	10.98506700	-4.70391100	-0.62487800
H	9.19594400	-3.79712900	-1.34594300
C	12.37462600	-3.33910600	0.79167700
H	11.64848200	-1.38197900	1.22187700
C	12.17065000	-4.58015300	0.14014800
H	10.76152100	-5.62739100	-1.14541500
H	13.26353100	-3.17162800	1.38788500

N	10.72160700	6.52780100	-0.45273200
N	13.08281700	-5.61790000	0.24534400
C	9.74057100	7.51148300	0.03510400
C	9.33818900	7.27468600	1.48989300
C	15.47288600	-4.88637700	0.50290300
H	8.66128400	8.06825600	1.82576100
H	8.82181500	6.31790500	1.61678100
H	10.22197600	7.27370300	2.13690000
H	15.26349900	-3.85722200	0.19423600
H	16.30669500	-4.86987900	1.21487300
H	15.79580000	-5.44255200	-0.38446900
C	11.30990200	6.92362300	-1.74263100
C	14.23667400	-5.53910400	1.13687900
C	12.94076500	-6.84704800	-0.52989600
C	12.53118100	6.08651300	-2.12026800
H	12.26955100	5.03451400	-2.27262000
H	12.97014000	6.46230800	-3.05150100
H	13.28998300	6.13807100	-1.33206600
C	12.06802900	-7.91445400	0.14489500
H	11.05029600	-7.54723900	0.31130000
H	12.01206700	-8.81536800	-0.47774900
H	12.48355300	-8.20014800	1.11785900
H	10.21519400	8.49657700	-0.05015700
H	8.83458600	7.54630700	-0.59978800
H	10.56925900	6.89063500	-2.56488800
H	11.61245900	7.97295000	-1.64144000
H	13.95187200	-5.01040300	2.05288200
H	14.48188700	-6.56115700	1.44854800
H	12.54983000	-6.60566100	-1.52424600
H	13.94699700	-7.24904700	-0.69647900

NS-5-TiO₂

Ti	7.95294200	2.55880000	-0.90114300
Ti	10.28441100	1.02971500	-1.45229200
Ti	7.89424100	-0.76275200	-1.46256100
Ti	9.69851400	1.69103600	1.24551900
Ti	5.47722300	-2.28448600	-1.00563500
Ti	5.57225000	1.24105000	-0.47705500
Ti	2.90350300	-0.68027100	-0.22041300
Ti	7.32300000	-0.27538500	1.54971500
Ti	4.88227500	-2.40783700	2.02977200
O	9.45771500	2.47904300	-2.07321600
O	6.25584100	3.01890200	-0.88243700
O	9.60615300	-0.47150500	-2.18197500
O	8.82865800	0.59008900	2.34685200
O	11.16351400	1.34942800	0.13790600
O	8.83053500	3.15356500	0.67558900
O	3.84752000	-1.74377600	-1.45732000
O	7.01232600	0.89674500	-1.80766400
O	3.82896200	0.91048700	-0.58435400
O	6.14345700	-0.71750300	-0.20490400
O	3.47179800	-1.30152600	1.30312100
O	7.01370500	-2.14754700	-2.12872200
O	8.44852100	-1.51433000	0.34532200
O	5.49339800	-3.30326700	0.42294600
O	6.34158100	1.26732200	1.16677300

O	4.37781600	-3.41763000	3.18857400
O	6.42384100	-1.32246900	2.58004600
O	8.78231500	0.89046300	-0.21477900
H	8.31587000	-2.46839000	0.48768600
C	-6.96379300	0.60175200	0.31541800
C	-7.44974200	-0.71127200	0.21832000
C	-8.82860200	-0.94821400	0.10545400
C	-9.71422800	0.14141000	0.09644100
C	-9.23431200	1.45731800	0.16523700
C	-7.85513800	1.68561000	0.27119600
H	-6.76671000	-1.55228700	0.25413300
H	-10.78158900	-0.03610400	0.04367600
H	-7.48248400	2.70249100	0.28555400
C	-5.52615500	0.86419000	0.43357900
C	-4.91376000	1.97815800	0.99740500
S	-4.34451600	-0.26644900	-0.16467400
C	-3.51435500	1.91663600	0.96016100
H	-5.47165000	2.79024200	1.44830500
C	-3.01528700	0.75621800	0.36521400
H	-2.86026100	2.68289400	1.36387500
C	-1.63195400	0.47757900	0.22721100
H	-0.97325600	1.25004700	0.61950400
C	-0.97886400	-0.60481200	-0.31673900
C	-1.64188300	-1.72965700	-0.89086500
N	-2.20098900	-2.63719700	-1.35949200
C	0.48048700	-0.61544400	-0.30771700
O	1.16034100	-1.59569600	-0.78226700
O	1.17036100	0.35650700	0.17600600
N	-9.32376600	-2.26910800	0.03668900
N	-10.13794100	2.54691100	0.14205800
C	-8.67520800	-3.31944700	0.75385800
C	-8.38115000	-4.53314700	0.11517000
C	-8.33425700	-3.15440700	2.10500600
C	-7.76014100	-5.56324700	0.82021000
H	-8.63978500	-4.66091500	-0.93127200
C	-7.69714300	-4.18317100	2.79762400
H	-8.56994300	-2.21972400	2.60458400
C	-7.41021200	-5.39322400	2.16164600
H	-7.53476100	-6.49687100	0.31208600
H	-7.43611300	-4.04125300	3.84295100
H	-6.91746600	-6.19424600	2.70498100
C	-10.47083400	-2.57509800	-0.75082000
C	-11.47052300	-3.41953800	-0.24335600
C	-10.61007900	-2.05278800	-2.04640000
C	-12.58282600	-3.73681500	-1.02140200
H	-11.36779000	-3.82440600	0.75844200
C	-11.73494400	-2.36068400	-2.81000600
H	-9.83251300	-1.41183000	-2.44989000
C	-12.72526500	-3.20660200	-2.30567100
H	-13.34767700	-4.39289000	-0.61438900
H	-11.82788800	-1.94883200	-3.81138600
H	-13.59642300	-3.45085100	-2.90669800
C	-11.28766900	2.51035900	-0.69873700
C	-12.53493600	2.93013700	-0.21080200
C	-11.18740200	2.06476200	-2.02604400
C	-13.65561500	2.90951600	-1.03959000

