

Charge transfer properties of novel linear carbon chain-based dyes

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Electronic Supplementary Information:

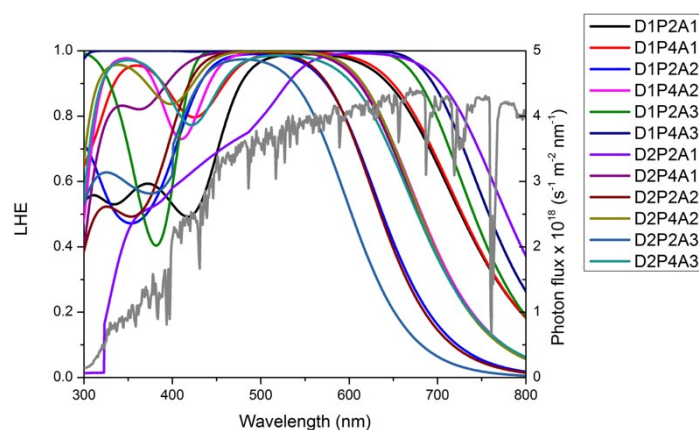


Figure 1: LHE curves of all dyes ($I = 20 \text{ nmol cm}^{-2}$). AM 1.5G solar spectrum is reported in grey.

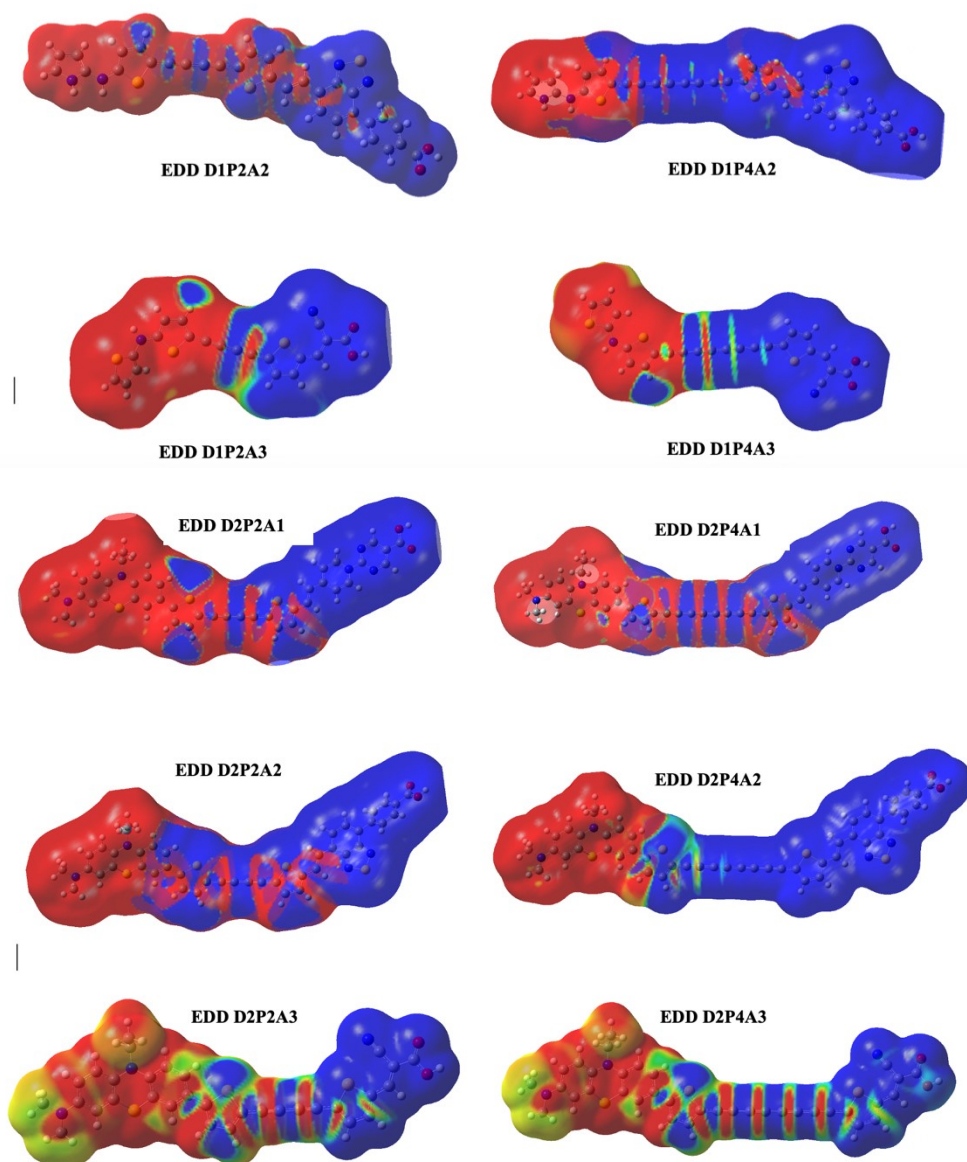
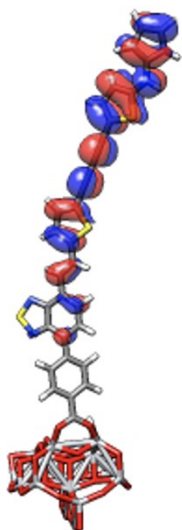
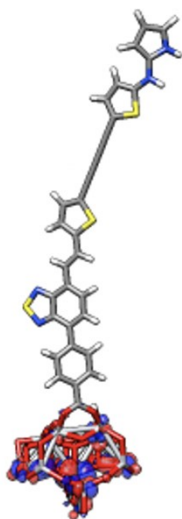


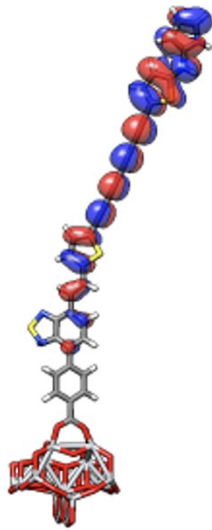
Figure 2. Electron density difference (EDD) maps of $D_xP_yA_z$ ($x=1,2$, $y=2,4$, $z=2,3$) dyes simulated by Gaussview (the red and blue colors indicate a decrease and increase of charge densities respectively). The density differences are 0.0001 a.u.



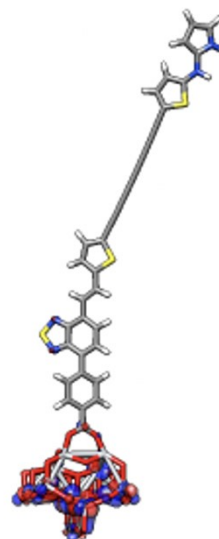
D1P2A2@TiO2 H



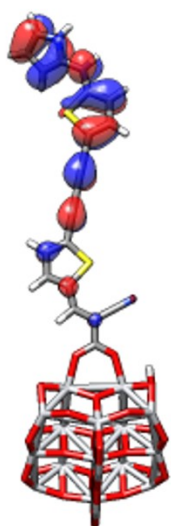
D1P2A2@TiO2 L



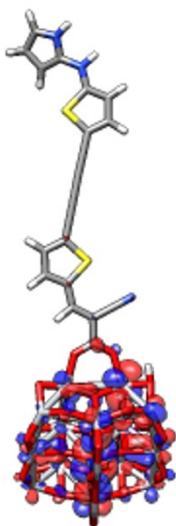
D1P4A2@TiO2 H



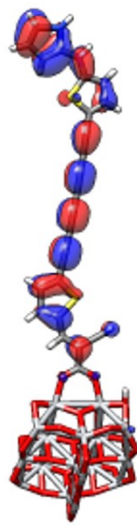
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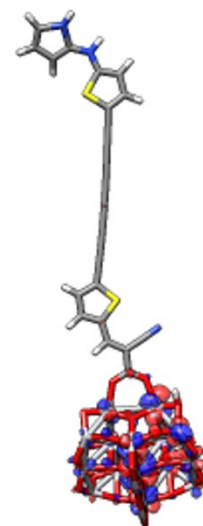
D1P2A3@TiO2 H



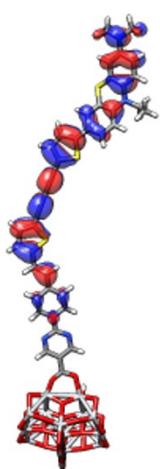
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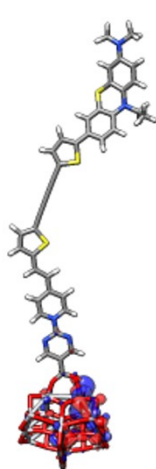
D1P4A3@TiO2 H



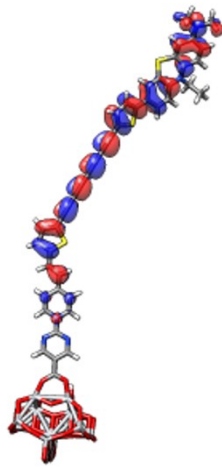
D1P4A3@TiO2 L



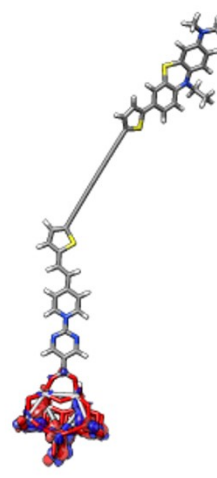
D2P2A1@TiO2 H



D2P2A1@TiO2 L



D2P4A1@TiO2 H



D2P4A1@TiO2 L

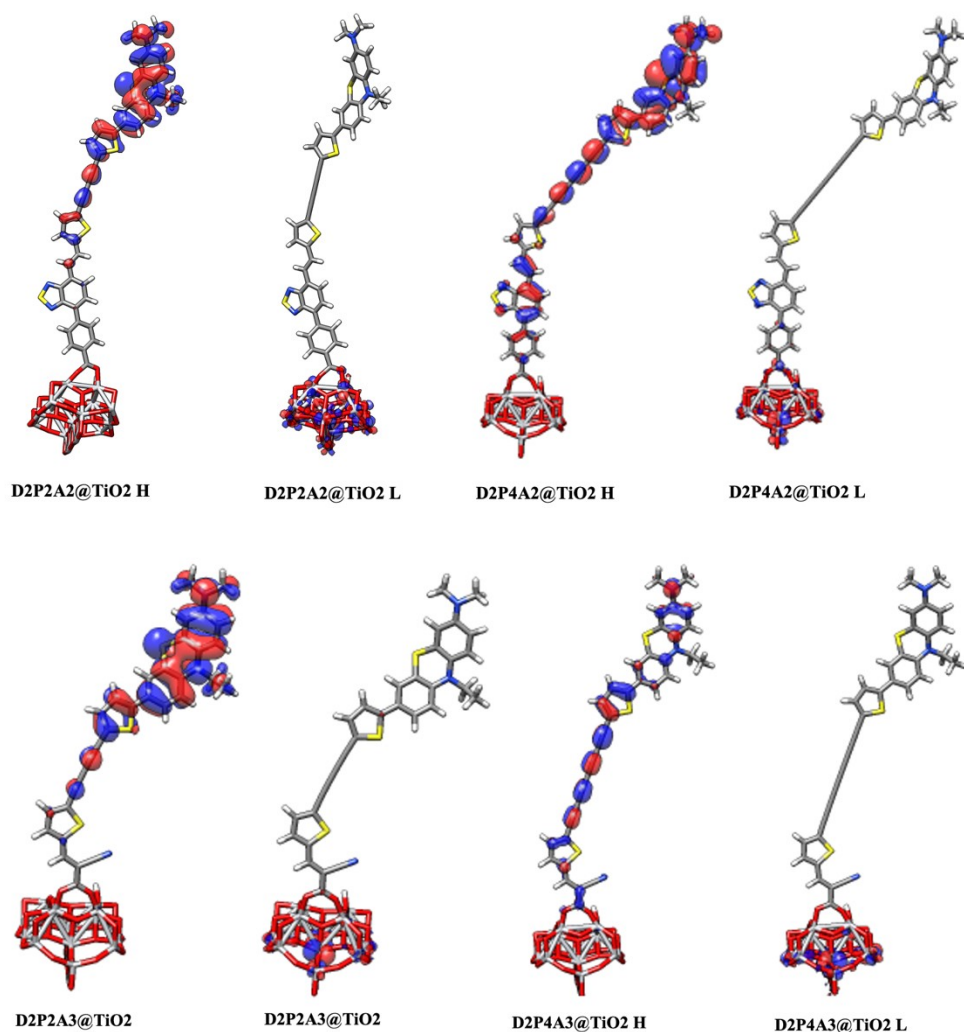


Figure 3: Optimized geometries of bidentate binding mode of $D_xP_yA_z$ ($x=1,2, y=2,4, z=2,3$) dyes on $(TiO_2)_{14}$. HOMOs (H) and LUMOs (L) are also visualized.

Optimized geometries of Dyes

D1P2A1

C	4.97764400	1.19180800	-0.01856000
C	3.67505900	1.52522100	0.00116300
C	1.14675900	2.17493200	0.01893500
C	0.58356300	3.44488400	-0.01886600
S	-0.09923600	0.94185100	0.06544000
C	-0.81303900	3.42635400	-0.01455300
H	1.18524900	4.34242200	-0.05017700
C	-1.36718900	2.15345100	0.02882000
H	-1.42869300	4.31618500	-0.04230200
C	-2.75726600	1.86138700	0.03281000
H	-3.38662600	2.74432500	-0.01362600
C	-3.33272700	0.62791600	0.08396100
H	-2.70551400	-0.25605200	0.13787800
C	-4.74148200	0.37594800	0.06707600
C	-5.73709400	1.37983700	-0.01385000

C	-5.20883400	-0.95834000	0.12676700
C	-7.05862400	1.05456100	-0.03771500
H	-5.48233900	2.42901300	-0.05754500
C	-6.54109900	-1.24560800	0.10382600
H	-4.50635300	-1.77890000	0.18915200
H	-7.84075700	1.79338700	-0.09783300
H	-6.92581300	-2.25147500	0.14536700
N	-7.47138200	-0.24884900	0.01760000
C	-8.87425500	-0.56248800	-0.00762800
C	-10.99536100	0.16716600	-0.21196100
C	-10.49629400	-2.11961600	0.15346300
C	-11.46221000	-1.13332600	-0.03377400
H	-11.68489600	0.98823300	-0.36782100
H	-10.76765600	-3.15840000	0.29595800
N	-9.19612500	-1.83343100	0.16980000
N	-9.69800800	0.45661600	-0.20118600
C	-12.92091900	-1.40127700	-0.05478700
O	-13.76202100	-0.54333200	-0.19606100
O	-13.21154000	-2.70342100	0.09759200
H	-14.18099000	-2.80601500	0.07004700
C	2.49360100	1.83320800	0.01409300
C	6.16370300	0.89292400	-0.04083500
C	7.49899200	0.53521800	-0.06479300
C	9.68426200	-0.72615600	-0.05697500
C	9.83850600	0.64544300	-0.19840000
H	10.79894600	1.12474100	-0.30755300
S	7.99404100	-1.16152900	0.09138500
C	8.61939500	1.33574300	-0.20593800
H	8.54144700	2.40908800	-0.31923700
C	12.01040600	-1.51436000	0.04673500
C	12.79371300	-0.54052300	0.63502300
C	14.14985700	-0.90472500	0.39335700
H	12.44049800	0.31471300	1.18725000
C	14.14913000	-2.08092100	-0.31796400
H	15.02481700	-0.36230700	0.71705900
H	14.95623100	-2.69062200	-0.68925400
N	12.84019300	-2.43927700	-0.53043900
H	12.53117000	-3.24831600	-1.05128100
N	10.62826300	-1.70452000	-0.01550000
H	10.31310300	-2.66688000	-0.00602700

