

A Density Functional Study on Ethylene Trimerization and Tetramerization Using Real Sasol Cr-PNP Catalyst

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Cartesian Coordinates (Å) of B3LYP/6-31G*/LanL2DZ Optimized Geometries in Figures 3 and 4

1	1R				33	C	-1.96929800	-2.07634100	-1.96105100
2	N	-0.04670600	0.20396100	-1.00746100	34	C	-2.65185700	-3.20529800	-2.42208400
3	P	1.28325600	-0.05068200	0.07383300	35	C	-3.84845400	-3.57921800	-1.81418600
4	P	-1.56445600	0.11172700	-0.14939400	36	C	-3.67407800	-1.71423600	-0.28828600
5	Cr	-0.25086200	-0.59025600	2.14317900	37	C	-4.36457000	-2.84052800	-0.74560500
6	C	-0.45554600	1.25724100	3.75855200	38	O	-4.08494000	-0.93290700	0.75532100
7	C	-1.29954600	0.28310000	4.18214900	39	C	4.56257600	-1.71795300	2.24091200
8	C	-0.21906800	-3.05555200	1.75118900	40	C	4.19552600	1.07796800	-3.20228900
9	C	-0.70394400	-2.91853400	3.00692500	41	C	-0.61989200	4.22665500	0.94381400
10	C	0.06011600	0.85032000	-2.33094100	42	C	-5.35276300	-1.19250800	1.35161100
11	C	2.24931100	-1.46621900	-0.59125000	43	H	0.53466600	1.37286100	4.19404600
12	C	2.42094700	1.39257500	0.00583500	44	H	-1.01865500	-0.40824600	4.97289600
13	C	-2.52696600	1.57081300	-0.72651400	45	H	-2.32975900	0.23858600	3.83475400
14	C	-2.46598500	-1.30897500	-0.90221700	46	H	-0.88010400	-3.11444600	0.88968900
15	C	3.27937700	-1.98473600	0.22484600	47	H	-1.77315000	-2.86873900	3.20033700
16	C	4.01166100	-3.10645600	-0.17761500	48	H	-0.05172300	-2.96169800	3.87664500
17	C	3.71479600	-3.72344000	-1.39533300	49	H	-0.77899100	2.01283800	3.04719800
18	C	1.96786900	-2.11236000	-1.79830000	50	H	0.84115700	-3.20572600	1.56309800
19	C	2.69278900	-3.23394800	-2.20661500	51	H	4.80611800	-3.50250300	0.44429000
20	O	3.47711400	-1.32470600	1.40654200	52	H	4.28763900	-4.59384000	-1.70205400
21	C	2.46176200	2.20052400	1.15115800	53	H	1.17758300	-1.72868900	-2.43330400
22	C	3.32204900	3.29318700	1.25648100	54	H	2.46185500	-3.71667300	-3.15131600
23	C	4.17046800	3.58767900	0.19043700	55	H	1.80907000	1.94837000	1.98249700
24	C	3.29785400	1.70331800	-1.06238900	56	H	3.33847900	3.89650000	2.15910700
25	C	4.16364700	2.80111100	-0.96190200	57	H	4.85098900	4.43241200	0.24979800
26	O	3.24591200	0.89601800	-2.15453500	58	H	4.83418500	3.04753100	-1.77663200
27	C	-2.18116700	2.85907500	-0.25635800	59	H	-2.66759400	4.96682600	-0.28714300
28	C	-2.92546900	3.97796100	-0.64627900	60	H	-4.58530400	4.70125200	-1.79882000
29	C	-4.01536400	3.82430200	-1.50534000	61	H	-3.89435300	0.47191000	-1.96952700
30	C	-3.62333400	1.45168600	-1.59102600	62	H	-5.21144800	2.44519400	-2.65580200
31	C	-4.36831900	2.56436900	-1.98252400	63	H	-1.03352500	-1.78953300	-2.42703600