H	-12.61800600	3.27139100	0.81625500
C	-12.31732100	2.03014100	-2.84190300
H	-10.22242200	1.75146800	-2.41210200
C	-13.55594600	2.45570400	-2.35682100
H	-14.61440200	3.23767200	-0.64702700
H	-12.22351300	1.68320600	-3.86754100
H	-14.43279000	2.43420900	-2.99749400
C	-9.89417800	3.69663200	0.94627300
C	-10.06759500	4.98449700	0.41520900
C	-9.48425300	3.55905900	2.28254200
C	-9.84025100	6.10811000	1.20879400
H	-10.38125000	5.09713200	-0.61773400
C	-9.24169200	4.68847800	3.06290000
H	-9.36122500	2.56596300	2.70314800
C	-9.42124200	5.96898900	2.53387400
H	-9.97962600	7.09789400	0.78214600
H	-8.92701000	4.56448400	4.09583200
H	-9.23930300	6.84675500	3.14725000

NS-6-TiO₂

Ti	-8.38045000	1.84831500	-0.98591300
Ti	-10.45045500	2.34394900	0.95904300
Ti	-8.53750100	0.24575500	1.87558600
Ti	-11.13202000	0.99180800	-1.41444200
Ti	-6.48670400	-2.10614100	2.13741300
Ti	-6.32842900	0.05635800	-0.88802200
Ti	-4.71763700	-2.27858300	-0.07807900
Ti	-9.42730600	-1.42287100	-0.88238500
Ti	-7.45789800	-4.08976200	-0.21251400
O	-9.19119400	3.22114100	0.08969100
O	-6.72028600	1.82772000	-1.56938900
O	-9.75740900	1.52732700	2.44710100
O	-11.00639900	-0.81630600	-1.65287700
O	-11.91595100	2.11445900	-0.14933600
O	-9.84707600	1.82950000	-2.26851100
O	-4.84083800	-2.66452300	1.83606400
O	-7.47968600	1.07831200	0.67607200
O	-5.04528700	-0.89169700	-1.52906000
O	-6.33332900	-1.21779400	0.52912700
O	-5.65193400	-3.62190200	-0.70098900
O	-7.47530600	-0.66432600	2.96768300
O	-9.35887400	-1.40018300	1.08392900
O	-7.60853200	-3.38208500	1.60423500
O	-8.06567500	-0.34330700	-1.50604000
O	-7.73915000	-5.67974300	-0.29019500
O	-8.89548900	-3.05190200	-1.08477100
O	-9.86684500	0.78692400	0.00291300
H	-9.01417700	-2.25764300	1.45182500
C	5.12346200	-0.78437100	-0.42154900
C	5.29700400	0.60795500	-0.36370600
C	6.57341600	1.17607900	-0.24552000
C	7.68202700	0.31624500	-0.19036400
C	7.54362700	-1.07974100	-0.25425000
C	6.25413600	-1.61647200	-0.36742700
H	4.43447500	1.26011400	-0.46110500
H	8.67008400	0.74039300	-0.04176800

H	6.12869300	-2.69330400	-0.41209400
C	3.78927800	-1.37705700	-0.55951100
C	3.45458700	-2.60468100	-1.11616100
S	2.37075200	-0.54384900	0.01537400
C	2.07616700	-2.86707800	-1.08972700
H	4.18656900	-3.27186400	-1.55570700
C	1.31817600	-1.84898400	-0.51266000
H	1.62065900	-3.76766100	-1.48908100
C	-0.09701400	-1.89601700	-0.38369100
H	-0.55336700	-2.80632400	-0.76623500
C	-0.98335400	-0.98846700	0.14184400
C	-0.59590400	0.26839600	0.69531000
N	-0.26234000	1.29079500	1.14213600
C	-2.41967200	-1.29430500	0.15190100
O	-3.28209600	-0.52378500	0.62137800
O	-2.82009200	-2.44712800	-0.36227400
C	6.74542000	2.64708800	-0.17723500
C	5.81171200	3.46256000	0.48594200
C	7.84772200	3.28258400	-0.77467300
C	5.97129900	4.84156500	0.55786800
H	4.96436300	3.00755400	0.99135800
C	8.00922100	4.66229800	-0.72284500
H	8.57214600	2.69119700	-1.32802800
C	7.07343400	5.46824400	-0.05034900
H	5.24533800	5.44065000	1.09737900
H	8.85726000	5.12570100	-1.21607700
C	8.73096100	-1.96582400	-0.18133400
C	8.68801600	-3.19493500	0.49933700
C	9.94571500	-1.60894500	-0.79187200
C	9.80088300	-4.02488800	0.57510000
H	7.77951700	-3.48896100	1.01791300
C	11.06039900	-2.43794900	-0.73605600
H	10.00897400	-0.68282300	-1.35662800
C	11.00881200	-3.66208900	-0.04630700
H	9.74370900	-4.95574500	1.12961800
H	11.97677100	-2.14560900	-1.23810200
N	7.23571700	6.87251900	0.01089300
N	12.14277200	-4.50624900	0.02139500
C	8.53451500	7.44112300	0.13898400
C	8.89839600	8.55981600	-0.62766000
C	9.46686000	6.89822000	1.03802000
C	10.16570000	9.12390800	-0.49015600
H	8.18348100	8.98146300	-1.32704800
C	10.73795500	7.45824900	1.15557300
H	9.18843800	6.03980300	1.64115600
C	11.09490900	8.57560000	0.39698700
H	10.43086600	9.98973500	-1.09125200
H	11.44710400	7.02607700	1.85677900
H	12.08377400	9.01391100	0.49679900
C	6.10010800	7.73014800	-0.05619400
C	5.98841300	8.82795200	0.81166500
C	5.08159800	7.49420500	-0.99337000
C	4.88262500	9.67338800	0.73570900
H	6.77034800	9.01197300	1.54162400
C	3.97053800	8.33421500	-1.04936500
H	5.16605800	6.65179400	-1.67259900