D1P4A1

C	-7.69346600	0.69384300	0.02796800
C	-6.38367900	0.95935000	0.03546600
C	1.20333000	2.51099600	0.04394800
C	1.83895700	3.74449300	0.04394200
S	2.37266800	1.20492900	0.03935300
C	3.23379000	3.64218500	0.04018200
H	1.29109000	4.67631100	0.04640300
C	3.70662400	2.33774000	0.03781200

H	3.90250000	4.49311600	0.03951600
C	5.08105200	1.95986100	0.03412000
H	5.76318000	2.80426100	0.03135400
C	5.57507300	0.69434800	0.03316100
H	4.89451100	-0.15158800	0.03585500
C	6.97005400	0.35429400	0.02702000
C	8.02412200	1.29694400	0.02310000
C	7.35053800	-1.00640600	0.02362500
C	9.32498200	0.89166800	0.01430300
H	7.83391100	2.36027000	0.02587800
C	8.66411100	-1.37450900	0.01454500
H	6.59833900	-1.78397800	0.02780800
H	10.15290200	1.58138100	0.00987100
H	8.98675300	-2.40266100	0.01102300
N	9.65328400	-0.43495800	0.00913300
C	11.03648200	-0.83723800	-0.00554800
C	13.20597400	-0.23512200	-0.00445800
C	12.54626400	-2.50980400	-0.05901800
C	13.58016000	-1.57624900	-0.04505500
H	13.95221400	0.55040200	0.01131600
H	12.74364500	-3.57428100	-0.08624500
N	11.26760000	-2.13882600	-0.03858600
N	11.93004200	0.13921000	0.01481400
C	15.01854700	-1.93974900	-0.07314300
O	15.91884700	-1.13314200	-0.02992300
O	15.21577300	-3.26523100	-0.15447600
H	16.17663600	-3.43225800	-0.16695400
C	-5.17960400	1.20718500	0.03786300
C	-3.87215200	1.47754900	0.04262600
C	-2.67044900	1.72801600	0.04377700
C	-1.35721900	1.99724600	0.04584200
C	-0.16169300	2.24683600	0.04542600
C	-8.89738400	0.45904500	0.02297900
C	-10.24899900	0.18574100	0.01599300
C	-12.51501300	-0.92155200	0.06191400
C	-12.57828700	0.46366300	-0.01896100
H	-13.50611500	1.01347600	-0.04391200
S	-10.85536300	-1.48193800	0.08645600
C	-11.31712900	1.06773200	-0.03799300
H	-11.16704800	2.13830100	-0.08358300
C	-14.88358900	-1.57545100	-0.05992900
C	-15.57137900	-0.64440800	-0.81359300
C	-16.95854800	-0.90418600	-0.61794600
H	-15.13746500	0.11278300	-1.44523900
C	-17.06977100	-1.97816800	0.23256000
H	-17.77877700	-0.36262300	-1.06342400
H	-17.93204400	-2.49252500	0.62351800
N	-15.79940900	-2.37368000	0.57351200
H	-15.57050700	-3.13290000	1.20020400
N	-13.52212000	-1.83091600	0.11791400
H	-13.27352700	-2.79951700	0.27617500

D1P2A2

C	8.42134100	0.35485900	-0.04872300
C	10.72992500	-0.66677600	-0.01964100
C	10.74017500	0.71447400	-0.09632200
H	11.64479000	1.29937600	-0.15528300
S	9.09111800	-1.28390200	0.05960900
C	9.44958400	1.27288100	-0.11748300
H	9.26079500	2.33595900	-0.18997300
C	13.12053700	-1.23919700	0.14008400
C	13.78508900	-0.18522900	0.73737100
C	15.17986400	-0.43954100	0.58214300
H	13.33281900	0.65161500	1.24267800
C	15.31900100	-1.62903300	-0.09046900
H	15.98580900	0.18526500	0.93538800
H	16.19368600	-2.17783800	-0.39810600
N	14.05713200	-2.10345700	-0.36312600
H	13.84838800	-2.95389400	-0.86739100
N	11.76802200	-1.55117500	0.00438100
H	11.54582700	-2.53602600	-0.06131300
C	7.04899700	0.56558300	-0.06067800
C	5.83965100	0.73521300	-0.07038400
C	4.50394400	0.92978500	-0.08135600
C	3.29825700	1.11298000	-0.09110000
C	-4.40601200	0.66165100	-0.09122700
C	-5.51763400	1.57064300	-0.08544900
C	-4.74408800	-0.67980600	-0.08427200
C	-6.88700600	1.09865700	-0.05305800
C	-6.07901300	-1.13804400	-0.06050000
H	-3.96412600	-1.43066700	-0.08814400
C	-7.17838100	-0.30200000	-0.03501300
H	-6.23686400	-2.20935000	-0.03604000
C	-8.55523200	-0.83542000	0.00694100
C	-8.89152700	-1.98206000	-0.73102500
C	-9.55029700	-0.24014900	0.79693900
C	-10.16876200	-2.51353300	-0.67868200
H	-8.14932900	-2.44921100	-1.36625800
C	-10.82807200	-0.77436700	0.85503000
H	-9.31838100	0.63645300	1.38556900
C	-11.15155300	-1.91617400	0.11575100
H	-10.41643200	-3.39238800	-1.25992500
H	-11.57389100	-0.30398400	1.48138500
C	-12.50565800	-2.51730200	0.14439300
O	-12.83578500	-3.50924300	-0.47248100
O	-13.37088700	-1.85121500	0.93833700
H	-14.22589500	-2.31585300	0.89585100
N	-5.42342100	2.90348500	-0.12073200
N	-7.78007200	2.09642000	-0.07554000
S	-6.94157400	3.49027800	-0.12055000
C	-0.58846000	1.03436700	-0.10344100

C	1.91857500	1.31408600	-0.10107700
C	1.22214300	2.51237600	-0.12861600
H	1.72479500	3.46988500	-0.14686200
S	0.79785300	-0.03227500	-0.07720100
C	-0.17136600	2.35367200	-0.13006700
H	-0.86142800	3.18645500	-0.14961900
C	-1.91374400	0.47091100	-0.09328600
C	-3.05584300	1.19365900	-0.10349300
H	-1.96623400	-0.61302700	-0.07386300
H	-2.98753900	2.27536500	-0.11931600

D1P4A2

C	11.39271300	0.11112800	-0.05203400
C	13.78046600	-0.70458200	-0.00219500
C	13.66903800	0.67800400	-0.00568700
H	14.52025900	1.34073400	-0.00191400
S	12.20341400	-1.46812000	-0.01451600
C	12.34002600	1.12027800	-0.03901100
H	12.05843000	2.16483700	-0.05944100
C	16.20908500	-1.04380200	0.18866700
C	16.75495300	0.01757200	0.88395100
C	18.16830100	-0.07083100	0.72283800
H	16.21298600	0.75371600	1.45385700
C	18.43554000	-1.17558500	-0.04970600
H	18.90195200	0.60258300	1.13860600
H	19.36496000	-1.59822800	-0.39384500
N	17.23384700	-1.75580200	-0.37723800
H	17.11778500	-2.57621000	-0.95587000
N	14.89564700	-1.48372900	0.01100600
H	14.77374700	-2.48419000	-0.08215000
C	8.79217200	0.29107800	-0.10955700
C	7.45743800	0.39643000	-0.13221300
C	6.23373000	0.50132400	-0.14627000
C	4.90255800	0.62969200	-0.15894000
C	3.68246300	0.75973600	-0.16338500
C	2.34918600	0.91376200	-0.16714200
C	1.13780900	1.07174900	-0.16320400
C	10.01462300	0.20992800	-0.08425400
C	-6.55768900	0.57979900	-0.08237200
C	-7.66788800	1.48951200	-0.06416900
C	-6.89491100	-0.76149800	-0.07760100
C	-9.03664700	1.01751300	-0.02515500
C	-8.22977300	-1.22009700	-0.04772300
H	-6.11458900	-1.51197800	-0.08593000
C	-9.32796600	-0.38333100	-0.01206400
H	-8.38798800	-2.29136700	-0.02638300
C	-10.70510700	-0.91575600	0.03620700
C	-11.04769400	-2.05583000	-0.70863900
C	-11.69291000	-0.32588000	0.83896900
C	-12.32526500	-2.58611100	-0.65127700

H	-10.31049200	-2.51858000	-1.35287000
C	-12.97083200	-0.85922000	0.90226300
H	-11.45524100	0.54528500	1.43334800
C	-13.30107500	-1.99416800	0.15556600
H	-12.57842100	-3.45985100	-1.23783000
H	-13.71129800	-0.39355400	1.53838600
C	-14.65582900	-2.59419100	0.18954200
O	-14.99154200	-3.58026000	-0.43351100
O	-15.51364500	-1.93487300	0.99686800
H	-16.36940600	-2.39845900	0.95769000
N	-7.57358600	2.82255300	-0.09209500
N	-9.92990800	2.01521800	-0.03524500
S	-9.09176200	3.40904400	-0.07741700
C	-2.74213000	0.95880600	-0.13752300
C	-0.24071400	1.25576600	-0.15539700
C	-0.94524700	2.45103800	-0.14275600
H	-0.44792800	3.41143600	-0.14103500
S	-1.35247300	-0.09932100	-0.15572100
C	-2.33535800	2.28320900	-0.13287900
H	-3.03148300	3.11087300	-0.12287300
C	-4.06535400	0.38884700	-0.12697200
C	-5.20706800	1.11119000	-0.10037000
H	-4.11568900	-0.69518500	-0.13982700
H	-5.13882400	2.19301100	-0.08834800

D1P2A3

C	1.74465013	0.72886806	0.04718000
C	0.59326704	0.31820002	0.03262300
C	-0.67502505	-0.12070501	0.01275000
C	-1.82804614	-0.51918004	-0.00702500
C	-3.14746324	-0.95168208	-0.03198400
C	-3.62419428	-2.25811517	-0.08702101
S	-4.45650634	0.19423701	0.00451600
C	-5.01403838	-2.32402818	-0.10121901
H	-2.96718822	-3.11349624	-0.11586901
C	-5.64705543	-1.08336808	-0.05687500
H	-5.57634840	-3.24569725	-0.14301401
C	-7.05366756	-0.93282607	-0.06484900
H	-7.58369456	-1.87527114	-0.11491801
C	-7.84069362	0.18651901	-0.02028900
C	-7.31311353	1.50130211	0.05373100
C	-9.31356271	0.11647601	-0.04213300
O	-9.79099473	-1.13864309	-0.11514001
H	-10.76089985	-1.08624908	-0.12493401
O	-10.03561776	1.08922909	0.00033300
N	-6.87850650	2.56893319	0.11457801
C	3.04972023	1.18230109	0.06109500
C	3.52113127	2.48536519	0.05538100
S	4.40205834	0.04905300	0.10813001
C	4.91363938	2.58848220	0.09164601

H	2.85473822	3.33489425	0.02742700
C	5.54816141	1.35453911	0.11296001
H	5.46090939	3.51942127	0.08997101
H	7.44229559	2.00939215	-0.04396000
C	7.58597457	-0.03810800	0.15648001
C	7.32349456	-1.15227909	0.90806707
S	8.98699071	-0.28026902	-0.85360007
C	8.26143663	-2.19684917	0.67963805
H	6.51913250	-1.21528809	1.62450712
C	9.22589968	-1.86876915	-0.22408202
H	8.22907464	-3.14699724	1.19244209
H	10.07125579	-2.45308319	-0.54889604
N	6.89848453	1.16856309	0.09606701

D1P4A3

C	-4.26104730	-1.12322208	-0.00083200
C	-3.06220622	-0.85332206	-0.00171600
C	-1.75938413	-0.56007604	-0.00192500
C	-0.55859904	-0.28590102	-0.00319800
C	0.74140205	0.01329000	-0.00331900
C	1.93959114	0.29054802	-0.00416300
C	3.24432023	0.59358304	-0.00355000
C	4.43536632	0.87284706	-0.00329700
C	5.79175641	1.18213308	-0.00224900
C	6.38302446	2.44184518	-0.00119700
S	6.99879251	-0.09057801	-0.00187500
C	7.77957058	2.38496817	0.00002400
H	5.80350044	3.35458024	-0.00123100
C	8.29996057	1.09209308	-0.00007300
H	8.42156762	3.25684023	0.00104500
C	9.69531372	0.82018706	0.00134900
H	10.30461772	1.71780213	0.00251100
C	10.38298876	-0.36445603	0.00158400
C	9.74618570	-1.63484812	0.00017400
C	11.86196286	-0.41677003	0.00334200
O	12.43678387	0.80091506	0.00440900
H	13.40221495	0.67761005	0.00565400
O	12.50189591	-1.44832610	0.00382200
N	9.22319765	-2.66712019	-0.00104000
C	-5.61081139	-1.40808410	-0.00024500
C	-6.25433744	-2.64125319	0.00017000
S	-6.81348549	-0.09689201	0.00016300
C	-7.64884755	-2.56166618	0.00069700
H	-5.70325241	-3.57257026	0.00004700
C	-8.12461256	-1.25145909	0.00071400
H	-8.31316561	-3.41606124	0.00103300
H	-10.06379571	-1.72690412	0.00147900
C	-10.06467674	0.32250402	0.00120900
C	-9.54867071	1.59621112	0.00112400
S	-11.82299684	0.35361103	0.00142600

C	-10.56775576	2.59822519	0.00124100
H	-8.49827663	1.84308413	0.00103500
C	-11.83289886	2.09626015	0.00141400
H	-10.35136476	3.65892826	0.00120700
H	-12.77743490	2.61931719	0.00154600
N	-9.44842369	-0.92051006	0.00114600

D2P2A1

C	13.36563800	-2.11646100	0.41325000
C	12.04920500	-2.56036500	0.43057300
C	10.98783200	-1.77831100	-0.03816700
C	11.33034700	-0.51138000	-0.52776300
C	12.63637800	-0.03911900	-0.51469900
C	13.70196500	-0.82942800	-0.04230500
C	8.64918100	-0.05814600	-0.47105500
C	8.55793300	-1.39167200	-0.01214700
C	7.29501300	-1.80665900	0.45088900
H	7.14971500	-2.81302100	0.81110100
C	6.20648700	-0.95133800	0.46774600
C	7.56907800	0.80433400	-0.41157800
H	14.12746200	-2.79079800	0.77626900
H	11.86975800	-3.55365000	0.81322100
H	12.81913600	0.95344300	-0.90099100
N	15.00732900	-0.35054200	-0.00977200
H	5.26619900	-1.33568400	0.84589800
H	7.69426100	1.81490900	-0.78026000
C	9.42242700	-3.69538500	0.15954700
C	9.35206100	-4.16675800	1.61466100
H	10.22130400	-4.22221100	-0.36216000
H	8.49906400	-3.95505200	-0.35892100
H	9.17864100	-5.24615800	1.62845100
H	10.27650200	-3.96913700	2.15838800
H	8.53829300	-3.69054700	2.16283500
N	9.64935300	-2.25558600	-0.04806200
S	10.10526400	0.50414400	-1.32064800
C	16.08859800	-1.31260800	0.16254400
C	15.33939000	0.82117600	-0.81062900
H	16.14860900	-2.03453500	-0.66450400
H	15.97453900	-1.86677300	1.09497400
H	17.03164400	-0.77130500	0.21599000
H	15.20463700	0.64876700	-1.88825700
H	16.38133400	1.08160600	-0.63213200
H	14.73318200	1.68066600	-0.52137200
C	6.31162400	0.38079300	0.05011800
C	0.30488200	2.73220900	0.23268000
C	-1.03134800	2.90365200	0.27166300
C	-3.62658300	3.18474100	0.32152400
C	-4.38067900	4.34798400	0.37726500
S	-4.66109800	1.77124100	0.26427500
C	-5.75890600	4.10868800	0.37264400