32	O	-1.09236200	2.93304800	0.57023700	64	H	-2.25188000	-3.78224100	-3.25013800

65	H	-4.39032000	-4.45284200	-2.16472600	109	C	-3.68188000	3.00661700	-2.02118200
66	H	-5.29417800	-3.14748600	-0.28049700	110	O	-0.87054900	2.62744400	1.04514100
67	H	1.00529000	0.57688400	-2.79947500	111	C	-1.98310000	-2.37426800	-1.51412800
68	H	-0.76552800	0.52738000	-2.97115900	112	C	-2.78885500	-3.45944300	-1.86038100
69	H	0.01915900	1.94236100	-2.24294200	113	C	-4.12772800	-3.46780700	-1.47333800
70	H	4.43485500	-2.74375700	2.60823300	114	C	-3.84587000	-1.32867400	-0.37526100
71	H	5.51858100	-1.63615100	1.71069000	115	C	-4.65845400	-2.41199700	-0.73060100
72	H	4.55534000	-1.02632600	3.08447800	116	O	-4.27322800	-0.27810100	0.37824900
73	H	5.22145900	1.00114300	-2.82435500	117	C	0.47629900	-3.80402600	1.77127300
74	H	4.00839000	0.27009000	-3.91062500	118	C	5.65727500	0.26987400	0.71179200
75	H	4.05852700	2.04370600	-3.70336300	119	C	-0.40350300	3.78137000	1.74724800
76	H	0.30316100	4.05887200	1.49842300	120	C	-5.63410200	-0.23509000	0.80316400
77	H	-0.39949600	4.83606100	0.05994700	121	H	2.14360700	-4.93915600	0.27465800
78	H	-1.34577600	4.74959200	1.57818800	122	H	3.76855600	-5.08983800	-1.55930900
79	H	-5.37558700	-2.17883800	1.83140200	123	H	3.42351000	-0.86742500	-2.25302600
80	H	-5.49168400	-0.41710000	2.10618500	124	H	4.41684500	-3.05944400	-2.84869300
81	H	-6.15839300	-1.12793900	0.61100300	125	H	0.85223200	2.38827300	-1.70582100
82					126	H	2.23601500	4.34060400	-2.32233700
83	1SC1				127	H	4.65163700	4.38082400	-1.70512900
84	N	-0.00326500	-0.02875300	-1.29708900	128	H	5.64910100	2.50378500	-0.46822600
85	P	1.36349300	-0.07488800	-0.24349200	129	H	-2.06938300	4.93795300	0.26686800
86	P	-1.37010900	0.05917200	-0.24722000	130	H	-3.71179900	5.10950300	-1.54977600
87	Cr	0.00195900	-0.01068800	1.86510800	131	H	-3.44291000	0.88077900	-2.23414600
88	C	0.01269900	-0.07000700	-2.76683400	132	H	-4.40879600	3.08525400	-2.82343900
89	C	2.20378000	-1.64536300	-0.66302800	133	H	-0.93802600	-2.37396700	-1.80464300
90	C	2.45876200	1.29585800	-0.78081600	134	H	-2.37365400	-4.28502600	-2.42983000
91	C	-2.19060300	1.64302200	-0.66183500	135	H	-4.76947100	-4.30252800	-1.74007000
92	C	-2.49393000	-1.28509700	-0.79281100	136	H	-5.69768600	-2.44225700	-0.42573300
93	C	1.83942700	-2.80702500	0.05389300	137	H	0.41098400	0.85502800	-3.19466000
94	C	2.40932900	-4.04234900	-0.27170700	138	H	0.62717500	-0.90800000	-3.11461300
95	C	3.33402800	-4.12470800	-1.31530500	139	H	-1.00389300	-0.21439900	-3.13874600
96	C	3.13406800	-1.75869100	-1.70406100	140	H	0.00610500	-4.52791800	1.09666800
97	C	3.69898500	-2.98956900	-2.03753800	141	H	1.30874100	-4.27682100	2.30427600