C	3.86527500	9.43034200	-0.18996600
H	4.81099100	10.51850900	1.41532000
H	3.18990400	8.13637900	-1.77911700
H	3.00096800	10.08626100	-0.24069600
C	13.44681400	-3.94837000	0.14719700
C	13.68804600	-2.88980400	1.03782900
C	14.51201300	-4.45551300	-0.61407000
C	14.96644800	-2.34601400	1.15269000
H	12.87096400	-2.49957900	1.63639300
C	15.79078100	-3.91723600	-0.47905100
H	14.33060300	-5.27058200	-1.30749000
C	16.02615000	-2.85741700	0.39984400
H	15.13609800	-1.52731600	1.84711700
H	16.60418100	-4.32164200	-1.07576600
H	17.02253300	-2.43604000	0.49750600
C	11.98844800	-5.92081700	-0.03284200
C	11.11767200	-6.50872600	-0.96450600
C	12.71168300	-6.74791900	0.84127800
C	10.96828600	-7.89395800	-1.00955900
H	10.56315700	-5.87510700	-1.64954200
C	12.56922100	-8.13312900	0.77675600
H	13.38267700	-6.29886500	1.56666400
C	11.69467600	-8.71508800	-0.14388200
H	10.29061400	-8.33301300	-1.73708400
H	13.13639100	-8.75895600	1.46076300
H	11.58118000	-9.79450300	-0.18674900

NS-8-TiO₂

Ti	-10.50264400	-1.53204600	-2.43012400
Ti	-12.87479300	-0.15171700	-1.69208700
Ti	-10.52415500	1.13238700	-0.36870100
Ti	-12.23326900	-2.56739000	-0.34636300
Ti	-8.13337400	1.88957100	1.07246400
Ti	-8.14452500	-0.88954100	-1.16136100
Ti	-5.51306800	0.29296500	0.44022100
Ti	-9.89581800	-1.39729100	1.31792200
Ti	-7.49344200	-0.24286100	3.22420300
O	-12.02702200	-0.65581200	-3.17419900
O	-8.79631100	-1.81392600	-2.74736600
O	-12.24043000	1.41958400	-1.07963400
O	-11.37041700	-2.60849400	1.21416200
O	-13.72237600	-1.55989500	-0.85401800
O	-11.34321200	-3.11681200	-1.80334300
O	-6.49949700	1.89779300	0.37761500
O	-9.61263500	0.28437100	-1.81825100
O	-6.41146600	-0.54095100	-0.98163300
O	-8.75388800	0.22270600	0.45919300
O	-6.07083600	-0.42235400	1.92587000
O	-9.68373400	2.58311900	0.20240400
O	-11.06606700	0.29866800	1.40658000
O	-8.14920000	1.52889600	2.78948700
O	-8.88792100	-2.13569200	-0.07055800
O	-6.99412400	-0.39712700	4.75504000
O	-9.00309000	-1.42216000	2.79051900
O	-11.35728500	-0.92777400	-0.74269100
H	-10.95050300	0.84381400	2.20505600

C	4.82319600	0.69891000	-0.24991700
C	6.18855400	1.01027500	-0.18008000
C	7.10925900	-0.04920300	-0.13058100
C	6.70198900	-1.39343000	-0.15290100
C	5.32969300	-1.67033600	-0.21757400
C	4.38119100	-0.63429900	-0.26492800
H	4.10239900	1.50551100	-0.34305800
H	8.16486800	0.17773700	-0.01923400
H	4.99772600	-2.70311000	-0.22976800
C	2.95511400	-0.95748300	-0.35445300
C	2.37350300	-2.13085500	-0.82480100
S	1.73941900	0.17712300	0.16490500
C	0.97382400	-2.11283700	-0.77648900
H	2.95165400	-2.95810200	-1.21849500
C	0.44011800	-0.92586800	-0.26975300
H	0.34268500	-2.93012700	-1.11077000
C	-0.94954300	-0.68256400	-0.13811000
H	-1.58565000	-1.50896500	-0.44942900
C	-1.63389100	0.42274400	0.31570800
C	-1.00328200	1.62014700	0.76616600
C	-3.09169100	0.38011500	0.33709200
O	-3.79983600	1.36980400	0.74717600
O	-3.75412800	-0.65012100	-0.05702300
N	-0.46945500	2.59068800	1.12539500
C	6.64430000	2.41967900	-0.15428300
C	5.90972000	3.41471100	0.51481000
C	7.82736000	2.82008700	-0.79878100
C	6.33274700	4.73748700	0.54659700
H	5.00849400	3.14287200	1.05776100
C	8.25383800	4.14274400	-0.78779600
H	8.40668700	2.08965200	-1.35736700
C	7.51496100	5.13171900	-0.10993400
H	5.75336600	5.47316700	1.09373600
H	9.15781700	4.42041000	-1.31905600
C	7.69617600	-2.49125500	-0.08879700
C	7.43631400	-3.67901500	0.61720500
C	8.94073800	-2.38850200	-0.73375700
C	8.36741200	-4.70840000	0.68349900
H	6.50318300	-3.78375700	1.16446100
C	9.87550600	-3.41598300	-0.68692400
H	9.16848200	-1.50147300	-1.31881100
C	9.60898400	-4.59931700	0.02799300
H	8.14403900	-5.59995500	1.25965200
H	10.81612100	-3.31200400	-1.21708700
N	7.94435100	6.47314000	-0.08848000
C	6.99914700	7.54018800	-0.01450800
C	5.88463600	7.57749800	-0.85929000
C	7.17944200	8.58790100	0.90516200
C	4.95579300	8.61811500	-0.78320800
H	5.73427900	6.77956600	-1.58001100
C	6.27371200	9.63732800	0.97069500
H	8.03941600	8.57289400	1.56754300
C	5.14869400	9.65977400	0.13181000
H	4.10000600	8.60901200	-1.44849800
H	6.40803800	10.44852900	1.67944400
C	9.33205200	6.79551300	-0.15826100