H	-3.92833500	5.32890300	0.41750900
C	-6.10217000	2.76564000	0.31349800
H	-6.50791100	4.88918100	0.40860000
C	-7.43053600	2.25378900	0.28106400
H	-8.19518400	3.02371900	0.31403600
C	-7.79404100	0.94609300	0.20221200
H	-7.03024100	0.17541700	0.16452700
C	-9.14445500	0.46710400	0.14046600
C	-10.29318800	1.29140300	0.18979900
C	-9.37914600	-0.92088300	0.01207000
C	-11.54297700	0.75577200	0.10348400
H	-10.21622900	2.36363300	0.29837800
C	-10.64488500	-1.42059800	-0.07272000
H	-8.54870800	-1.61304800	-0.02794000
H	-12.43829400	1.35436700	0.13669500
H	-10.85637100	-2.47211400	-0.17710600
N	-11.72852700	-0.59182000	-0.03313600
C	-13.05814200	-1.13390800	-0.13143300
C	-15.27562500	-0.75952900	-0.24712700
C	-14.38314400	-2.95408500	-0.24127500
C	-15.50764700	-2.13285500	-0.28398600
H	-16.09853300	-0.05508700	-0.27974100
H	-14.46789600	-4.03343300	-0.26764900
N	-13.15216700	-2.45286400	-0.16258600
N	-14.04778700	-0.25535000	-0.16986300
C	-16.89793700	-2.64493800	-0.36326800
O	-17.87802400	-1.93621400	-0.37807700
O	-16.95509300	-3.98551200	-0.41631300
H	-17.89333500	-4.24857800	-0.46312400
C	-2.24110900	3.05131200	0.30043000
C	1.51288100	2.56758000	0.18798000
C	2.88381300	2.34372600	0.12853200
C	5.17969800	1.29760100	0.06589700
C	5.18648800	2.67777900	-0.02234100
H	6.09692300	3.25660000	-0.09524100
S	3.53798000	0.71252800	0.18634400
C	3.91058800	3.26332900	0.01426900
H	3.72910200	4.32858000	-0.03382600

D2P4A1

C	-15.76442200	2.34127900	0.32688800
C	-14.56524900	2.60526400	-0.32258200
C	-13.58498800	1.62541000	-0.51381400
C	-13.87959400	0.35498400	-0.00376400
C	-15.05833500	0.08503000	0.67965400
C	-16.05489000	1.06644700	0.84572900
C	-11.23746100	-0.12421500	-0.40518000
C	-11.20105000	1.19049700	-0.92434700
C	-9.92381800	1.72364600	-1.18155500
H	-9.81892400	2.71369200	-1.59649200

C	-8.76851000	1.01421100	-0.90296400
C	-10.07949900	-0.81197900	-0.09090900
H	-16.46946600	3.15318100	0.42969800
H	-14.40875300	3.61113900	-0.68141700
H	-15.20426900	-0.91476200	1.06301900
N	-17.26353200	0.77919600	1.46776300
H	-7.81950000	1.49414400	-1.11280800
H	-10.16897000	-1.81485700	0.30760000
C	-12.27692500	3.14339500	-1.98011600
C	-11.88832800	4.41058400	-1.21241900
H	-13.24547400	3.28374400	-2.45976800
H	-11.56209900	2.96431600	-2.78363600
H	-11.86284500	5.25130500	-1.91094600
H	-12.60252900	4.65114700	-0.42432400
H	-10.90329000	4.32822300	-0.75196900
N	-12.36588100	1.90304600	-1.19105000
S	-12.77789700	-1.00610300	-0.31026500
C	-18.10263200	1.89048100	1.89742100
C	-17.36463500	-0.43375000	2.26894400
H	-18.38483000	2.51875000	1.05123500
H	-17.61232400	2.52470000	2.64979500
H	-19.01798500	1.48995700	2.32945600
H	-17.15547100	-1.31960400	1.66760400
H	-18.38392500	-0.52286800	2.64042800
H	-16.67980500	-0.43113800	3.12915100
C	-8.80767900	-0.26379000	-0.33114300
C	-2.64345100	-2.14468000	0.11448900
C	-1.31313200	-2.29027600	0.04809700
C	6.38624400	-3.01466900	-0.34179400
C	7.14687100	-4.14499500	-0.59952200
S	7.41079300	-1.61444200	-0.09087700
C	8.52311800	-3.89170200	-0.59703600
H	6.70052400	-5.11261900	-0.78168100
C	8.85404400	-2.56969500	-0.34040300
H	9.27733400	-4.64614000	-0.77818200
C	10.18222100	-2.04849300	-0.28603400
H	10.94982000	-2.79463700	-0.46454800
C	10.53471100	-0.76231500	-0.03612400
H	9.76654800	-0.01818800	0.14915700
C	11.88393900	-0.26833400	0.01349000
C	13.03431100	-1.05325400	-0.22586200
C	12.10754400	1.09196200	0.31766900
C	14.28067900	-0.50462400	-0.15946800
H	12.96372800	-2.10340700	-0.47005400
C	13.37039300	1.60556600	0.37755900
H	11.27305800	1.75248500	0.51105100
H	15.17934700	-1.07184900	-0.33843500
H	13.57514300	2.63805400	0.60854700
N	14.45677100	0.81628500	0.14116100
C	15.78513400	1.37354200	0.20851500
C	18.00584900	1.05973000	0.01265600

C	17.09270800	3.17030500	0.58203100
C	18.22458700	2.39790700	0.33172700
H	18.83493500	0.39441400	-0.19692000
H	17.16710300	4.22020700	0.83675000
N	15.86602300	2.65576400	0.51995200
N	16.78209100	0.54260000	-0.04949900
C	19.61038000	2.92602300	0.39147700
O	20.59668400	2.25689800	0.18565200
O	19.65404200	4.23183700	0.70031000
H	20.58912300	4.50916900	0.72149700
C	-0.09434600	-2.41667600	-0.01456500
C	1.23434200	-2.55136100	-0.07931600
C	2.45309800	-2.67016300	-0.14184700
C	3.78731400	-2.79353500	-0.20757700
C	5.00087800	-2.90740400	-0.27153800
C	-3.85731200	-2.01235900	0.18135400
C	-5.23284900	-1.84451000	0.24739500
C	-7.60209900	-1.00766900	0.00462100
C	-7.48174000	-2.14608300	0.78345800
H	-8.32587700	-2.62219000	1.26249300
S	-6.03217100	-0.51386400	-0.58123000
C	-6.16673700	-2.61329900	0.92078400
H	-5.88813800	-3.48252900	1.50119600

D2P2A2

C	-14.29534100	1.87099200	0.76789600
C	-13.01395400	2.40708700	0.73013800
C	-11.94572500	1.75191100	0.10843200
C	-12.24548800	0.51979800	-0.48712900
C	-13.51267800	-0.04536600	-0.42658800
C	-14.58214400	0.61074600	0.21359600
C	-9.55190600	0.22638900	-0.61540900
C	-9.50449200	1.51255800	-0.03257300
C	-8.24499300	1.94611900	0.41900700
H	-8.12973300	2.92396600	0.85937400
C	-7.12134200	1.14048700	0.32995100
C	-8.43505100	-0.58888700	-0.66597700
H	-15.06693400	2.44821200	1.25585500
H	-12.86763700	3.36974900	1.19602000
H	-13.66243000	-1.00439600	-0.90201100
N	-15.84037700	0.02827300	0.31144900
H	-6.18667100	1.53298200	0.71340200
H	-8.53078800	-1.56698700	-1.12097800
C	-10.48373200	3.73875500	0.39425800
C	-10.35618200	4.08322700	1.88166700
H	-11.34002000	4.26101900	-0.03286000
H	-9.60664600	4.10036700	-0.14331000
H	-10.26888900	5.16819600	1.98481800
H	-11.22468700	3.76187500	2.45736000
H	-9.47315200	3.63312100	2.33689800

N	-10.64140800	2.31386400	0.05957200
S	-11.01688000	-0.31728900	-1.46288900
C	-16.96597600	0.86680400	0.70084800
C	-16.16254800	-1.08836700	-0.56733100
H	-17.17876200	1.65940900	-0.03094400
H	-16.78858200	1.33430400	1.67034900
H	-17.85183100	0.24089700	0.79575800
H	-16.13823200	-0.81110200	-1.63098800
H	-17.16327300	-1.44367800	-0.32791000
H	-15.47366900	-1.92049500	-0.41416900
C	-7.18440500	-0.15542200	-0.19549500
C	-1.11523100	-2.38585800	-0.10876700
C	0.21877400	-2.57554100	-0.01745500
C	1.42102600	-2.75367500	0.07447200
C	-2.32092400	-2.22186200	-0.18462100
C	-3.69777100	-2.02117600	-0.26181100
C	-6.02285300	-1.03486100	-0.25968700
C	-5.98987700	-2.39990400	-0.46660000
H	-6.88309600	-2.99533000	-0.59638500
S	-4.39725800	-0.41951100	-0.07022600
C	-4.69663000	-2.95265200	-0.46861900
H	-4.48639100	-4.00476700	-0.60627800
C	8.43637400	-0.42754600	-0.06879000
C	9.62461700	-1.18251400	0.22385000
C	8.65011500	0.90121900	-0.39459300
C	10.93471000	-0.55797500	0.18942800
C	9.92660400	1.50338600	-0.43733500
H	7.78980700	1.51967900	-0.62304700
C	11.09144300	0.82584000	-0.14696300
H	9.97760600	2.55593300	-0.68787100
C	12.40679700	1.49755000	-0.18880100
C	12.68530300	2.43273800	-1.19841300
C	13.39064000	1.25372600	0.78063700
C	13.89827700	3.09876500	-1.23645000
H	11.95079100	2.62423900	-1.97057700
C	14.60297300	1.92557900	0.74853000
H	13.19937000	0.54794500	1.57705400
C	14.86982200	2.85459800	-0.26175400
H	14.10351900	3.80999800	-2.02606900
H	15.34086200	1.72923700	1.51450800
C	16.15394900	3.59078300	-0.33863300
O	16.43996700	4.39337300	-1.20298900
O	17.00649100	3.28882000	0.66348900
H	17.81497300	3.81523900	0.52858700
N	9.67850000	-2.48073800	0.53404200
N	11.92560200	-1.41304600	0.46494000
S	11.24649200	-2.86312200	0.75151900
C	5.29916800	-2.64461100	0.24728100
C	2.79772900	-2.94465800	0.18402000
C	3.48480100	-4.10578100	0.48467200
H	2.98013600	-5.04321500	0.67483200

S	3.91931500	-1.61364000	-0.06516500
C	4.87899200	-3.93371800	0.51834100
H	5.57796200	-4.72997700	0.73915200
C	6.66454700	-2.19381500	0.22803500
C	7.08037700	-0.93666200	-0.04453700
H	7.38966600	-2.96407400	0.45911700
H	6.33538600	-0.18063500	-0.27992100

D2P4A2

C	-16.86695100	1.88642700	0.79778500
C	-15.59947900	2.45086400	0.72727400
C	-14.52409300	1.80316000	0.10965300
C	-14.80117800	0.54651200	-0.44349500
C	-16.05339100	-0.04664300	-0.34843800
C	-17.13069500	0.60392300	0.28400900
C	-12.10249300	0.31931300	-0.61067700
C	-12.07994000	1.62463200	-0.06897200
C	-10.82344500	2.10761500	0.34119700
H	-10.72744200	3.10140300	0.74911200
C	-9.67961700	1.33290000	0.25017600
C	-10.96394600	-0.46438300	-0.66189500
H	-17.64587600	2.45922600	1.27937900
H	-15.46989800	3.42968800	1.16352100
H	-16.18629700	-1.02327700	-0.79172900
N	-18.37448900	-0.00231700	0.41167700
H	-8.74861500	1.76503800	0.59860100
H	-11.04166100	-1.45833600	-1.08467100
C	-13.10879900	3.83294400	0.32255900
C	-12.96142200	4.21056200	1.79965000
H	-13.98637900	4.32312300	-0.09894200
H	-12.25247400	4.20495300	-0.24066600
H	-12.89113700	5.29875900	1.87931300
H	-13.81393800	3.88533600	2.39658800
H	-12.06289100	3.78418000	2.24710600
N	-13.23505000	2.39638800	0.02446700
S	-13.56703000	-0.29116000	-1.41152800
C	-19.51880000	0.82975700	0.76022300
C	-18.66921600	-1.16985000	-0.40845600
H	-19.73696900	1.59051900	-0.00301700
H	-19.35846600	1.33681300	1.71268100
H	-20.39409000	0.19199600	0.87078500
H	-18.65249500	-0.94687900	-1.48501200
H	-19.66026600	-1.53815500	-0.14917200
H	-17.95835000	-1.97465600	-0.21441800
C	-9.71569400	0.01981200	-0.23512800
C	-3.58301800	-2.01648700	-0.19750800
C	-2.25079800	-2.15709500	-0.13263000
C	-1.03242200	-2.28369500	-0.06800700
C	0.29647100	-2.42318100	0.00145000
C	1.51409500	-2.55238200	0.06897500

C	2.84651500	-2.69344200	0.14208700
C	4.05841000	-2.82897300	0.21262800
C	-4.79777400	-1.89402900	-0.25735900
C	-6.17603100	-1.73620100	-0.32139200
C	-8.52934000	-0.82206600	-0.30701200
C	-8.45478800	-2.18627700	-0.52503400
H	-9.32900400	-2.80819500	-0.65906300
S	-6.92478200	-0.15756100	-0.11512200
C	-7.14796200	-2.69782000	-0.53385700
H	-6.90491000	-3.74150300	-0.68113400
C	10.98922100	-0.26242300	0.01615300
C	12.20714100	-1.00978500	0.17548100
C	11.15630400	1.09421300	-0.20398000
C	13.49963400	-0.35100500	0.12122100
C	12.41528800	1.73101700	-0.26283000
H	10.27216700	1.70794200	-0.33113100
C	13.60830000	1.06063200	-0.09896900
H	12.42980900	2.80220400	-0.42177800
C	14.90618800	1.76446400	-0.15675800
C	15.11060600	2.78493700	-1.09898700
C	15.94838500	1.46142600	0.73167800
C	16.30891100	3.47639100	-1.14990800
H	14.32967100	3.02409100	-1.80986200
C	17.14672600	2.15710600	0.68610000
H	15.81499400	0.68917800	1.47648700
C	17.34003900	3.17063300	-0.25735800
H	16.45716100	4.25435500	-1.88762700
H	17.93129600	1.91284800	1.38933500
C	18.60635600	3.93601900	-0.34691100
O	18.81989200	4.82748100	-1.14237500
O	19.53236900	3.54959700	0.55595600
H	20.32254100	4.10289200	0.42004300
N	12.30604600	-2.32842100	0.36494500
N	14.52243000	-1.20109300	0.26106200
S	13.89207500	-2.68763700	0.45554500
C	7.92730700	-2.58397200	0.31106300
C	5.43936900	-2.97018200	0.29075700
C	6.17349400	-4.11803400	0.53257700
H	5.70529700	-5.07914800	0.69571100
S	6.50845800	-1.59038500	0.07057700
C	7.55916300	-3.89820800	0.54148100
H	8.29109700	-4.67651100	0.71341800
C	9.27730300	-2.09043500	0.27238100
C	9.64771600	-0.80707900	0.06405100
H	10.03197600	-2.85068200	0.42963900
H	8.87505900	-0.05749200	-0.08904400