98	O	0.91300600	-2.64634100	1.05602900	142	H	-0.26038400	-3.44767500	2.49205300
99	C	1.90696100	2.39724000	-1.45201700	143	H	5.89607500	1.10670400	1.37865000
100	C	2.68253900	3.50645700	-1.79024900	144	H	5.79377700	-0.67168800	1.24458300
101	C	4.03247600	3.52767200	-1.44337900	145	H	6.31867200	0.29376600	-0.16200100
102	C	3.81976400	1.35436000	-0.39707200	146	H	0.33141700	3.41546300	2.46498600
103	C	4.60257000	2.46204700	-0.74554700	147	H	0.07646300	4.48915400	1.06254200
104	O	4.28579600	0.29558300	0.32118000	148	H	-1.22115400	4.27599200	2.28325000
105	C	-1.80267400	2.80032700	0.04959100	149	H	-5.87298500	-1.08226900	1.45676400
106	C	-2.35546100	4.04401000	-0.27388400	150	H	-5.73918400	0.69646100	1.36012500
107	C	-3.29009000	4.13826900	-1.30750500	151	H	-6.31660600	-0.22624000	-0.05448900
108	C	-3.13213500	1.76838400	-1.69084200	152	C	2.00138300	0.62089300	2.67862300

153	H	2.73591900	-0.13124400	2.40829600	197	C	-4.66588500	-2.35652600	-0.60290400
154	H	2.15003600	1.59897400	2.22586000	198	O	-4.18557500	-0.24241500	0.50958300
155	C	1.22087400	0.47538100	3.80858800	199	C	0.07594400	-3.79755000	1.51333700
156	H	1.33929100	-0.38701200	4.45578400	200	C	5.56231900	0.14128300	0.94498100
157	H	0.74429800	1.33763800	4.26588200	201	C	-0.09346500	3.84237300	1.42952800
158	C	-1.20120400	-0.50796900	3.81628000	202	C	-5.50455900	-0.20576000	1.05034000
159	H	-0.72084800	-1.37141000	4.26728800	203	H	1.83663700	-5.00011500	0.17027400
160	H	-1.31530500	0.35229200	4.46713200	204	H	3.59083500	-5.20915900	-1.53615300
161	C	-1.98840500	-0.64930600	2.69066200	205	H	3.52779200	-0.96284400	-2.16696000
162	H	-2.72385900	0.10392600	2.42672400	206	H	4.44696000	-3.19674400	-2.72749600
163	H	-2.13896100	-1.62559200	2.23444400	207	H	1.00810200	2.35475000	-1.84015400
164					208	H	2.49488900	4.24676900	-2.40682800
165	1TS1				209	H	4.86384800	4.22525800	-1.63110800
166	N	0.00571300	-0.00248800	-1.34559900	210	H	5.71684900	2.34644300	-0.29147700
167	P	1.36538100	-0.09864100	-0.28717000	211	H	-1.87464600	5.00729300	0.08022600
168	P	-1.36294200	0.10292500	-0.29948500	212	H	-3.65907200	5.16992900	-1.59990100
169	Cr	0.00266000	0.02236600	1.81637500	213	H	-3.56787800	0.91416500	-2.15602000
170	C	0.02539700	-0.06681500	-2.81517400	214	H	-4.51827700	3.12854500	-2.73830300
171	C	2.15065000	-1.69946700	-0.69006400	215	H	-1.03234400	-2.31090400	-1.94540800
172	C	2.51688600	1.23260100	-0.79411600	216	H	-2.51907100	-4.20359800	-2.50017900
173	C	-2.16828300	1.68955100	-0.72047200	217	H	-4.85705500	-4.22775700	-1.63653600
174	C	-2.50698500	-1.23578900	-0.80437100	218	H	-5.68033000	-2.38919100	-0.22363600
175	C	1.66873700	-2.85113800	-0.02766800	219	H	0.51432500	-0.98709300	-3.15467200