C	10.26458700	6.15285900	0.67583600
C	9.79284100	7.77790200	-1.04080000
C	11.61278100	6.47571300	0.61262900
H	9.92258200	5.39504600	1.37393400
C	11.14523000	8.12431000	-1.09439200
H	9.08488500	8.28449100	-1.68943800
C	12.06642200	7.46822300	-0.27013500
H	12.33636000	5.98214900	1.25398000
H	11.46388200	8.89439000	-1.78765800
O	4.31333300	10.72886700	0.28494100
O	13.40931200	7.71799200	-0.24524200
C	3.14931400	10.78995300	-0.52234600
C	13.92048400	8.71357900	-1.11479500
H	14.99576500	8.75078100	-0.93001400
H	13.74317300	8.46055700	-2.16892700
H	13.48275800	9.69876800	-0.90409100
H	2.49256100	9.92668500	-0.35064300
H	2.62800700	11.70300900	-0.22879700
H	3.39982300	10.84411300	-1.59048900
N	10.55633700	-5.64093800	0.08908500
C	10.13777400	-7.00162400	0.18069500
C	10.71951400	-7.86384300	1.12664300
C	9.15588000	-7.51409700	-0.67417200
C	10.33173400	-9.19390200	1.20687200
H	11.48299700	-7.48123500	1.79685900
C	8.74397100	-8.84609200	-0.58455700
H	8.70277200	-6.86357200	-1.41602100
C	9.33578000	-9.69744700	0.35580200
H	10.77856000	-9.86364600	1.93503300
H	7.97741100	-9.20651000	-1.26112900
C	11.95353700	-5.35720300	0.04048700
C	12.79975600	-6.07909900	-0.80746700
C	12.51559300	-4.36271700	0.86112100
C	14.17409300	-5.83000300	-0.83968900
H	12.38122200	-6.85101500	-1.44588200
C	13.87633200	-4.09407800	0.81823000
H	11.87465900	-3.79949600	1.53236100
C	14.72056100	-4.82824600	-0.02949400
H	14.79904000	-6.41352900	-1.50612100
H	14.31469700	-3.32690900	1.44889500
O	9.02005200	-11.01562300	0.52366300
O	16.04391400	-4.49318000	0.01338400
C	8.02096900	-11.57624300	-0.31086900
C	16.94146400	-5.20373700	-0.82241500
H	17.92970300	-4.78224600	-0.62905700
H	16.95261500	-6.27619300	-0.58517200
H	16.69429400	-5.07391300	-1.88477600
H	8.30664500	-11.53171200	-1.37058900
H	7.92717300	-12.62062900	-0.00740300
H	7.05369800	-11.07275000	-0.17860400

Cb-1-TiO₂

Ti	8.06164600	1.20660700	-2.00216400
Ti	10.20296900	-0.62459400	-1.48765700
Ti	7.65010100	-1.76058600	-0.44861600
Ti	9.89383700	1.63778000	0.18390700

Ti	5.06750900	-2.30463800	0.75714100
Ti	5.59064400	0.58716100	-1.21843200
Ti	2.71286000	-0.33675600	0.13740100
Ti	7.29255500	0.64263300	1.42988900
Ti	4.56985500	-0.29016200	3.03998700
O	9.48566400	0.25532100	-2.85270900
O	6.46621000	1.60967700	-2.62536400
O	9.33484700	-2.18021000	-1.13209600
O	8.88874100	1.62604000	1.67078700
O	11.23360200	0.49708800	-0.44915700
O	9.17299200	2.52947800	-1.16968300
O	3.48878400	-2.04498500	-0.02308500
O	6.96651800	-0.65562300	-1.83239800
O	3.81873500	0.49795200	-1.13130900
O	5.90979600	-0.68137200	0.36214400
O	3.25024600	0.18218000	1.70891900
O	6.57154900	-3.12128000	-0.08432100
O	8.11512300	-1.22299000	1.47266300
O	5.01778400	-2.09857400	2.50192000
O	6.65293000	1.59289300	-0.09575000
O	4.00683600	-0.19752300	4.55385300
O	6.22955600	0.72978300	2.78087400
O	8.80377100	0.18716300	-0.43869700
H	7.79266500	-1.80937600	2.18070600
C	-7.25068700	-0.52159200	0.05434200
C	-7.56749000	0.84411200	0.02034700
C	-8.90449500	1.26108100	-0.11141700
C	-9.90525200	0.27974300	-0.24873000
C	-9.59617000	-1.09078700	-0.23871000
C	-8.26131200	-1.48870900	-0.06239600
H	-6.77878300	1.58140600	0.08550000
H	-10.93653500	0.58487400	-0.36198200
H	-8.01747200	-2.54106900	-0.01041200
C	-5.85973400	-0.95984800	0.21870300
C	-5.40550200	-2.17675800	0.71647100
S	-4.52642700	0.07012800	-0.22441000
C	-4.00837600	-2.27446700	0.75057400
H	-6.07114900	-2.95413600	1.07165100
C	-3.35033100	-1.13641700	0.28031400
H	-3.46788100	-3.14057200	1.11897400
C	-1.93935700	-1.00827800	0.23438500
H	-1.39399700	-1.88256300	0.58457000
C	-1.14025700	0.03595600	-0.17288200
C	-1.64154500	1.27772000	-0.66392200
N	-2.07003500	2.28343100	-1.06479400
C	0.30807100	-0.11977100	-0.09168100
O	1.11778200	0.81802800	-0.42433600
O	0.85878400	-1.20829300	0.32096700
C	-8.24896500	6.08275700	-0.27058600
C	-6.78231400	5.01761500	1.33035900
C	-8.88646000	4.86678400	-0.47778100
H	-8.57928800	6.97154800	-0.80339200
C	-7.41612400	3.78598300	1.13233100
H	-5.96793600	5.07962000	2.04694900
C	-8.45590000	3.71330600	0.19894400
H	-7.11449200	2.92149500	1.71218900