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C	7.56037200	-1.51104900	0.17325800
C	8.43198100	-2.58628300	0.29374400

S	8.42953200	0.00094200	0.05530400
C	9.77169500	-2.20019600	0.29110000
H	8.08582000	-3.60653700	0.37919500
C	9.97247900	-0.82832500	0.16975000
H	10.60102900	-2.89045900	0.37489500
C	3.60352000	-1.55370100	0.08175700
C	4.95027500	-1.54230000	0.11281400
C	11.25948500	-0.23528300	0.14559300
H	12.06386500	-0.95736600	0.23080700
C	11.64653400	1.07225700	0.03526900
C	6.16879100	-1.53472000	0.14161100
C	2.38377900	-1.56775600	0.05532400
C	10.72294600	2.14616700	-0.08136100
N	9.96433000	3.01157000	-0.17567600
C	13.06593100	1.47730400	0.02711200
O	13.43728800	2.62879200	-0.06774800
O	13.92077200	0.44257900	0.13454400
H	14.82531000	0.80421000	0.12219200
C	-10.00391200	1.15597900	0.57359500
C	-8.80374300	1.80217900	0.30547800
C	-7.67346500	1.12101800	-0.15926000
C	-7.82373000	-0.25866400	-0.34797900
C	-9.00545100	-0.92438500	-0.04944700
C	-10.13731000	-0.23693800	0.43008900
C	-5.11837200	-0.25779000	-0.55396400
C	-5.22611200	1.14074900	-0.37831700
C	-4.02223700	1.83617200	-0.15936800
H	-4.02626900	2.90704700	-0.03024900
C	-2.80482400	1.18090400	-0.08776400
C	-3.90483100	-0.91175900	-0.44038000
H	-10.83350500	1.75763700	0.91529500
H	-8.77243300	2.86992600	0.46025000
H	-9.04070200	-1.99204900	-0.21298100
N	-11.30859100	-0.90542900	0.76337600
H	-1.91968300	1.77810300	0.09887100
H	-3.88279900	-1.98507000	-0.58292000
C	-6.47531400	3.26168900	-0.55043300
C	-6.35106200	4.03631400	0.76496600
H	-7.40405100	3.53184000	-1.05316800
H	-5.66925800	3.54907400	-1.22601900
H	-6.37671400	5.10734600	0.54669900
H	-7.16701700	3.81507600	1.45365700
H	-5.41488600	3.82250900	1.28180600
N	-6.45428400	1.79266800	-0.44805400
S	-6.52037000	-1.19954000	-1.10778700
C	-12.52997900	-0.12705500	0.92264600
C	-11.48741100	-2.27498200	0.30037200
H	-12.83206800	0.38082600	-0.00449900
H	-12.41529900	0.62611900	1.70355300
H	-13.33352800	-0.79578200	1.22620800
H	-11.50826400	-2.35253400	-0.79624000

H	-12.43022200	-2.65505200	0.68977700
H	-10.69233000	-2.92209600	0.67430000
C	-2.70917500	-0.21116300	-0.20707300
C	-1.44156900	-0.92016400	-0.10065200
C	-1.22577800	-2.27581500	0.07251200
S	0.08611100	-0.07688100	-0.19034800
C	0.12789900	-2.63904400	0.14194600
H	-2.03087800	-2.99130400	0.16688600
C	0.99462600	-1.56738500	0.02213900
H	0.47862600	-3.65229700	0.28462800

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C	10.55056400	-1.37288500	0.16636100
C	11.45228200	-2.42120500	0.29163100
S	11.37147000	0.16845400	0.09492300
C	12.77888100	-1.99091300	0.33053100
H	11.13801100	-3.45353000	0.35180000
C	12.93463800	-0.61187700	0.23577000
H	13.62830800	-2.65464000	0.42536000
C	1.47960500	-1.57355600	-0.21395800
C	2.81793500	-1.56346200	-0.16827400
C	14.20261700	0.02825000	0.25705200
H	15.03013700	-0.66450100	0.36377600
C	14.53871200	1.34904500	0.16578900
C	4.04424500	-1.54866600	-0.12718000
C	5.37946300	-1.52831400	-0.07229200
C	6.60416700	-1.50450000	-0.02016600
C	7.94355000	-1.46961500	0.04141400
C	9.16183200	-1.43697400	0.09971500
C	0.25683400	-1.58543000	-0.24326500
C	13.57601700	2.38499900	0.01628100
N	12.78708100	3.21901500	-0.10441300
C	15.94042200	1.81617600	0.21114200
O	16.26131000	2.98240900	0.12078700
O	16.83340100	0.82194700	0.36365600
H	17.72202400	1.22149600	0.38054400
C	-12.04554200	1.35972900	0.75184000
C	-10.85644700	1.95361400	0.34829900
C	-9.76796300	1.20964700	-0.11978200
C	-9.94738200	-0.17878300	-0.16149100
C	-11.11694600	-0.78939100	0.27194500
C	-12.20776000	-0.03749100	0.74962100
C	-7.26150500	-0.24550300	-0.55956600
C	-7.34224900	1.16557400	-0.51765100
C	-6.11741200	1.85857900	-0.46980000
H	-6.10012600	2.93704500	-0.45483800
C	-4.90493700	1.19284100	-0.43407000
C	-6.04892100	-0.90507900	-0.47927300
H	-12.84229800	2.00805200	1.08608100
H	-10.80096100	3.03030400	0.39866700

H	-11.17687400	-1.86686300	0.21437800
N	-13.36674100	-0.64768100	1.21354400
H	-4.00263000	1.79220700	-0.39545100
H	-6.05116100	-1.98753200	-0.50389800
C	-8.57932600	3.27920600	-0.81133300
C	-8.35686800	4.18840800	0.40055200
H	-9.53807900	3.51002600	-1.27582300
H	-7.82024500	3.47877700	-1.56776500
H	-8.37657500	5.22954500	0.06725700
H	-9.13154700	4.06598200	1.15835400
H	-7.39412700	4.01036700	0.88132500
N	-8.56429500	1.82892800	-0.55428400
S	-8.70946700	-1.21682600	-0.90303100
C	-14.56611900	0.16632200	1.36261400
C	-13.59708100	-2.04929600	0.88874200
H	-14.91941500	0.57853300	0.40661400
H	-14.39495900	0.99475300	2.05103200
H	-15.35732300	-0.45178300	1.78357000
H	-13.70139000	-2.22270100	-0.19196400
H	-14.51304800	-2.37516700	1.37883500
H	-12.78567900	-2.67658100	1.26071900
C	-4.83066100	-0.20587600	-0.41983500
C	-3.56501700	-0.92095200	-0.35615700
C	-3.35056100	-2.28643600	-0.26290800
S	-2.03566600	-0.07646100	-0.39028900
C	-1.99956400	-2.65581600	-0.21783100
H	-4.15518900	-3.00713100	-0.22120300
C	-1.12904400	-1.58020400	-0.27453200
H	-1.65099500	-3.67697700	-0.14206700

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C	14.10960000	-2.07050000	1.42560000
C	13.74290000	-3.16410000	2.19760000
S	12.70130000	-1.28800000	0.62120000
C	12.38250000	-3.41510000	2.18270000
H	14.44400000	-3.76800000	2.76000000
C	11.64770000	-2.52960000	1.40230000
H	11.92530000	-4.23270000	2.73240000
C	10.23810000	-2.60460000	1.24660000
H	9.75650000	-3.40460000	1.77720000
C	9.52040000	-1.74170000	0.48750000
H	10.03820000	-0.94740000	-0.03310000
C	8.09770000	-1.79540000	0.31080000
C	7.29320000	-2.76190000	0.91740000
C	7.49310000	-0.82370000	-0.51720000
C	5.97680000	-2.75810000	0.71010000
H	7.66270000	-3.53620000	1.56160000
C	6.16190000	-0.84810000	-0.70580000
H	8.05030000	-0.05800000	-1.00810000
H	5.35890000	-3.51470000	1.18590000

H	5.66980000	-0.11550000	-1.33540000
N	5.42060000	-1.80280000	-0.09670000
C	3.98260000	-1.86880000	-0.26120000
C	1.90340000	-2.84430000	0.12730000
C	2.12010000	-0.94450000	-1.35200000
C	1.30780000	-1.92080000	-0.77690000
H	1.31610000	-3.59580000	0.64680000
H	1.78260000	-0.15570000	-2.00370000
N	3.36350000	-1.07240000	-1.00840000
N	3.24810000	-2.79750000	0.35210000
C	-0.10700000	-1.96540000	-1.01550000
O	-0.78850000	-2.75260000	-0.35440000
O	-0.54290000	-1.16840000	-1.87960000
C	18.81660000	-0.20520000	0.70300000
C	17.70770000	-0.67240000	0.89560000
C	16.51420000	-1.16300000	1.09330000
C	15.40210000	-1.60850000	1.26750000
C	20.10560000	0.38370000	0.44560000
C	22.05780000	1.73940000	-0.29350000
C	22.41520000	0.66430000	0.51000000
H	23.42670000	0.44800000	0.81660000
S	20.27780000	1.87160000	-0.55250000
C	21.33240000	-0.08900000	0.91230000
H	21.41420000	-0.96780000	1.53500000
C	24.30290000	2.76300000	-0.77300000
C	25.20490000	1.77990000	-0.84930000
C	26.45400000	2.38000000	-0.91100000
H	25.00380000	0.71030000	-0.90480000
C	26.26300000	3.70190000	-0.89190000
H	27.41420000	1.89150000	-0.97840000
H	27.01640000	4.47020000	-0.93890000
N	24.94380000	3.96650000	-0.81480000
H	24.49040000	4.89810000	-0.80690000
N	22.88400000	2.69340000	-0.82280000
H	22.41000000	3.50490000	-1.26500000
Ti	-5.33450000	2.16210000	3.73520000
O	-3.91900000	1.13710000	2.82170000
O	-7.27490000	2.09340000	3.47350000
O	-5.62460000	1.20830000	5.48230000
O	-6.25370000	-0.84520000	1.39340000
O	-6.00770000	1.38860000	-1.54740000
O	-4.77430000	0.19570000	-0.01620000
O	-4.66530000	-1.87090000	3.12960000
O	-6.98120000	4.21530000	0.47960000
O	-5.79360000	3.63680000	2.46760000
Ti	-9.46140000	1.39050000	0.41880000
O	-9.47000000	2.97940000	1.65240000
O	-7.50180000	1.49270000	0.72470000
O	-7.58120000	-1.34180000	4.11390000
O	-6.50760000	-3.99090000	1.85530000
Ti	-6.68880000	0.05920000	-0.27490000

Ti	-8.75410000	-1.62490000	-1.79900000
O	-8.60390000	-0.14570000	-0.50360000
O	-6.80440000	-1.48140000	-1.44040000
Ti	-6.49650000	-2.17240000	2.66250000
Ti	-7.55030000	2.97700000	1.80880000
Ti	-7.34290000	0.58980000	4.69240000
O	-3.67410000	3.14940000	0.16150000
O	-2.63990000	-1.21820000	1.30370000
Ti	-4.08560000	1.68820000	-1.05170000
O	-2.35490000	0.97270000	-1.48150000
Ti	-4.33800000	-0.44790000	1.78150000
Ti	-5.07180000	4.39010000	0.77360000
O	-5.07640000	5.90200000	-0.54680000
O	-4.08430000	2.51720000	-2.84760000
O	-6.78100000	4.03990000	-2.97470000
O	-5.85770000	0.96960000	-4.72790000
Ti	-5.93890000	2.23940000	-3.20250000
Ti	-6.76950000	5.09530000	-1.22870000
Ti	-2.62450000	-2.64510000	-0.00360000
O	-5.57280000	-4.50850000	-1.48800000
O	-3.24250000	-4.33730000	0.73480000
O	-5.36990000	-2.39460000	-4.22760000
O	-3.45750000	-2.16150000	-1.65650000
O	-8.08560000	-3.20320000	-2.81050000
Ti	-6.14280000	-2.89860000	-2.47840000
Ti	-5.15360000	-4.31320000	0.42790000
Ti	-2.33680000	-0.77600000	-2.36100000
O	-2.71610000	-0.52240000	-4.27220000
Ti	-4.67080000	-0.58970000	-4.43730000
H	-1.64280000	1.09750000	-0.81690000

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C	14.23400000	-1.48990000	1.16630000
C	13.04720000	-1.98180000	1.29650000
C	10.62470000	-2.87330000	1.50010000
C	10.22890000	-3.98710000	2.21810000
S	9.25280000	-2.02040000	0.68420000
C	8.86650000	-4.21430000	2.16450000
H	10.90480000	-4.62550000	2.77390000
C	8.16370000	-3.28400000	1.40270000
H	8.39380000	-5.04370000	2.67450000
C	6.76330000	-3.33570000	1.23400000
H	6.25510000	-4.13760000	1.73690000
C	6.06940000	-2.44200000	0.48950000
H	6.61530000	-1.65470000	-0.01100000
C	4.65220000	-2.45130000	0.30920000
C	3.80950000	-3.40340000	0.90500000
C	4.07410000	-1.45420000	-0.49950000
C	2.48600000	-3.34720000	0.70480000
H	4.15620000	-4.19970000	1.53250000

C	2.74170000	-1.43120000	-0.67790000
H	4.66330000	-0.69490000	-0.98800000
H	1.85940000	-4.09270000	1.17370000
H	2.31850000	-0.64800000	-1.30620000
N	1.97000000	-2.36190000	-0.07790000
C	0.51720000	-2.33580000	-0.26920000
C	-1.63540000	-3.20160000	0.20190000
C	-1.35030000	-1.42010000	-1.37090000
C	-2.18130000	-2.32860000	-0.74480000
H	-2.23800000	-3.88300000	0.77070000
H	-1.73160000	-0.66990000	-2.06090000
N	-0.00440000	-1.44290000	-1.14080000
N	-0.27680000	-3.18090000	0.39800000
C	-3.63410000	-2.29470000	-0.98190000
O	-4.36800000	-2.92140000	-0.30000000
O	-4.00610000	-1.44670000	-1.89030000
C	11.92590000	-2.42590000	1.41000000
C	15.34810000	-1.02380000	1.04470000
C	21.51710000	1.54280000	0.39950000
C	23.43410000	2.89150000	-0.28850000
C	23.75460000	1.89380000	0.61070000
H	24.74290000	1.71660000	1.01990000
S	21.67910000	2.96370000	-0.68500000
C	22.64670000	1.14210000	0.97110000
H	22.70390000	0.30680000	1.65500000
C	25.69830000	3.94520000	-0.63630000
C	26.59670000	2.98570000	-0.60950000
C	27.84120000	3.60290000	-0.59440000
H	26.42400000	1.90740000	-0.64690000
C	27.61370000	4.90410000	-0.63720000
H	28.80690000	3.12900000	-0.56720000
H	28.38080000	5.67900000	-0.64810000
N	26.31160000	5.16280000	-0.67350000
H	25.83460000	6.08720000	-0.73900000
N	24.28540000	3.83070000	-0.81620000
H	23.82320000	4.60360000	-1.34610000
H	-4.95660000	0.98510000	-0.77870000
C	16.66040000	-0.49000000	0.91620000
C	17.79300000	-0.05130000	0.82240000
C	19.11300000	0.46190000	0.71230000
C	20.22410000	0.92580000	0.59620000
Ti	-8.60170000	2.39800000	3.69680000
O	-7.26390000	1.24380000	2.79880000
O	-10.52360000	2.53770000	3.38120000
O	-9.03890000	1.42220000	5.42790000
O	-9.79700000	-0.43590000	1.27240000
O	-9.20630000	1.79420000	-1.59420000
O	-8.19550000	0.40700000	-0.09570000
O	-8.39190000	-1.70330000	3.02310000
O	-9.90480000	4.66090000	0.46370000
O	-8.89740000	3.96760000	2.49210000