176	C	2.19330200	-4.11061200	-0.33483300	220	H	-0.99925700	-0.05918700	-3.19337000
177	C	3.19149600	-4.22576800	-1.30526000	221	H	0.55795800	0.78584500	-3.24616800
178	C	3.15164200	-1.84544000	-1.65813000	222	H	-0.37282100	-4.45153700	0.75791700
179	C	3.67331800	-3.10036600	-1.97228300	223	H	0.80528700	-4.35818600	2.10858900
180	O	0.67804300	-2.65325000	0.90340900	224	H	-0.70554900	-3.40768000	2.16614200
181	C	2.04458400	2.33455200	-1.52124500	225	H	5.77526400	0.98812400	1.60791900
182	C	2.87744000	3.41099900	-1.82933800	226	H	5.62622000	-0.78923700	1.50973300
183	C	4.20157400	3.39776200	-1.39360500	227	H	6.29019600	0.12173000	0.12554300
184	C	3.84997700	1.25685400	-0.32066500	228	H	0.69702800	3.47071600	2.08208700
185	C	4.69015100	2.33107400	-0.63739800	229	H	0.34253700	4.49354600	0.66425200
186	O	4.22722500	0.19870300	0.44723900	230	H	-0.82686600	4.40033800	2.02232100
187	C	-1.68919100	2.85685900	-0.08381000	231	H	-5.68986500	-1.06723700	1.70263400
188	C	-2.23078600	4.10580600	-0.40358700	232	H	-5.55771900	0.71280700	1.63536600
189	C	-3.24627200	4.19456500	-1.35886800	233	H	-6.25799400	-0.17608500	0.25468500
190	C	-3.18945700	1.80892000	-1.67055000	234	C	1.78779500	0.32577100	2.80385200
191	C	-3.72936600	3.05296200	-1.99663000	235	H	2.54205500	-0.39483900	2.49540600
192	O	-0.68384000	2.68326200	0.83661600	236	H	2.12753800	1.35968600	2.71236300
193	C	-2.05324200	-2.31135500	-1.58054500	237	C	0.97992100	-0.01181700	3.96904900
194	C	-2.88748000	-3.38780100	-1.88613500	238	H	1.11095000	-1.03696200	4.31455900
195	C	-4.19434900	-3.39979600	-1.40184200	239	H	1.02117600	0.68834900	4.80100200
196	C	-3.82450700	-1.28275700	-0.28967300	240	C	-0.95929200	0.09498800	3.97643700

241	H	-0.99552100	-0.59717000	4.81534100	285	C	4.94853400	-0.61193200	1.85287000
242	H	-1.08381400	1.12388700	4.31279700	286	C	3.89731200	-0.24523600	-3.66330200
243	C	-1.77694000	-0.25126600	2.82112800	287	C	-0.98112200	3.64358700	1.84375600
244	H	-2.52262800	0.47402100	2.50343200	288	C	-5.35482200	-0.99278100	1.68312000
245	H	-2.12942000	-1.28207000	2.74610900	289	H	1.71319300	1.83917100	3.12336400
246					290	H	2.32918800	-0.52843400	3.60131200
247	1INT1				291	H	1.84911500	0.15693100	5.15561700
248	N	-0.20660100	-0.19737800	-1.17795500	292	H	-1.15850600	-1.88821600	2.78273600
249	P	1.16681300	-0.03241600	-0.12867000	293	H	-0.45395700	-0.76054500	4.86046100
250	P	-1.65069100	-0.16235600	-0.21552800	294	H	0.70087100	-2.07937200	4.72360500
251	Cr	-0.26140400	0.39473000	1.88846800	295	H	0.18230700	1.63218800	4.01520800
252	C	0.93785100	1.10927500	3.39042700	296	H	0.53281700	-2.05365400	2.23745700