C	-9.72986500	-5.09680100	-2.34019500
C	-11.95314100	-5.23000800	-1.40220800
C	-9.53202200	-3.83378500	-1.76951200
H	-8.93634600	-5.52618200	-2.94639600
C	-11.77260000	-3.97922800	-0.82996200
H	-12.89455500	-5.75886600	-1.27161000
C	-10.55995500	-3.28259100	-0.99586500
H	-8.61241200	-3.29250000	-1.95691300
N	-10.62279700	-2.03547400	-0.35390900
C	-12.71872800	-3.15400800	0.00468400
C	-11.99634300	-1.77190000	0.12974000
C	-12.08296600	-1.36495400	1.62594100
C	-12.94503700	-3.61962900	1.46561500
C	-13.14639100	-2.30333400	2.23163400
C	-10.07862200	4.54741100	-1.35578200
C	-10.42040700	3.07302700	-0.94671100
C	-11.34694600	5.36841000	-1.03054800
C	-11.75570200	3.15898900	-0.14693700
H	-12.57749900	2.81069500	-0.78676700
C	-11.95094000	4.65050500	0.18593700
N	-9.25788600	2.61113900	-0.15480400
H	-10.52501700	2.41286800	-1.81252300
H	-9.81284100	4.62762000	-2.41722000
H	-11.73734500	2.52255700	0.74287500
H	-12.99989000	4.91156500	0.36113000
H	-11.38954600	4.91369100	1.09030800
H	-12.04321100	5.32474400	-1.87859700
H	-11.12290300	6.42393100	-0.84460200
H	-12.47763600	-1.02294900	-0.51388100
H	-13.69126700	-3.03002800	-0.48598900
H	-12.32355900	-0.30620500	1.76447400
H	-11.11186400	-1.54210100	2.10136800
H	-14.15359000	-1.90966700	2.03907300
H	-13.04246900	-2.41275300	3.31647800
H	-13.78681400	-4.31394200	1.55798200
H	-12.04881400	-4.13608500	1.83190000
C	-7.18087000	6.15876900	0.63271600
C	-10.92066600	-5.80099600	-2.15930400
H	-6.67205600	7.10396900	0.79658400
H	-11.05269800	-6.77896700	-2.61257500

Cb-7-TiO₂

Ti	8.04806800	0.36317300	2.52595200
Ti	10.20000100	2.13860400	1.79655500
Ti	8.43400800	1.51196300	-0.52483200
Ti	10.80674600	-0.55629900	2.33901300
Ti	6.50378100	0.22316600	-2.62753300
Ti	6.08357800	-0.68934700	0.95589700
Ti	4.62241900	-1.55447200	-1.45687900
Ti	9.24061200	-1.68401500	0.03810700
Ti	7.42877100	-2.86613500	-2.56126800
O	8.85769900	2.05917900	2.93760400
O	6.36075700	-0.07139900	2.77209500
O	9.62679700	2.75847200	0.16900800
O	10.74653800	-1.90407000	1.10517400
O	11.61040500	1.12297400	2.43606500