Ti	-12.71590000	2.17330000	0.26410000
O	-12.58300000	3.73430000	1.54200000
O	-10.76890000	2.02040000	0.60710000
O	-11.31910000	-0.85920000	3.95740000
O	-10.48800000	-3.57950000	1.65610000
Ti	-10.08630000	0.52720000	-0.38920000
Ti	-12.31840000	-0.87810000	-1.96910000
O	-12.00340000	0.58350000	-0.68200000
O	-10.37210000	-0.96390000	-1.58420000
Ti	-10.26050000	-1.76450000	2.49860000
Ti	-10.65420000	3.47510000	1.73650000
Ti	-10.83020000	1.04390000	4.59070000
O	-6.71020000	3.24450000	0.23850000
O	-6.20520000	-1.22810000	1.29000000
Ti	-7.30840000	1.86680000	-1.05200000
O	-5.65160000	0.94500000	-1.48340000
Ti	-7.88770000	-0.28570000	1.70870000
Ti	-8.00060000	4.61870000	0.82970000
O	-7.78450000	6.15800000	-0.47570000
O	-7.13210000	2.72040000	-2.83910000
O	-9.68120000	4.58510000	-3.02190000
O	-9.07210000	1.45240000	-4.82680000
Ti	-9.02480000	2.67780000	-3.23850000
Ti	-9.57610000	5.58720000	-1.21200000
Ti	-6.25370000	-2.66020000	-0.07020000
O	-9.47430000	-4.14810000	-1.69910000
O	-7.17890000	-4.26450000	0.62630000
O	-8.97950000	-2.00210000	-4.40710000
O	-7.09290000	-2.08550000	-1.71660000
O	-11.82720000	-2.48940000	-3.03590000
Ti	-9.84650000	-2.42880000	-2.65420000
Ti	-9.09750000	-3.98600000	0.24910000
Ti	-5.75890000	-0.80370000	-2.33190000
O	-6.08170000	-0.43450000	-4.26900000
Ti	-8.05170000	-0.25680000	-4.50640000

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C	20.46030000	0.20640000	0.70370000
C	22.65720000	1.42170000	0.43730000
C	22.77380000	0.21260000	1.09930000
H	23.70850000	-0.16810000	1.48070000
S	20.99770000	1.72490000	-0.03900000
C	21.54390000	-0.45320000	1.24730000
H	21.43760000	-1.40450000	1.75220000
C	24.99060000	2.18940000	0.25310000
C	25.81610000	1.08170000	0.22470000
C	27.15090000	1.56140000	0.37480000
H	25.50820000	0.05840000	0.09030000
C	27.09730000	2.92970000	0.48170000
H	28.04680000	0.96010000	0.39400000

H	27.87330000	3.66820000	0.59790000
N	25.77480000	3.30140000	0.41520000
H	25.42900000	4.24820000	0.48630000
N	23.61070000	2.34590000	0.12540000
H	23.29930000	3.22930000	-0.25680000
C	19.12160000	-0.16140000	0.68730000
C	17.94060000	-0.47150000	0.66510000
C	16.63670000	-0.82040000	0.64400000
C	15.46060000	-1.14220000	0.62800000
C	7.81580000	-1.76550000	-0.22550000
C	6.79590000	-2.73390000	0.06370000
C	7.36960000	-0.60700000	-0.83590000
C	5.40830000	-2.50600000	-0.28500000
C	6.01600000	-0.38300000	-1.16820000
H	8.07570000	0.17420000	-1.08760000
C	5.00470000	-1.29250000	-0.92690000
H	5.77290000	0.54930000	-1.66310000
C	3.60590000	-1.01410000	-1.31110000
C	3.07780000	0.27940000	-1.16800000
C	2.77980000	-2.01120000	-1.85170000
C	1.77880000	0.56500000	-1.55230000
H	3.68580000	1.06310000	-0.73330000
C	1.48090000	-1.72550000	-2.24250000
H	3.16200000	-3.01360000	-1.98540000
C	0.96570000	-0.43420000	-2.09490000
H	1.38200000	1.56420000	-1.42770000
H	0.86840000	-2.50890000	-2.66810000
C	-0.41820000	-0.08630000	-2.49440000
O	-0.94970000	1.10560000	-2.38520000
O	-1.08480000	-1.09400000	-2.97900000
N	6.99680000	-3.90550000	0.67510000
N	4.60780000	-3.51330000	0.08650000
S	5.54740000	-4.63630000	0.79650000
C	11.61480000	-1.58570000	0.27230000
C	14.11400000	-1.50330000	0.60500000
C	13.52390000	-2.66270000	1.08390000
H	14.09870000	-3.44920000	1.55390000
S	12.89690000	-0.45190000	-0.08980000
C	12.13450000	-2.70550000	0.89780000
H	11.52100000	-3.53860000	1.21320000
C	10.26010000	-1.26000000	-0.09190000
C	9.19220000	-2.05850000	0.12930000
H	10.11930000	-0.30020000	-0.57860000
H	9.34890000	-3.01570000	0.61320000
Ti	-5.94770000	-2.23160000	3.43990000
O	-4.64890000	-1.99210000	2.08750000
O	-7.93680000	-1.95260000	3.30900000
O	-6.39680000	-4.06460000	3.54740000
O	-6.62390000	-1.46270000	-0.35730000
O	-6.28770000	2.23070000	0.23250000
O	-4.98210000	0.19190000	0.23880000

O	-5.16190000	-3.49370000	-0.25460000
O	-7.54420000	1.79200000	3.83270000
O	-6.16210000	-0.30410000	3.97700000
Ti	-9.78030000	0.49870000	1.08460000
O	-9.84190000	0.21700000	3.00340000
O	-7.86820000	0.23330000	1.50080000
O	-7.80070000	-3.87540000	0.60580000
O	-6.47260000	-3.15150000	-2.69720000
Ti	-6.98460000	0.45780000	-0.23680000
Ti	-8.88030000	1.01720000	-2.59070000
O	-8.91970000	0.66110000	-0.67230000
O	-6.95890000	0.72390000	-2.16170000
Ti	-6.79510000	-3.23990000	-0.85850000
Ti	-8.06340000	-0.01390000	3.31800000
Ti	-7.83180000	-3.65770000	2.44620000
O	-4.39100000	1.62450000	2.60450000
O	-3.09320000	-1.70460000	-0.58310000
Ti	-4.32500000	1.83270000	0.85460000
O	-2.49480000	1.67180000	0.23360000
Ti	-4.68890000	-1.70570000	0.32760000
Ti	-5.58480000	1.60410000	4.07570000
O	-5.66690000	3.31230000	4.87920000
O	-4.37770000	3.76490000	0.82260000
O	-6.85940000	4.40100000	2.00800000
O	-5.76190000	4.53860000	-1.44470000
Ti	-6.05310000	4.05890000	0.35190000
Ti	-7.06810000	3.64560000	3.69540000
Ti	-2.80550000	-1.33550000	-2.34060000
O	-5.65530000	-0.63600000	-4.46980000
O	-3.32780000	-2.55540000	-3.59980000
O	-5.39400000	2.56840000	-3.81680000
O	-3.07100000	0.50040000	-2.60130000
O	-8.02680000	1.21070000	-4.35050000
Ti	-6.31670000	0.96420000	-3.89100000
Ti	-5.17330000	-2.26030000	-3.70840000
Ti	-2.35370000	1.90920000	-1.76540000
O	-2.79470000	3.44410000	-2.62150000
Ti	-4.62850000	3.78200000	-2.69880000
H	-1.74400000	1.30160000	0.73480000

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C	-24.54500000	-0.56430000	0.47060000
C	-26.83160000	-1.61500000	0.27800000
C	-26.86420000	-0.29490000	0.70260000
H	-27.77720000	0.22810000	0.94110000
S	-25.18790000	-2.14630000	-0.01580000
C	-25.58990000	0.27720000	0.81140000
H	-25.41740000	1.29350000	1.14020000
C	-29.21930000	-2.17770000	0.10010000
C	-29.92630000	-1.03200000	-0.20920000

C	-31.30530000	-1.33830000	-0.02030000
H	-29.51090000	-0.09750000	-0.54800000
C	-31.39380000	-2.64850000	0.38510000
H	-32.13580000	-0.66680000	-0.17530000
H	-32.24390000	-3.26620000	0.62320000
N	-30.11610000	-3.14760000	0.46400000
H	-29.86960000	-4.08320000	0.75590000
N	-27.85730000	-2.48530000	0.07490000
H	-27.62520000	-3.44440000	-0.15030000
C	-21.98090000	-0.09090000	0.46510000
C	-20.66680000	0.16630000	0.45960000
C	-19.46340000	0.41210000	0.45090000
C	-18.15610000	0.69380000	0.44320000
C	-16.95960000	0.96570000	0.43330000
C	-15.65350000	1.27470000	0.42510000
C	-14.46920000	1.57450000	0.41600000
C	-23.18650000	-0.31080000	0.47040000
C	-6.79560000	2.08220000	-0.15470000
C	-5.79070000	3.08470000	0.05900000
C	-6.32250000	0.85670000	-0.58770000
C	-4.38800000	2.81880000	-0.18440000
C	-4.95390000	0.59670000	-0.81680000
H	-7.01760000	0.04840000	-0.77630000
C	-3.95480000	1.53400000	-0.64150000
H	-4.68770000	-0.39050000	-1.17430000
C	-2.53820000	1.21470000	-0.91280000
C	-2.02080000	-0.04520000	-0.57180000
C	-1.68440000	2.13590000	-1.53780000
C	-0.70370000	-0.37200000	-0.84640000
H	-2.65200000	-0.76760000	-0.06930000
C	-0.36730000	1.80810000	-1.81930000
H	-2.05800000	3.10940000	-1.82350000
C	0.13770000	0.55080000	-1.47420000
H	-0.31520000	-1.34360000	-0.56970000
H	0.26760000	2.53110000	-2.31310000
C	1.54020000	0.16070000	-1.75160000
O	2.06290000	-1.00200000	-1.45720000
O	2.23250000	1.09880000	-2.33270000
N	-6.02030000	4.32530000	0.50070000
N	-3.60510000	3.86940000	0.09290000
S	-4.57720000	5.07130000	0.59990000
C	-10.61310000	1.95370000	0.18430000
C	-13.12240000	1.92090000	0.40410000
C	-12.54890000	3.14170000	0.72920000
H	-13.14170000	3.98910000	1.04560000
S	-11.87950000	0.77640000	-0.06270000
C	-11.15410000	3.15730000	0.60620000
H	-10.55070000	4.02880000	0.82090000
C	-9.24300000	1.58090000	-0.06020000
C	-8.18810000	2.41280000	0.08630000
H	-9.07960000	0.55820000	-0.38440000

H	-8.36910000	3.43100000	0.41130000
Ti	7.21200000	2.39700000	3.18240000
O	5.87260000	2.10180000	1.88160000
O	9.18520000	2.02880000	3.03290000
O	7.73340000	4.21320000	3.13110000
O	7.76630000	1.29870000	-0.55300000
O	7.30320000	-2.31880000	0.34210000
O	6.07720000	-0.23540000	0.21000000
O	6.38600000	3.38830000	-0.58520000
O	8.66220000	-1.64270000	3.86750000
O	7.36530000	0.51190000	3.86990000
Ti	10.87920000	-0.66550000	0.97690000
O	10.99780000	-0.23310000	2.86470000
O	8.98930000	-0.29100000	1.41020000
O	9.05750000	3.73190000	0.18580000
O	7.62330000	2.79850000	-3.01880000
Ti	8.05590000	-0.61880000	-0.28440000
Ti	9.87140000	-1.44130000	-2.62420000
O	9.97070000	-0.93400000	-0.74240000
O	7.97360000	-1.03750000	-2.18030000
Ti	7.99320000	3.02150000	-1.20060000
Ti	9.23770000	0.09360000	3.19690000
Ti	9.12470000	3.66170000	2.03670000
O	5.48900000	-1.44820000	2.69620000
O	4.24300000	1.66310000	-0.72360000
Ti	5.37290000	-1.79360000	0.97070000
O	3.53560000	-1.61000000	0.37730000
Ti	5.85900000	1.67330000	0.15030000
Ti	6.71790000	-1.35750000	4.13540000
O	6.75390000	-2.99750000	5.07320000
O	5.35070000	-3.72270000	1.09480000
O	7.83410000	-4.36050000	2.27570000
O	6.64910000	-4.73110000	-1.13050000
Ti	7.00180000	-4.12060000	0.61460000
Ti	8.11220000	-3.48090000	3.89140000
Ti	3.89900000	1.16580000	-2.43890000
O	6.66770000	0.18340000	-4.56350000
O	4.43710000	2.25840000	-3.80380000
O	6.29970000	-2.94510000	-3.64670000
O	4.08760000	-0.69430000	-2.55490000
O	8.96890000	-1.74130000	-4.34410000
Ti	7.28100000	-1.39020000	-3.87050000
Ti	6.26670000	1.88170000	-3.92670000
Ti	3.33730000	-2.00150000	-1.59240000
O	3.69840000	-3.61670000	-2.32990000
Ti	5.51550000	-4.03300000	-2.41790000
H	2.81190000	-1.17080000	0.86240000

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Ti	-5.12380000	2.52780000	-2.87310000
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O	-3.36830000	2.24670000	-2.49170000
O	-6.83250000	2.44260000	-1.74480000
O	-5.48500000	4.31500000	-2.85020000
O	-3.89810000	1.80250000	0.62700000
O	-4.15110000	-1.81470000	-0.03930000
O	-3.08190000	0.12230000	-0.76140000
O	-2.62750000	3.72620000	-0.21650000
O	-7.08040000	-1.18190000	-2.40610000
O	-5.82710000	0.78800000	-3.35240000
Ti	-7.36100000	0.09470000	1.03680000
O	-8.44280000	0.44780000	-0.51030000
O	-5.98870000	0.24250000	-0.31960000
O	-5.30400000	4.31530000	0.50650000
O	-2.78300000	3.50990000	2.64190000
Ti	-4.33630000	-0.05600000	0.67390000
Ti	-4.67360000	-0.58330000	3.59920000
O	-5.83610000	-0.20510000	2.11300000
O	-3.35300000	-0.40910000	2.20310000
Ti	-3.74290000	3.56880000	1.12830000
Ti	-7.14320000	0.57220000	-1.68980000
Ti	-6.07550000	4.03280000	-1.13730000
O	-3.60580000	-1.19540000	-3.12530000
O	-0.82550000	1.68500000	-0.56750000
Ti	-2.81550000	-1.60730000	-1.55890000
O	-1.05740000	-1.70730000	-1.19040000
Ti	-2.57080000	1.97080000	-0.89960000
Ti	-5.37330000	-1.08660000	-3.53700000
O	-5.97010000	-2.69870000	-4.14190000
O	-3.12640000	-3.46430000	-1.53980000
O	-5.86990000	-3.91520000	-1.00710000
O	-3.31710000	-4.25340000	1.21520000
Ti	-4.24010000	-3.64810000	-0.19750000
Ti	-6.55680000	-2.97070000	-2.42490000
Ti	-0.03420000	1.25120000	1.00430000
O	-1.15370000	0.87570000	3.89100000
O	0.28840000	2.65790000	2.11760000
O	-1.36740000	-2.48470000	3.26160000
O	-0.61410000	-0.46830000	1.46410000
O	-3.13860000	-0.87920000	4.59090000
Ti	-1.85070000	-0.72650000	3.35490000
Ti	-1.24860000	2.48100000	3.04100000
Ti	-0.23530000	-1.98030000	0.40180000
Ti	-1.66170000	-3.66520000	1.91130000
C	13.44460000	-0.57000000	-0.28760000
C	12.28880000	-0.23070000	-0.13780000
C	10.99050000	0.10350000	0.03600000
C	9.82600000	0.40710000	0.18050000
C	8.48820000	0.75970000	0.36090000
C	7.97580000	2.00050000	0.63540000
S	7.18900000	-0.47470000	0.23510000
C	6.56930000	2.01760000	0.75970000