O	9.44119000	-0.64943300	3.43817900
O	4.87058300	-0.34453300	-2.97503500
O	7.27627700	1.14958700	0.80906600
O	4.81025100	-1.77321600	0.55784800
O	6.22104400	-0.42698600	-0.92581100
O	5.58074400	-2.91025900	-2.01411100
O	7.47416100	1.77401600	-1.99421900
O	9.28004600	-0.16715900	-1.21444400
O	7.64927000	-1.02379400	-3.17887100
O	7.80075000	-1.44272300	1.16831800
O	7.77345800	-3.95562900	-3.70483200
O	8.76979700	-2.88318500	-1.10991700
O	9.63281800	0.41207900	1.18339200
H	8.99306100	-0.43484100	-2.12854600
C	-5.27682000	-0.72878000	-0.78545700
C	-5.53618800	0.65056800	-0.74231300
C	-6.82776500	1.13960700	-0.49779100
C	-7.86149900	0.20946400	-0.29957000
C	-7.63908000	-1.17679000	-0.34839100
C	-6.33542700	-1.63169500	-0.59045300
H	-4.73483600	1.35254800	-0.95134300
H	-8.85363600	0.57228600	-0.04992800
H	-6.14189500	-2.69884700	-0.62439400
C	-3.92773500	-1.23549800	-1.05304300
C	-3.56798300	-2.45285600	-1.61821600
S	-2.51798900	-0.29396500	-0.64891900
C	-2.18011300	-2.62058300	-1.73481800
H	-4.29445000	-3.17847500	-1.96432900
C	-1.43769100	-1.53841600	-1.26186000
H	-1.70737200	-3.49819800	-2.16431100
C	-0.01825100	-1.48639400	-1.28467500
H	0.45763400	-2.37291600	-1.69808600
C	0.85452700	-0.50783200	-0.87365000
C	0.44239700	0.73441500	-0.30531900
N	0.08965600	1.74361400	0.15670700
C	2.30005800	-0.71615100	-1.01424800
O	3.15367500	0.12832100	-0.67145300
O	2.72355800	-1.85923100	-1.53331600
C	-7.08969700	2.59747600	-0.44418900
C	-6.13202900	3.49038200	0.08403300
C	-8.29000700	3.13961800	-0.93220600
C	-6.38719000	4.84905700	0.12757900
H	-5.19340400	3.10661900	0.47650000
C	-8.56314000	4.50824600	-0.89589000
H	-9.02262100	2.47919900	-1.38804000
C	-7.60606900	5.36990200	-0.34499200
H	-9.48661300	4.88584900	-1.31835800
C	-8.74968200	-2.13391300	-0.12453500
C	-10.03839100	-1.87670400	-0.61996700
C	-8.54513500	-3.33882100	0.58160700
C	-11.10558500	-2.75603800	-0.42639400
H	-10.20917000	-0.97826900	-1.20676800
C	-9.59153400	-4.22105300	0.78331800
H	-7.56270600	-3.56523500	0.98889100
C	-10.88263600	-3.93534500	0.29523400
H	-12.07239300	-2.53459300	-0.86217300

N	-11.76248100	-4.97642300	0.59699100
C	-9.61102800	-5.54496100	1.50540300
C	-11.03136500	-6.11959700	1.18705600
C	-11.61380400	-6.62478700	2.53455400
C	-9.53894200	-5.49334400	3.05307200
C	-10.40514000	-6.68466900	3.49029000
C	-13.13760500	-5.03409900	0.31521700
C	-13.73834600	-6.25648000	-0.03917400
C	-13.95479800	-3.89231200	0.42092000
C	-15.10599400	-6.32537900	-0.29876700
H	-13.13242300	-7.15275600	-0.12169900
C	-15.31854800	-3.97065100	0.14551000
H	-13.52393700	-2.95297100	0.74869200
C	-15.90600600	-5.18422300	-0.21819900
H	-15.54547500	-7.28062800	-0.57427500
H	-15.92856800	-3.07541500	0.23515500
H	-16.97044000	-5.24127200	-0.42602900
C	-5.50346800	5.97015400	0.62542800
C	-6.30862300	7.26339400	0.25058000
C	-5.31272900	6.02741200	2.17094100
C	-6.41478400	8.08006100	1.55454000
H	-5.53549500	8.73336600	1.63384200
C	-6.38030100	7.01874200	2.66570800
N	-7.62334800	6.75842900	-0.21862100
C	-8.68780000	7.61915500	-0.53854700
C	-10.02202600	7.26099100	-0.26665900
C	-8.43688100	8.88255400	-1.10588200
C	-11.06680000	8.12576200	-0.58700900
H	-10.23365200	6.31597400	0.22108500
C	-9.48880000	9.74576700	-1.40785700
H	-7.41756100	9.18577100	-1.32109900
C	-10.81127400	9.37297200	-1.16075100
H	-12.08836300	7.82611900	-0.36726800
H	-9.26905600	10.71461300	-1.84898100
H	-11.62824800	10.04630700	-1.40309100
H	-5.82223800	7.82988300	-0.55263800
H	-4.53083200	5.94563600	0.12301800
H	-7.30199400	8.71966500	1.57733200
H	-6.14995200	7.43847400	3.65060200
H	-7.35618300	6.52269300	2.73901000
H	-4.31230700	6.41440700	2.40181700
H	-5.39434100	5.03681100	2.62948100
H	-10.96619700	-6.93393300	0.45326600
H	-8.83457600	-6.22325600	1.13268100
H	-12.12940800	-7.58539300	2.43958200
H	-12.34674700	-5.89750000	2.90111900
H	-9.85174400	-7.62221400	3.34423600
H	-10.69891600	-6.64182500	4.54457800
H	-8.51028300	-5.53875500	3.42589000
H	-9.97947500	-4.55490900	3.41257400

H-4-TiO₂

Ti	-7.36975700	2.03000500	-0.96665800
Ti	-9.44188700	2.47329700	0.98900200
Ti	-7.52709700	0.35468900	1.85276600
Ti	-10.12053800	1.18224100	-1.41886000