H	8.60210000	2.87190000	0.74710000
C	5.96440000	0.79830000	0.58310000
H	5.99890000	2.90980000	0.97900000
C	4.55890000	0.57740000	0.66130000
H	3.96050000	1.45570000	0.89010000
C	3.85760000	-0.56310000	0.49650000
C	4.41890000	-1.82990000	0.20200000
C	2.38930000	-0.50770000	0.64450000
O	1.85360000	0.63390000	0.90680000
O	1.71920000	-1.58900000	0.50170000
N	4.88360000	-2.86480000	-0.03490000
C	14.77150000	-0.94020000	-0.47740000
C	15.27960000	-2.19370000	-0.64850000
S	16.09920000	0.30150000	-0.56680000
C	16.67990000	-2.24540000	-0.86360000
H	14.64940000	-3.07040000	-0.62960000
C	17.28750000	-1.01950000	-0.84960000
H	17.22450000	-3.16350000	-1.02730000
H	19.22610000	-1.59400000	-0.96990000
C	19.23660000	0.46190000	-1.14800000
C	18.78380000	1.67980000	-1.57700000
C	19.89970000	2.56530000	-1.51040000
H	17.79740000	1.92220000	-1.93080000
C	20.94560000	1.82790000	-1.05220000
H	19.89890000	3.60780000	-1.78390000
H	21.97320000	2.07840000	-0.86350000
N	18.62790000	-0.77460000	-0.97740000
H	21.10490000	-0.17230000	-0.46450000
N	20.52460000	0.56530000	-0.82700000
H	0.83670000	-3.66070000	1.11810000
O	-0.14610000	-3.71350000	0.94080000

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Ti	-6.20080000	1.97810000	-3.18280000
O	-4.42700000	1.74660000	-2.81980000
O	-7.93330000	2.08130000	-2.07690000
O	-6.53480000	3.74830000	-3.45470000
O	-4.99630000	1.89080000	0.36890000
O	-5.18060000	-1.84790000	0.31260000
O	-4.10400000	-0.01100000	-0.70380000
O	-3.72620000	3.66880000	-0.82620000
O	-8.11450000	-1.68380000	-2.13330000
O	-6.92680000	0.16610000	-3.41020000
Ti	-8.39270000	0.17270000	1.00920000
O	-9.51160000	0.24800000	-0.58740000
O	-7.01390000	0.12520000	-0.36740000
O	-6.41330000	4.36910000	-0.13480000
O	-3.86870000	3.94310000	2.04270000
Ti	-5.35680000	0.02750000	0.71100000
Ti	-5.65560000	0.00780000	3.67970000

O	-6.87010000	0.09360000	2.16380000
O	-4.32530000	-0.04560000	2.23410000
Ti	-4.82540000	3.71110000	0.54320000
Ti	-8.18940000	0.20030000	-1.73920000
Ti	-7.14340000	3.73370000	-1.71760000
O	-4.58890000	-1.66530000	-2.86510000
O	-1.89460000	1.59460000	-0.97570000
Ti	-3.83930000	-1.85740000	-1.24190000
O	-2.05220000	-1.81440000	-1.02580000
Ti	-3.66800000	1.81680000	-1.19150000
Ti	-6.37500000	-1.71420000	-3.23560000
O	-6.87760000	-3.43260000	-3.56530000
O	-4.07900000	-3.70250000	-0.93220000
O	-6.82570000	-4.16280000	-0.26560000
O	-4.26170000	-4.04570000	1.92680000
Ti	-5.18390000	-3.68150000	0.43330000
Ti	-7.48800000	-3.41620000	-1.82860000
Ti	-1.09420000	1.43990000	0.64570000
O	-2.09870000	1.52210000	3.64820000
O	-0.77270000	3.00200000	1.51800000
O	-2.26960000	-1.86060000	3.60310000
O	-1.60810000	-0.17110000	1.41360000
O	-4.08690000	-0.08650000	4.73110000
Ti	-2.84610000	-0.13560000	3.45720000
Ti	-2.29620000	2.93910000	2.49550000
Ti	-1.22620000	-1.80100000	0.58860000
Ti	-2.59740000	-3.21700000	2.40480000
C	17.57310000	-1.18300000	-0.63890000
C	16.37210000	-0.96440000	-0.54030000
C	15.04100000	-0.72750000	-0.43570000
C	13.84080000	-0.49940000	-0.34260000
C	12.51610000	-0.22610000	-0.23900000
C	11.32500000	0.03600000	-0.14520000
C	10.00390000	0.34920000	-0.04040000
C	8.82730000	0.65190000	0.05480000
C	7.47100000	1.01200000	0.16570000
C	6.96070000	2.29160000	0.29640000
S	6.21650000	-0.18570000	0.15160000
C	5.55910000	2.29930000	0.38420000
H	7.59200000	3.17000000	0.32570000
C	4.99250000	1.03700000	0.32230000
H	4.95650000	3.19440000	0.49210000
C	3.57550000	0.82060000	0.39620000
H	2.98070000	1.72630000	0.49870000
C	2.86250000	-0.33190000	0.36450000
C	3.47230000	-1.62150000	0.24130000
C	1.37870000	-0.27780000	0.47680000
O	0.84950000	0.87020000	0.54400000
O	0.76100000	-1.37750000	0.49820000
N	4.00390000	-2.64510000	0.13600000
C	18.94540000	-1.39430000	-0.74480000

C	19.62310000	-2.57150000	-1.01570000
S	20.07890000	-0.06410000	-0.55580000
C	21.01460000	-2.43160000	-1.08410000
H	19.10140000	-3.51010000	-1.16070000
C	21.42710000	-1.12450000	-0.85210000
H	21.72770000	-3.22690000	-1.26990000
C	23.22020000	0.53530000	-0.59150000
C	22.68280000	1.77200000	-0.78030000
C	23.59550000	2.79490000	-0.37680000
H	21.71690000	1.95520000	-1.22930000
C	24.76130000	2.29200000	0.07980000
H	23.38480000	3.85480000	-0.44990000
H	25.64620000	2.80680000	0.42380000
H	23.41840000	-1.49050000	-0.89480000
N	22.72540000	-0.72710000	-0.82010000
N	24.73780000	0.65670000	0.03810000
H	25.36730000	0.01510000	0.28380000
H	-0.12900000	-3.32450000	1.70670000
O	-1.08440000	-3.39870000	1.42080000

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C	-27.19400000	3.29100000	0.24650000
C	-25.83290000	3.53720000	0.37730000
C	-24.86170000	2.68630000	-0.16190000
C	-25.34340000	1.56190000	-0.84430000
C	-26.69990000	1.28220000	-0.94870000
C	-27.67440000	2.14130000	-0.40500000
C	-22.75550000	0.73020000	-0.75600000
C	-22.51150000	1.95990000	-0.10330000
C	-21.23260000	2.12290000	0.46170000
H	-20.97370000	3.03790000	0.97070000
C	-20.27200000	1.12820000	0.39280000
C	-21.80660000	-0.27610000	-0.78400000
H	-27.87750000	4.00890000	0.67630000
H	-25.54330000	4.43170000	0.90780000
H	-26.99240000	0.38960000	-1.48280000
N	-29.03200000	1.85220000	-0.49110000
H	-19.31150000	1.31870000	0.85770000
H	-22.04570000	-1.19700000	-1.30130000
C	-23.06600000	4.31570000	0.37240000
C	-23.01560000	4.56370000	1.88260000
H	-23.75570000	5.01820000	-0.09530000
H	-22.08820000	4.51220000	-0.06790000
H	-22.69930000	5.59500000	2.06100000
H	-23.98760000	4.42470000	2.35710000
H	-22.30600000	3.90490000	2.38450000
N	-23.47280000	2.96600000	-0.05230000
S	-24.22340000	0.50450000	-1.73190000
C	-29.98190000	2.92390000	-0.21950000
C	-29.47300000	0.86320000	-1.46690000

H	-29.89690000	3.75580000	-0.93330000
H	-29.84720000	3.32020000	0.78780000
H	-30.99060000	2.51940000	-0.28070000
H	-29.25520000	1.16410000	-2.50190000
H	-30.54880000	0.73050000	-1.36700000
H	-29.00550000	-0.10540000	-1.28480000
C	-20.53180000	-0.10380000	-0.21920000
C	-14.91700000	-3.28400000	-0.16260000
C	-13.62050000	-3.64660000	-0.10010000
C	-11.09380000	-4.29640000	0.00350000
C	-10.50770000	-5.55100000	-0.08430000
S	-9.87670000	-3.04970000	0.19230000
C	-9.11190000	-5.51090000	-0.00320000
H	-11.08980000	-6.45380000	-0.20520000
C	-8.58790000	-4.23510000	0.14810000
H	-8.47820000	-6.38690000	-0.05450000
C	-7.20300000	-3.91700000	0.24010000
H	-6.55220000	-4.78430000	0.18780000
C	-6.66280000	-2.67590000	0.36730000
H	-7.31230000	-1.80720000	0.41500000
C	-5.25870000	-2.38910000	0.42620000
C	-4.23630000	-3.36630000	0.39640000
C	-4.83220000	-1.04410000	0.51170000
C	-2.92280000	-3.00630000	0.43560000
H	-4.46310000	-4.42140000	0.34350000
C	-3.50790000	-0.72170000	0.54770000
H	-5.55820000	-0.24270000	0.54310000
H	-2.11970000	-3.72430000	0.41360000
H	-3.15100000	0.29340000	0.60650000
N	-2.55000000	-1.69280000	0.50510000
C	-1.15600000	-1.33600000	0.53640000
C	0.99380000	-2.00060000	0.44870000
C	0.40630000	0.27550000	0.74360000
C	1.41050000	-0.68240000	0.62230000
H	1.71480000	-2.80280000	0.34340000
H	0.63710000	1.32490000	0.87900000
N	-0.88340000	-0.05240000	0.70260000
N	-0.29310000	-2.33160000	0.40590000
C	2.85940000	-0.36640000	0.67020000
O	3.73430000	-1.19750000	0.58770000
O	3.09970000	0.94670000	0.81660000
C	-12.44520000	-3.96660000	-0.04890000
C	-16.08730000	-2.94540000	-0.22720000
C	-17.40990000	-2.52360000	-0.30350000
C	-19.53660000	-1.16470000	-0.29650000
C	-19.72430000	-2.50390000	-0.58640000
H	-20.69870000	-2.93200000	-0.77690000
S	-17.84050000	-0.84060000	-0.03120000
C	-18.54310000	-3.26350000	-0.58910000
H	-18.50440000	-4.32630000	-0.78630000
Ti	10.15770000	-0.84910000	-3.59740000

O	8.40090000	-0.90680000	-3.10470000
O	11.96420000	-0.90730000	-2.61890000
O	10.67670000	-2.49110000	-4.19090000
O	9.20990000	-1.49880000	-0.03010000
O	8.94580000	2.21940000	0.53290000
O	8.02360000	0.43020000	-0.70970000
O	8.06660000	-3.20160000	-1.44380000
O	11.69610000	2.81090000	-2.05380000
O	10.64680000	1.05150000	-3.55610000
Ti	12.43420000	0.52910000	0.71680000
O	13.42810000	0.85280000	-0.92960000
O	10.95940000	0.61720000	-0.55100000
O	10.86820000	-3.65840000	-1.02660000
O	8.46600000	-3.90380000	1.33460000
Ti	9.36430000	0.32680000	0.61910000
Ti	9.96240000	-0.08900000	3.57220000
O	11.02190000	0.22940000	1.96600000
O	8.43760000	0.03230000	2.12460000
Ti	9.26620000	-3.32450000	-0.16890000
Ti	12.02260000	0.91220000	-1.97870000
Ti	11.40670000	-2.68520000	-2.51200000
O	8.15720000	2.45430000	-2.58940000
O	6.00270000	-1.38060000	-1.13300000
Ti	7.50520000	2.28800000	-0.92260000
O	5.75430000	1.98480000	-0.62180000
Ti	7.77110000	-1.33330000	-1.47640000
Ti	9.89280000	2.79130000	-3.04230000
O	10.16490000	4.58970000	-3.11940000
O	7.53950000	4.08380000	-0.33390000
O	10.26060000	4.78760000	0.25180000
O	7.90540000	3.98290000	2.53340000
Ti	8.74110000	3.99410000	0.94170000
Ti	10.89790000	4.38410000	-1.44260000
Ti	5.30910000	-1.58850000	0.52950000
O	6.57970000	-2.01420000	3.41210000
O	5.23860000	-3.29660000	1.15310000
O	6.34670000	1.32490000	3.92300000
O	5.67350000	-0.07060000	1.52870000
O	8.42360000	-0.36000000	4.65660000
Ti	7.11090000	-0.26480000	3.45450000
Ti	6.82060000	-3.20030000	2.02820000
Ti	5.05440000	1.60680000	1.00690000
O	4.78720000	3.01750000	2.10710000
Ti	6.38660000	2.88740000	2.95190000
H	4.93390000	2.08410000	-1.36290000

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C	30.40580000	3.72560000	-0.99460000
C	29.13930000	3.99390000	-0.49120000
C	28.31190000	2.99230000	0.02840000