Ti	-5.47234500	-2.00030500	2.05366300
Ti	-5.31468700	0.23938900	-0.91440300
Ti	-3.70137700	-2.11386100	-0.16457900
Ti	-8.41268000	-1.24259100	-0.94834900
Ti	-6.44024900	-3.92386700	-0.34740400
O	-8.18323100	3.37404700	0.14339000
O	-5.70908900	2.02785400	-1.54872000
O	-8.74911700	1.62001700	2.45635500
O	-9.99219400	-0.61903700	-1.70413400
O	-10.90666500	2.27123600	-0.12597000
O	-8.83622400	2.04326700	-2.25003800
O	-3.82623500	-2.54991700	1.73928200
O	-6.46999300	1.21940400	0.67626800
O	-4.03204800	-0.69084500	-1.58088100
O	-5.31829700	-1.06991400	0.46952600
O	-4.63497700	-3.44128500	-0.82236500
O	-6.46358300	-0.58191600	2.92102000
O	-8.34492900	-1.27144900	1.01789100
O	-6.59273600	-3.26301300	1.48682800
O	-7.05232900	-0.14475300	-1.54258100
O	-6.71983300	-5.51171200	-0.46584100
O	-7.87852200	-2.86505500	-1.19303600
O	-8.85640700	0.94193900	-0.00619400
H	-7.99876500	-2.13770000	1.36329800
C	4.80214200	-1.17923400	-0.61601300
C	4.47285400	-2.38950300	-1.21317500
S	3.38016300	-0.37162200	-0.01497400
C	3.09548900	-2.65751900	-1.19732800
H	5.20835100	-3.03681900	-1.67608700
C	2.33202600	-1.66159100	-0.58827700
H	2.64374800	-3.54548600	-1.62812500
C	0.91781700	-1.71577300	-0.46269700
H	0.46333500	-2.61524500	-0.87219800
C	0.02878200	-0.82487400	0.08847800
C	0.41419100	0.41679800	0.67657500
N	0.74773700	1.42677400	1.15102200
C	-1.40589800	-1.13329800	0.08984800
O	-2.27099800	-0.37752600	0.57918300
O	-1.80477700	-2.27327400	-0.45426100
C	7.72977400	2.83555500	-0.13519200
C	8.83336300	3.62971700	-0.40266100
C	7.11595200	4.98229900	0.24223800
C	8.46749800	4.98786900	-0.17351800
N	6.68356400	3.67506700	0.23300600
H	5.81781400	3.35774200	0.64115300
H	9.78545900	3.27170100	-0.76991600
C	6.41492400	6.16970600	0.58027600
C	9.15425000	6.23836700	-0.27892300
C	8.46668900	7.42728000	0.05284800
C	7.11779200	7.39320300	0.47974000
C	10.47882800	6.62093400	-0.66429600
C	5.08851800	6.48198600	1.02733700
C	5.02067300	7.84361000	1.18293700
C	10.56153600	7.98820700	-0.56125500
H	11.38530400	8.65864000	-0.76067300
H	4.20135200	8.47196000	1.50117000

H	11.27662600	5.96296600	-0.98026600
H	4.27818600	5.78902700	1.20894400
N	9.34529800	8.48031600	-0.12590500
N	6.24536400	8.39687300	0.85250600
H	6.45494000	9.38121100	0.88581100
H	9.14281200	9.45535500	0.02240700
C	9.73419400	-1.71015100	-0.18317000
C	11.05209900	-1.44363400	-0.51235800
C	11.81490500	-2.62578200	-0.27723300
C	10.91595900	-3.60301400	0.20656800
N	9.65836300	-3.03841100	0.22537900
H	8.86552600	-3.43192500	0.70843000
C	13.19493000	-2.96907900	-0.42934400
C	11.33203400	-4.91021900	0.57217100
C	12.70403000	-5.22322100	0.42621900
C	13.62143900	-4.26791300	-0.07155200
C	10.68684600	-6.08310000	1.08709100
C	14.35434200	-2.26489100	-0.88684900
H	15.57156300	-5.14104600	-0.15390700
H	14.39429000	-1.24329100	-1.23883300
C	15.42206400	-3.12447000	-0.79936000
H	16.46358200	-2.97736400	-1.04720500
C	11.65121300	-7.04802500	1.23707200
H	11.57550600	-8.06467500	1.59502900
H	9.63713800	-6.20521400	1.31755300
N	14.98283000	-4.33833500	-0.30481100
N	12.87071500	-6.53147200	0.83746200
H	13.73993300	-7.03951500	0.85671200
C	6.13077600	-0.58126700	-0.45515700
C	7.26487400	-1.40704400	-0.39978300
C	8.55037700	-0.85714900	-0.25592800
C	8.67679400	0.53779300	-0.15791800
C	7.56170100	1.38896200	-0.22739900
C	6.28880600	0.81118800	-0.37794800
H	7.14407200	-2.48297100	-0.47616400
H	9.65808200	0.96605000	0.01642700
H	5.41988900	1.45070100	-0.50067400
H	11.41506500	-0.51265000	-0.92599800

H-7-TiO₂

Ti	10.78865700	0.92768300	-2.05805700
Ti	12.90900500	-0.97911300	-1.80716500
Ti	10.37909700	-2.15978400	-0.76086000
Ti	12.71954800	1.12433300	0.07682000
Ti	7.84143300	-2.76929600	0.50665200
Ti	8.34092900	0.28859800	-1.20998700
Ti	5.50589000	-0.70862000	0.18352200
Ti	10.15557400	0.06239300	1.34875200
Ti	7.48947800	-0.97257200	2.99040000
O	12.15278700	0.03442400	-3.05445500
O	9.17520200	1.42067200	-2.55754800
O	12.02316500	-2.54438300	-1.55649500
O	11.78340400	0.99103900	1.60163600
O	14.00644800	0.02364100	-0.71733800
O	11.95942000	2.14929700	-1.15644200