C	28.83330000	1.69290000	0.00650000
C	30.08280000	1.40390000	-0.52670000
C	30.92450000	2.41830000	-1.02330000
C	26.27620000	0.94610000	0.53100000
C	26.00180000	2.33320000	0.54780000
C	24.64300000	2.69900000	0.58820000
H	24.35840000	3.73890000	0.62260000
C	23.63280000	1.75310000	0.57120000
C	25.26240000	0.00720000	0.47280000
H	30.98210000	4.55680000	-1.37410000
H	28.80530000	5.01990000	-0.51520000
H	30.40740000	0.37300000	-0.52790000
N	32.20210000	2.13990000	-1.49260000
H	22.60910000	2.10870000	0.58880000
H	25.53270000	-1.04130000	0.45830000
C	26.68880000	4.68350000	0.84770000
C	26.16150000	5.51740000	-0.32380000
H	27.58940000	5.14370000	1.25380000
H	25.95790000	4.67880000	1.65670000
H	25.95910000	6.53200000	0.02940000
H	26.88130000	5.58390000	-1.14020000
H	25.23430000	5.11440000	-0.73260000
N	27.02170000	3.27950000	0.55270000
S	27.93730000	0.35990000	0.76860000
C	32.88620000	3.15530000	-2.28300000
C	32.54350000	0.75900000	-1.80870000
H	33.01010000	4.07770000	-1.71370000
H	32.35550000	3.39400000	-3.21570000
H	33.87950000	2.78950000	-2.53690000
H	32.43400000	0.11760000	-0.93310000
H	33.58700000	0.71880000	-2.11590000
H	31.92610000	0.34520000	-2.61900000
C	23.90790000	0.38190000	0.49200000
C	18.15320000	-2.54660000	0.69590000
C	16.86000000	-2.88190000	0.79910000
C	9.35690000	-4.71130000	1.35980000
C	8.76470000	-5.79120000	1.99690000
S	8.14730000	-3.68130000	0.61870000
C	7.36920000	-5.79070000	1.89340000
H	9.34220000	-6.54390000	2.51520000
C	6.85580000	-4.71780000	1.18030000
H	6.73040000	-6.54970000	2.32520000
C	5.46970000	-4.48050000	0.93330000
H	4.81650000	-5.23510000	1.35960000
C	4.94000000	-3.44190000	0.23920000
H	5.59450000	-2.69150000	-0.19270000
C	3.53700000	-3.23150000	0.00610000
C	2.50850000	-4.06520000	0.50010000
C	3.12670000	-2.12190000	-0.76410000
C	1.19950000	-3.79290000	0.23280000
H	2.72420000	-4.93560000	1.10270000

C	1.80650000	-1.88240000	-1.01310000
H	3.85990000	-1.44010000	-1.17330000
H	0.38950000	-4.40460000	0.59460000
H	1.46040000	-1.04620000	-1.59800000
N	0.84180000	-2.71040000	-0.51980000
C	-0.54910000	-2.44430000	-0.79170000
C	-2.70250000	-3.03950000	-0.51480000
C	-2.09080000	-1.13950000	-1.79080000
C	-3.10380000	-1.95470000	-1.29100000
H	-3.43100000	-3.71910000	-0.08870000
H	-2.30950000	-0.27360000	-2.40310000
N	-0.80630000	-1.38520000	-1.53990000
N	-1.42060000	-3.28810000	-0.26280000
C	-4.54740000	-1.72250000	-1.54600000
O	-5.50900000	-2.49720000	-1.08550000
O	-4.76600000	-0.66210000	-2.28060000
C	15.67400000	-3.18200000	0.89300000
C	14.38090000	-3.50750000	0.99080000
C	13.19380000	-3.80070000	1.08180000
C	11.89340000	-4.11620000	1.17650000
C	10.71050000	-4.40350000	1.26700000
C	19.33360000	-2.24340000	0.59600000
C	20.66780000	-1.87980000	0.48560000
C	22.85730000	-0.62430000	0.43350000
C	22.96730000	-1.96610000	0.10990000
H	23.90540000	-2.43000000	-0.16140000
S	21.19400000	-0.22910000	0.79250000
C	21.75270000	-2.66640000	0.13750000
H	21.65170000	-3.71730000	-0.09770000
Ti	-9.81430000	0.96970000	4.15990000
O	-8.65430000	0.06790000	2.97060000
O	-11.77070000	1.37320000	3.91300000
O	-10.41910000	-0.24670000	5.47420000
O	-10.82620000	-0.87350000	0.83630000
O	-10.08200000	2.19140000	-1.20200000
O	-8.98100000	0.50560000	0.14210000
O	-9.55890000	-2.51220000	2.24390000
O	-10.97320000	4.42420000	1.79020000
O	-9.78660000	2.77630000	3.27380000
Ti	-13.60780000	1.97580000	0.65450000
O	-13.48550000	3.04360000	2.27000000
O	-11.69510000	1.78170000	1.10590000
O	-12.11200000	-1.84860000	3.18770000
O	-11.09070000	-3.68510000	0.22430000
Ti	-10.98950000	0.67380000	-0.35200000
Ti	-13.07020000	-0.19660000	-2.44020000
O	-12.93290000	0.81280000	-0.77570000
O	-11.14950000	-0.40430000	-1.96090000
Ti	-11.21720000	-2.49040000	1.65570000
Ti	-11.71290000	2.82690000	2.62520000
Ti	-11.92130000	-0.46870000	4.41040000

O	-8.00290000	3.03930000	0.93090000
O	-7.37970000	-1.70530000	0.76470000
Ti	-8.10930000	2.02810000	-0.51000000
O	-6.38110000	1.23810000	-0.89780000
Ti	-8.85920000	-0.87690000	1.47190000
Ti	-9.02540000	4.16600000	2.06000000
O	-8.85840000	5.96790000	1.51600000
O	-7.98350000	3.43940000	-1.82520000
O	-10.25000000	5.04570000	-1.32370000
O	-9.52840000	2.71100000	-4.00190000
Ti	-9.66520000	3.58490000	-2.34040000
Ti	-10.34290000	5.63240000	0.43950000
Ti	-7.25240000	-2.63460000	-0.79360000
O	-10.23940000	-3.11720000	-2.79080000
O	-8.02150000	-4.29070000	-0.90370000
O	-9.60850000	-0.36030000	-4.45380000
O	-7.37120000	-1.41490000	-2.21030000
O	-12.39960000	-1.33770000	-3.89320000
Ti	-10.68040000	-1.46060000	-3.41860000
Ti	-9.83180000	-3.88110000	-1.14740000
Ti	-6.43760000	0.07330000	-2.54480000
O	-6.82350000	0.70300000	-4.19940000
Ti	-8.61490000	1.16320000	-4.44880000
H	-5.61830000	1.18870000	-0.29170000

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C	16.14390000	-2.04190000	0.19650000
C	14.94360000	-2.24120000	0.11890000
C	13.61450000	-2.46730000	0.03890000
C	12.41590000	-2.67700000	-0.03040000
C	4.72320000	-2.34000000	-0.50640000
C	3.61630000	-3.23520000	-0.32170000
C	4.38000000	-1.03140000	-0.79480000
C	2.24460000	-2.78380000	-0.43620000
C	3.04250000	-0.59130000	-0.89840000
H	5.15680000	-0.29680000	-0.96510000
C	1.94680000	-1.41670000	-0.73600000
H	2.87860000	0.45060000	-1.14450000
C	0.56770000	-0.90290000	-0.86130000
C	0.24580000	0.37480000	-0.37500000
C	-0.44430000	-1.65040000	-1.48220000
C	-1.03450000	0.88440000	-0.50520000
H	1.00170000	0.96510000	0.12760000
C	-1.72580000	-1.13920000	-1.61820000
H	-0.22380000	-2.63210000	-1.87750000
C	-2.03520000	0.13320000	-1.12830000
H	-1.27090000	1.86660000	-0.11670000
H	-2.48530000	-1.73130000	-2.11050000
C	-3.39290000	0.71610000	-1.24290000
O	-3.71020000	1.81510000	-0.83670000

O	-4.27760000	-0.09980000	-1.85450000
N	3.71770000	-4.53230000	-0.01520000
N	1.35670000	-3.75880000	-0.20190000
S	2.20260000	-5.11150000	0.11790000
C	8.53950000	-2.66390000	-0.28680000
C	11.04220000	-2.90200000	-0.10670000
C	10.36210000	-4.10880000	-0.06210000
H	10.87500000	-5.05560000	0.04030000
S	9.90870000	-1.57800000	-0.27820000
C	8.97000000	-3.97390000	-0.16260000
H	8.29060000	-4.81530000	-0.14750000
C	7.21080000	-2.12020000	-0.40950000
C	6.07570000	-2.85240000	-0.38290000
H	7.15060000	-1.04210000	-0.52030000
H	6.14950000	-3.92540000	-0.24650000
C	28.02430000	2.47060000	-0.24010000
C	26.72120000	2.94200000	-0.34120000
C	25.63430000	2.26950000	0.22770000
C	25.93700000	1.08600000	0.91310000
C	27.22940000	0.58240000	0.99000000
C	28.31950000	1.25880000	0.40930000
C	23.25490000	0.67470000	0.84680000
C	23.20120000	1.92510000	0.19160000
C	21.96390000	2.27880000	-0.37630000
H	21.84720000	3.22390000	-0.88330000
C	20.86680000	1.43440000	-0.31960000
C	22.16860000	-0.18270000	0.86400000
H	28.80790000	3.05860000	-0.69500000
H	26.57050000	3.86840000	-0.87430000
H	27.38150000	-0.34180000	1.52920000
N	29.60930000	0.74090000	0.45660000
H	19.94840000	1.76430000	-0.79160000
H	22.26510000	-1.12880000	1.38250000
C	24.11580000	4.16910000	-0.28050000
C	24.09140000	4.42950000	-1.78990000
H	24.91150000	4.75390000	0.18170000
H	23.18400000	4.51570000	0.16750000
H	23.94120000	5.49920000	-1.95970000
H	25.02440000	4.14160000	-2.27510000
H	23.28110000	3.89530000	-2.28730000
N	24.30780000	2.77200000	0.14220000
S	24.67020000	0.24020000	1.83070000
C	30.72330000	1.63580000	0.17010000
C	29.89400000	-0.33350000	1.39860000
H	30.79510000	2.46510000	0.88870000
H	30.63960000	2.05800000	-0.83220000
H	31.64960000	1.06540000	0.20990000
H	29.76240000	-0.02560000	2.44600000
H	30.92500000	-0.65510000	1.26130000
H	29.25340000	-1.19670000	1.21220000
C	20.93980000	0.17400000	0.28460000

C	17.51340000	-1.80020000	0.28900000
C	19.80630000	-0.74300000	0.32770000
C	19.81030000	-2.10450000	0.55570000
H	20.71870000	-2.66920000	0.71590000
S	18.16810000	-0.18100000	0.08920000
C	18.53480000	-2.69740000	0.53430000
H	18.35360000	-3.75330000	0.68390000
Ti	-9.54310000	-2.07510000	3.19910000
O	-7.92060000	-1.80350000	2.40760000
O	-11.50770000	-1.96990000	2.60440000
O	-9.89160000	-3.86130000	3.27370000
O	-9.31750000	-1.40930000	-0.48220000
O	-9.26340000	2.29170000	0.23310000
O	-8.06630000	0.28360000	0.59430000
O	-7.87160000	-3.37290000	0.02620000
O	-11.45000000	1.73210000	3.31700000
O	-10.07690000	-0.32280000	3.90460000
Ti	-12.67490000	0.44590000	0.11190000
O	-13.32440000	0.10990000	1.91970000
O	-10.97750000	0.24190000	1.04340000
O	-10.68780000	-3.92030000	-0.00890000
O	-8.80510000	-3.14310000	-2.70290000
Ti	-9.64420000	0.50590000	-0.42300000
Ti	-10.81440000	1.04440000	-3.17840000
O	-11.53620000	0.71070000	-1.39750000
O	-9.03280000	0.81630000	-2.07890000
Ti	-9.30000000	-3.17390000	-0.97350000
Ti	-11.73830000	-0.05470000	2.65240000
Ti	-10.93980000	-3.55140000	1.79220000
O	-7.86810000	1.54460000	3.04760000
O	-5.95790000	-1.37080000	-0.00550000
Ti	-7.56120000	2.00370000	1.33700000
O	-5.89990000	1.98040000	0.63880000
Ti	-7.62140000	-1.60340000	0.64690000
Ti	-9.48460000	1.55040000	3.89470000
O	-9.77960000	3.18720000	4.63490000
O	-7.75740000	3.88180000	1.41990000
O	-10.55720000	4.48710000	1.61510000
O	-8.69070000	4.70860000	-1.18980000
Ti	-9.18880000	4.11200000	0.43130000
Ti	-10.83000000	3.48540000	3.15200000
Ti	-5.60840000	-0.94820000	-1.73400000
O	-7.42260000	-0.50440000	-4.30620000
O	-5.62310000	-2.33690000	-2.91000000
O	-7.37920000	2.82060000	-3.66800000
O	-6.20360000	0.77540000	-2.06530000
O	-9.51940000	1.29290000	-4.54890000
Ti	-7.99420000	1.10250000	-3.64620000
Ti	-7.35080000	-2.10060000	-3.39680000
Ti	-5.53340000	2.23260000	-1.11840000
O	-5.52790000	3.94760000	-1.69380000

Ti	-7.26100000	3.95970000	-2.22760000
H	-4.94980000	1.90230000	1.20720000

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C	-30.57610000	-3.37290000	-1.04340000
C	-29.23300000	-3.67930000	-1.22380000
C	-28.22240000	-3.10500000	-0.44530000
C	-28.64470000	-2.20140000	0.53820000
C	-29.97980000	-1.85710000	0.70570000
C	-30.99330000	-2.42910000	-0.08750000
C	-26.01520000	-1.55060000	0.69360000
C	-25.83370000	-2.55010000	-0.28910000
C	-24.56100000	-2.61340000	-0.88630000
H	-24.34510000	-3.36140000	-1.63270000
C	-23.55440000	-1.72320000	-0.55310000
C	-25.01900000	-0.63890000	0.99330000
H	-31.29470000	-3.87160000	-1.67710000
H	-28.98930000	-4.39720000	-1.99200000
H	-30.22580000	-1.14420000	1.47990000
N	-32.32540000	-2.05970000	0.05420000
H	-22.60380000	-1.82230000	-1.06410000
H	-25.21560000	0.10720000	1.75300000
C	-26.52410000	-4.62590000	-1.43070000
C	-26.46060000	-4.42040000	-2.94720000
H	-27.26590000	-5.38780000	-1.19120000
H	-25.56860000	-5.00740000	-1.06960000
H	-26.22290000	-5.37620000	-3.42210000
H	-27.40810000	-4.06910000	-3.35680000
H	-25.69040000	-3.70380000	-3.23470000
N	-26.85200000	-3.43890000	-0.62310000
S	-27.47510000	-1.54780000	1.70720000
C	-33.34790000	-2.91130000	-0.53940000
C	-32.72490000	-1.33570000	1.25390000
H	-33.36540000	-3.91970000	-0.10170000
H	-33.20020000	-3.00800000	-1.61590000
H	-34.32160000	-2.45050000	-0.38160000
H	-32.56850000	-1.91890000	2.17270000
H	-33.78290000	-1.09060000	1.17830000
H	-32.17580000	-0.39730000	1.34630000
C	-23.75590000	-0.69900000	0.38050000
C	-18.06670000	2.32080000	0.90230000
C	-16.78740000	2.72040000	0.85240000
C	-15.61760000	3.08590000	0.80110000
C	-14.34180000	3.48560000	0.74670000
C	-13.17350000	3.85440000	0.69370000
C	-11.89490000	4.25740000	0.63620000
C	-10.73350000	4.63200000	0.58290000
C	-19.23410000	1.96130000	0.95070000
C	-20.55590000	1.53760000	0.99490000
C	-22.72020000	0.26760000	0.71920000

C	-22.84710000	1.45400000	1.41950000
H	-23.79350000	1.81360000	1.79900000
S	-21.05530000	0.02530000	0.24770000
C	-21.64580000	2.16260000	1.57490000
H	-21.56190000	3.11180000	2.08660000
C	-3.49230000	3.49980000	-0.38870000
C	-2.43260000	4.46770000	-0.30060000
C	-3.08710000	2.20980000	-0.68620000
C	-1.05130000	4.08520000	-0.53130000
C	-1.74180000	1.83960000	-0.90370000
H	-3.84370000	1.43790000	-0.76550000
C	-0.69470000	2.73390000	-0.84720000
H	-1.53870000	0.80440000	-1.14870000
C	0.69960000	2.30990000	-1.09140000
C	1.15650000	1.07860000	-0.59530000
C	1.58830000	3.09660000	-1.83870000
C	2.45020000	0.64980000	-0.83840000
H	0.49690000	0.46200000	0.00220000
C	2.88220000	2.66590000	-2.08820000
H	1.26030000	4.04370000	-2.24430000
C	3.32720000	1.43850000	-1.58820000
H	2.79300000	-0.29720000	-0.44200000
H	3.54540000	3.28520000	-2.67680000
C	4.70360000	0.94100000	-1.82450000
O	5.16900000	-0.20360000	-1.38520000
O	5.43550000	1.75670000	-2.52450000
N	-2.56750000	5.76140000	0.00340000
N	-0.19820000	5.10390000	-0.38150000
S	-1.07670000	6.41760000	0.00180000
C	-6.90380000	5.16210000	0.28220000
C	-9.40770000	5.04600000	0.51940000
C	-8.89610000	6.32000000	0.69240000
H	-9.52730000	7.17140000	0.90730000
S	-8.11300000	3.90250000	0.18550000
C	-7.50040000	6.37940000	0.56080000
H	-6.92440000	7.28970000	0.66360000
C	-5.49430000	4.94720000	0.09570000
C	-4.90260000	3.76630000	-0.19230000
H	-4.89150000	5.84000000	0.20480000
H	-5.52510000	2.88150000	-0.30080000
Ti	10.33450000	1.52960000	3.52620000
O	9.06840000	1.60800000	2.12460000
O	12.22880000	0.85380000	3.44680000
O	11.14250000	3.22690000	3.72440000
O	10.98950000	0.76970000	-0.27650000
O	9.88580000	-2.79470000	0.14770000
O	9.02310000	-0.53310000	0.19790000
O	9.96830000	3.05220000	-0.13540000
O	11.06220000	-2.74670000	3.80110000
O	10.13080000	-0.41830000	3.98900000
Ti	13.62130000	-1.84510000	1.18130000

O	13.66310000	-1.64810000	3.11110000
O	11.78830000	-1.20820000	1.54760000
O	12.59350000	2.85570000	0.82330000
O	11.27730000	2.53310000	-2.54750000
Ti	10.94670000	-1.18700000	-0.22490000
Ti	12.78040000	-2.04150000	-2.53890000
O	12.81570000	-1.76720000	-0.60720000
O	10.94350000	-1.37570000	-2.15920000
Ti	11.53820000	2.49030000	-0.69740000
Ti	11.95780000	-1.06880000	3.37890000
Ti	12.50710000	2.57290000	2.65300000
O	8.06000000	-1.89490000	2.48180000
O	7.59350000	1.73720000	-0.60340000
Ti	8.02220000	-2.02470000	0.72350000
O	6.28890000	-1.47110000	0.05220000
Ti	9.11870000	1.38000000	0.35650000
Ti	9.17390000	-2.16990000	3.98950000
O	8.87500000	-3.88540000	4.72320000
O	7.68190000	-3.92440000	0.61250000
O	9.93350000	-5.09580000	1.84820000
O	8.96820000	-4.88680000	-1.64010000
Ti	9.27970000	-4.53900000	0.18320000
Ti	10.22470000	-4.45770000	3.57140000
Ti	7.30640000	1.49560000	-2.38310000
O	10.03600000	0.30090000	-4.44840000
O	8.11520000	2.62520000	-3.57310000
O	9.10260000	-2.80270000	-3.93840000
O	7.20280000	-0.34570000	-2.71160000
O	11.97560000	-1.99540000	-4.33140000
Ti	10.33460000	-1.41970000	-3.91640000
Ti	9.86490000	1.96230000	-3.63550000
Ti	6.18150000	-1.60570000	-1.95840000
O	6.33440000	-3.16790000	-2.86340000
Ti	8.06280000	-3.87140000	-2.89680000
H	5.61000000	-0.97240000	0.54450000

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C	4.87370000	-4.16890000	1.02450000
C	4.12160000	-5.16410000	1.63780000
S	3.86960000	-3.13000000	0.04910000
C	2.75460000	-5.07330000	1.33690000
H	4.56200000	-5.91390000	2.28350000
C	2.42810000	-4.01920000	0.48650000
H	2.00220000	-5.75050000	1.72600000
C	8.73960000	-3.35930000	1.19090000
C	7.43560000	-3.68490000	1.14560000
C	1.10760000	-3.71640000	0.06010000
H	0.34560000	-4.38260000	0.46560000
C	0.67420000	-2.71360000	-0.76270000
C	6.24250000	-3.93950000	1.10110000

C	9.92080000	-3.02880000	1.22890000
C	1.56860000	-1.78450000	-1.36310000
N	2.30050000	-1.03270000	-1.84750000
C	-0.74810000	-2.47760000	-1.08770000
O	-1.13130000	-1.49960000	-1.86340000
O	-1.60380000	-3.29180000	-0.52500000
C	21.15850000	2.34970000	-1.12950000
C	19.81810000	2.58500000	-1.36840000
C	18.80240000	2.04730000	-0.54690000
C	19.23040000	1.25610000	0.54530000
C	20.56330000	0.98040000	0.77870000
C	21.58560000	1.51450000	-0.05680000
C	16.62720000	0.53360000	0.71260000
C	16.43420000	1.41940000	-0.37720000
C	15.17100000	1.38040000	-1.00800000
H	14.95080000	2.03960000	-1.83860000
C	14.18330000	0.50040000	-0.60080000
C	15.65500000	-0.37560000	1.09230000
H	21.87970000	2.81000000	-1.79720000
H	19.56720000	3.21450000	-2.21510000
H	20.81630000	0.35810000	1.63150000
N	22.91420000	1.21510000	0.15050000
H	13.23800000	0.51410000	-1.13880000
H	15.85610000	-1.03250000	1.93530000
C	17.08520000	3.40260000	-1.72310000
C	17.06650000	3.02730000	-3.20690000
H	17.79750000	4.21850000	-1.55290000
H	16.10400000	3.79000000	-1.42380000
H	16.79160000	3.91090000	-3.79210000
H	18.04030000	2.68230000	-3.56040000
H	16.33910000	2.24270000	-3.42610000
N	17.43630000	2.30860000	-0.78680000
S	18.05800000	0.68670000	1.74460000
C	23.92850000	2.03510000	-0.50910000
C	23.31190000	0.62050000	1.42460000
H	23.89840000	3.08720000	-0.18040000
H	23.81120000	2.01490000	-1.59830000
H	24.92040000	1.63430000	-0.28150000
H	23.11620000	1.28790000	2.28050000
H	24.38310000	0.40060000	1.40130000
H	22.78970000	-0.32600000	1.60370000
C	14.39780000	-0.41640000	0.44850000
C	13.38650000	-1.35600000	0.86420000
C	13.52240000	-2.48820000	1.68130000
S	11.72210000	-1.16970000	0.35810000
C	12.33400000	-3.18540000	1.89130000
H	14.47190000	-2.80610000	2.09970000
C	11.22940000	-2.61060000	1.24470000
H	12.25500000	-4.08800000	2.48950000
Ti	-5.70780000	1.20300000	4.07620000
O	-4.59190000	0.11430000	2.99620000

O	-7.65740000	1.66250000	3.78780000
O	-6.35770000	0.15880000	5.51790000
O	-6.83490000	-0.95910000	0.97250000
O	-5.95430000	1.83260000	-1.40590000
O	-4.91610000	0.25160000	0.12720000
O	-5.62850000	-2.50230000	2.57120000
O	-6.72560000	4.43320000	1.32290000
O	-5.60160000	2.89980000	2.99360000
Ti	-9.48470000	1.99420000	0.47230000
O	-9.30750000	3.23310000	1.96480000
O	-7.56820000	1.75320000	0.93920000
O	-8.15100000	-1.60660000	3.43070000
O	-7.25260000	-3.81410000	0.67380000
Ti	-6.92900000	0.45830000	-0.38710000
Ti	-9.06400000	-0.54450000	-2.37610000
O	-8.87790000	0.64150000	-0.83060000
O	-7.14150000	-0.79020000	-1.87290000
Ti	-7.29660000	-2.45750000	1.97320000
Ti	-7.53730000	2.96710000	2.33780000
Ti	-7.89060000	-0.10400000	4.50060000
O	-3.81040000	2.81580000	0.62820000
O	-3.40900000	-1.96220000	1.00130000
Ti	-3.97490000	1.65890000	-0.69560000
O	-2.28300000	0.74740000	-0.99650000
Ti	-4.85030000	-0.98760000	1.61270000
Ti	-4.78180000	4.10950000	1.62880000
O	-4.52590000	5.82790000	0.87410000
O	-3.78340000	2.91440000	-2.16720000
O	-5.98460000	4.67150000	-1.84680000
O	-5.39330000	2.00840000	-4.25350000
Ti	-5.47310000	3.07450000	-2.69500000
Ti	-6.04410000	5.46300000	-0.15180000
Ti	-3.36270000	-3.06320000	-0.45980000
O	-6.39540000	-3.63580000	-2.40720000
O	-4.24380000	-4.68350000	-0.38900000
O	-5.63240000	-1.10340000	-4.37370000
O	-3.43490000	-1.99890000	-2.00470000
O	-8.46680000	-1.87780000	-3.70540000
Ti	-6.74970000	-2.02900000	-3.21510000
Ti	-6.02240000	-4.22190000	-0.67910000
Ti	-2.41850000	-0.60110000	-2.51030000
O	-2.79810000	-0.13780000	-4.23380000
Ti	-4.56410000	0.37010000	-4.52710000
H	-1.51510000	0.72690000	-0.39310000

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C	-3.52280000	-3.61030000	-0.74960000
C	-2.78060000	-4.67280000	-1.24770000
S	-2.50510000	-2.45460000	0.07740000
C	-1.41860000	-4.55860000	-0.96750000

H	-3.23090000	-5.49130000	-1.79110000
C	-1.07660000	-3.41490000	-0.25350000
H	-0.67530000	-5.28460000	-1.26980000
C	-12.46820000	-2.10880000	-1.18570000
C	-11.15000000	-2.34020000	-1.14110000
C	0.25650000	-3.11180000	0.13260000
H	0.97330000	-3.86450000	-0.17670000
C	0.76850000	-2.04600000	0.81620000
C	-9.94140000	-2.54740000	-1.09770000
C	-8.62560000	-2.77510000	-1.03960000
C	-7.41840000	-2.98090000	-0.98200000
C	-6.09730000	-3.20150000	-0.91010000
C	-4.89590000	-3.40260000	-0.84240000
C	-13.67420000	-1.90660000	-1.21770000
C	-0.03310000	-0.97000000	1.28730000
N	-0.69220000	-0.10130000	1.66620000
C	2.20890000	-1.91770000	1.12280000
O	2.72430000	-0.89870000	1.76660000
O	2.92860000	-2.92500000	0.68910000
C	-25.52740000	1.87520000	1.27460000
C	-24.23900000	2.39410000	1.28620000
C	-23.21810000	1.88390000	0.47700000
C	-23.57200000	0.81360000	-0.35410000
C	-24.84600000	0.26110000	-0.35080000
C	-25.86930000	0.77270000	0.47080000
C	-20.89240000	0.55620000	-0.71560000
C	-20.79230000	1.68630000	0.12850000
C	-19.49740000	2.02390000	0.56670000
H	-19.34140000	2.88460000	1.19780000
C	-18.39050000	1.27180000	0.21500000
C	-19.78870000	-0.21610000	-1.02710000
H	-26.26050000	2.33730000	1.91960000
H	-24.04870000	3.22720000	1.94550000
H	-25.04020000	-0.56790000	-1.01620000
N	-27.13560000	0.20150000	0.49930000
H	-17.42530000	1.59050000	0.59160000
H	-19.92950000	-1.07700000	-1.66840000
C	-21.71130000	3.75900000	1.09970000
C	-21.48540000	3.77220000	2.61410000
H	-22.58480000	4.36180000	0.85070000
H	-20.86600000	4.22760000	0.59550000
H	-21.33850000	4.80590000	2.93870000
H	-22.33610000	3.36770000	3.16370000
H	-20.60260000	3.20240000	2.90670000
N	-21.90900000	2.43850000	0.47790000
S	-22.41650000	0.19660000	-1.55570000
C	-28.22750000	0.96680000	1.08740000
C	-27.51550000	-0.71100000	-0.57130000
H	-28.43420000	1.89790000	0.54060000
H	-28.01440000	1.21940000	2.12680000
H	-29.12790000	0.35490000	1.07650000

H	-27.54110000	-0.22240000	-1.55590000
H	-28.50740000	-1.10580000	-0.35790000
H	-26.83050000	-1.55840000	-0.62580000
C	-18.50060000	0.12100000	-0.57590000
C	-17.35010000	-0.69530000	-0.93290000
C	-17.32480000	-1.88630000	-1.63980000
S	-15.72740000	-0.23740000	-0.47450000
C	-16.04340000	-2.42620000	-1.81350000
H	-18.21670000	-2.36420000	-2.02010000
C	-15.03870000	-1.66350000	-1.24170000
H	-15.83910000	-3.35040000	-2.33720000
Ti	7.50260000	0.53470000	-4.13040000
O	6.28830000	-0.33390000	-2.97090000
O	9.43630000	0.97820000	-3.79080000
O	8.19710000	-0.72660000	-5.35500000
O	8.34690000	-1.15110000	-0.67900000
O	7.44800000	1.98510000	1.18080000
O	6.44740000	0.22750000	-0.14990000
O	7.18330000	-2.86690000	-2.08430000
O	8.47960000	4.10330000	-1.84950000
O	7.40110000	2.37640000	-3.32560000
Ti	11.07650000	1.74560000	-0.46270000
O	11.03280000	2.74240000	-2.12690000
O	9.19530000	1.50330000	-1.01270000
O	9.77720000	-2.20460000	-2.90990000
O	8.61230000	-3.93020000	0.06710000
Ti	8.42200000	0.44710000	0.44920000
Ti	10.39120000	-0.30270000	2.68710000
O	10.33610000	0.63360000	0.97570000
O	8.50380000	-0.55990000	2.10940000
Ti	8.80490000	-2.79500000	-1.40490000
Ti	9.28630000	2.48380000	-2.57200000
Ti	9.63880000	-0.88050000	-4.19950000
O	5.48320000	2.71030000	-1.10060000
O	4.91290000	-2.03210000	-0.76660000
Ti	5.52020000	1.76240000	0.38610000
O	3.78310000	0.96300000	0.70920000
Ti	6.41960000	-1.21160000	-1.42390000
Ti	6.55380000	3.80410000	-2.21750000
O	6.33280000	5.62450000	-1.76160000
O	5.30130000	3.22570000	1.63030000
O	7.57180000	4.84410000	1.18910000
O	6.72870000	2.61340000	3.92000000
Ti	6.94890000	3.41870000	2.23300000
Ti	7.75770000	5.35740000	-0.58940000
Ti	4.70900000	-2.89680000	0.82050000
O	7.58310000	-3.24890000	3.00220000
O	5.49180000	-4.53470000	1.04480000
O	6.82260000	-0.43450000	4.50700000
O	4.73070000	-1.61680000	2.18800000
O	9.65360000	-1.39170000	4.14750000

Ti	7.96590000	-1.56080000	3.58230000
Ti	7.27980000	-4.08760000	1.37270000
Ti	3.76060000	-0.13040000	2.40520000
O	4.04310000	0.57430000	4.05040000
Ti	5.81130000	1.07200000	4.38070000
H	3.05680000	0.87640000	0.06360000