O	6.23658400	-2.40788900	-0.17210800
O	9.65953300	-0.91639300	-2.00297000
O	6.57250000	0.22248900	-1.05010900
O	8.70231500	-1.13151200	0.22625500
O	6.12214500	-0.35445000	1.77171100
O	9.28857300	-3.52949100	-0.47637300
O	10.94210600	-1.81260700	1.17681800
O	7.87357000	-2.72885300	2.26340900
O	9.46543300	1.16528300	-0.04429600
O	6.99700500	-1.01462100	4.53075000
O	9.15855500	0.03744200	2.75151900
O	11.57318100	-0.24191400	-0.62730400
H	10.64134800	-2.45782100	1.84192400
C	-4.73503700	0.63100400	0.33233000
C	-4.45012800	-0.74226100	0.31577400
C	-5.50552700	-1.65982200	0.19054100
C	-6.82999700	-1.21788300	0.07246500
C	-7.08697100	0.16212500	0.10202800
C	-6.05195000	1.10075700	0.23443500
H	-3.94295500	1.36276400	0.44145400
H	-5.31539500	-2.72537700	0.15475900
H	-8.11157000	0.50775000	0.02392700
C	-3.06894300	-1.22198100	0.42196400
C	-2.62836600	-2.48822800	0.79259800
S	-1.72649000	-0.17276600	0.06094400
C	-1.23242700	-2.60914800	0.79285600
H	-3.30223000	-3.28709100	1.07778000
C	-0.56390700	-1.43961300	0.42433400
H	-0.70018200	-3.51522800	1.06434600
C	0.84741500	-1.32344100	0.36269400
H	1.38902200	-2.23550900	0.60592500
C	1.65094400	-0.24998800	0.04967000
C	1.15673600	1.04444200	-0.29022300
N	0.73536800	2.09440000	-0.56585800
C	3.09852900	-0.43109500	0.07202700
O	3.91305800	0.52529800	-0.18752900
O	3.64320800	-1.56396100	0.35169500
C	-6.29892200	2.56350400	0.27586200
C	-7.58674100	3.09870300	0.53568200
C	-7.75333500	4.47929800	0.55358800
H	-8.42656400	2.44770700	0.74374200
C	-5.35453900	4.64769300	0.08582000
C	-7.91846700	-2.21366600	-0.08897600
C	-8.57759800	-4.38809400	0.23115700
C	-10.14786300	-2.82333600	-0.81175300
H	-9.31423500	-0.85882000	-1.07244300
N	-5.19862400	3.34327900	0.06624800
N	-6.60147000	5.18246600	0.30997300
N	-9.79148100	-4.05294500	-0.32002600
C	-5.34438200	6.99767200	0.07690300
C	-4.50314100	5.81126200	-0.07564900
C	-6.68842800	6.53830900	0.32632700
C	-8.06781700	6.80887500	0.60952500
C	-8.74428300	5.51486000	0.75558500
C	-8.72124200	-5.79711900	0.54716600
C	-10.71182300	-5.04842600	-0.42158000

C	-11.49293100	-3.03208900	-1.30471300
C	-11.84318900	-4.43422700	-1.05425400
C	-10.06307600	-6.20777200	0.13355600
C	-9.15544400	-1.85855300	-0.68816100
N	-7.63735400	-3.47441200	0.34966900
C	-4.76976700	8.25495100	-0.02954900
C	-3.14882100	5.91924800	-0.32335600
C	-8.80022100	7.98136800	0.75673300
C	-10.09916500	5.45388700	1.03654400
H	-10.60299300	4.49623300	1.14608500
H	-2.53447200	5.02951300	-0.43374600
H	-8.32174400	8.95159800	0.65330500
C	-10.17856500	7.92229300	1.04364300
C	-10.84065800	6.64307100	1.18642900
C	-3.38442200	8.37833100	-0.28260200
C	-2.56125400	7.19894700	-0.43155100
H	-5.36938400	9.15482500	0.07969600
C	-12.39521000	-2.17578200	-1.91331800
C	-13.09518000	-4.90245600	-1.43497700
C	-7.84594800	-6.69594800	1.12492000
C	-10.45943100	-7.52367800	0.32305600
H	-13.37835100	-5.93699300	-1.26023800
H	-12.13741400	-1.13594800	-2.10063500
C	-13.66450900	-2.65139100	-2.30018600
C	-14.01560000	-4.03397500	-2.05577900
C	-9.57107800	-8.45071900	0.91180800
C	-8.24728400	-8.03543600	1.31992400
H	-6.85265800	-6.37767800	1.43033800
H	-11.44996900	-7.85674200	0.02470600
C	-9.94568500	-9.81128300	1.12216000
C	-7.37707500	-8.99657900	1.91249300
C	-14.62024300	-1.80046700	-2.93139900
C	-15.30988300	-4.48267400	-2.45978700
C	-12.23741300	6.62090200	1.47778400
C	-10.96003500	9.10754700	1.20147400
C	-2.75922400	9.65505300	-0.39746500
C	-1.16741400	7.35733400	-0.68451000
C	-12.30182700	9.04266200	1.48115000
H	-12.87745700	9.95694900	1.59750800
C	-12.95115000	7.78389200	1.62175400
H	-14.01400500	7.74980600	1.84388400
C	-15.85362800	-2.27242000	-3.30413100
H	-16.57017400	-1.61188600	-3.78403600
C	-16.20078100	-3.63151900	-3.06400700
H	-17.18043800	-3.99380000	-3.36365100
C	-9.07758600	-10.70731500	1.69651300
H	-9.38352300	-11.73901600	1.84761800
C	-7.77670300	-10.29728100	2.09757500
H	-7.10188200	-11.01791300	2.55076400
C	-0.60453500	8.60601700	-0.78763200
H	0.45933000	8.71142600	-0.97993700
C	-1.41193200	9.76668400	-0.64230300
H	-0.95554300	10.74944100	-0.72576000
H	-12.72811100	5.65611800	1.58474700
H	-10.46595700	10.07032500	1.09493900
H	-3.37376400	10.54534000	-0.28627100

H	-0.55638500	6.46459600	-0.79349400
H	-15.57740100	-5.52078600	-2.27778200
H	-14.34903400	-0.76295400	-3.11280500
H	-10.94013500	-10.12783800	0.81666200
H	-6.38352100	-8.67620600	2.21731100