253	C	1.47855500	-0.10602300	4.15327300	297	H	4.94763400	-3.02352700	1.01860100
254	C	-0.15983300	-1.42954600	2.81543200	298	H	4.03472000	-4.96504000	-0.19019800
255	C	0.35918200	-1.15566000	4.23246400	299	H	0.62592800	-2.64466200	-1.39254600
256	C	-0.16373700	0.10221600	-2.62317100	300	H	1.86591600	-4.79440900	-1.40081100
257	C	2.08869600	-1.60404300	-0.21531900	301	H	1.61039500	2.62197300	0.80414500
258	C	2.21575600	1.31062400	-0.78529500	302	H	2.99173300	4.53639000	0.05317700
259	C	-2.51827800	1.38866800	-0.66243300	303	H	4.42969400	4.28569400	-1.96686600
260	C	-2.72142000	-1.51267600	-0.81282800	304	H	4.47079900	2.16991400	-3.21357900
261	C	3.30828400	-1.71783600	0.48726100	305	H	-2.64768800	4.66477200	0.33196600
262	C	4.00838500	-2.92833600	0.48656700	306	H	-4.27344500	4.75743100	-1.49525300
263	C	3.48613600	-4.02759700	-0.19926400	307	H	-3.70848400	0.56940800	-2.25127300
264	C	1.57777500	-2.72334200	-0.87867000	308	H	-4.82380600	2.71342400	-2.80977400
265	C	2.27230700	-3.93391100	-0.87872200	309	H	-1.43915700	-2.26240600	-2.37266600
266	O	3.71411800	-0.59265600	1.13894500	310	H	-2.92448400	-4.14155800	-2.98023900
267	C	2.21740100	2.52869300	-0.09035100	311	H	-5.05639500	-4.47933700	-1.74106200
268	C	3.00151500	3.60456300	-0.50333400	312	H	-5.69288300	-2.95967600	0.08914900
269	C	3.80877100	3.46023200	-1.63066900	313	H	0.54724200	-0.55803000	-3.12492200
270	C	3.04495200	1.17952400	-1.92657500	314	H	-1.15590700	-0.04948500	-3.05246400
271	C	3.83607200	2.25890000	-2.34009200	315	H	0.13269900	1.14120400	-2.80401400
272	O	3.00990800	-0.01545100	-2.56990300	316	H	4.92390200	-1.34551800	2.66697100
273	C	-2.22862500	2.55373500	0.07771200	317	H	5.78773600	-0.83125500	1.18240200
274	C	-2.85855000	3.76204700	-0.22675000	318	H	5.06486500	0.38945300	2.26811300
275	C	-3.78809600	3.81260100	-1.26937600	319	H	4.94206700	-0.11708000	-3.35822900
276	C	-3.46206600	1.46872500	-1.69434100	320	H	3.73004200	-1.28030900	-3.96280000
277	C	-4.09663200	2.67103200	-2.00512200	321	H	3.67422400	0.42170300	-4.50456900
278	O	-1.30293000	2.44019300	1.11704200	322	H	-0.24032500	3.35677400	2.58767900
279	C	-2.37215400	-2.39979000	-1.83774500	323	H	-0.56094300	4.39439500	1.16805900
280	C	-3.20681400	-3.46553100	-2.17949900	324	H	-1.87147300	4.03855100	2.34206100
281	C	-4.40004900	-3.65312600	-1.48396600	325	H	-5.35539300	-1.95846300	2.20179300
282	C	-3.92770700	-1.72662100	-0.10678700	326	H	-5.33127400	-0.18477300	2.41505000
283	C	-4.76588200	-2.79241300	-0.44627000	327	H	-6.25757700	-0.90177300	1.06826800
284	O	-4.17703500	-0.83462400	0.89285300	328				

329 **IINT2**

330 N -0.15576400 0.42423300 -1.26426900
331 P 1.31393700 0.03636500 -0.45888200
332 P -1.50520800 0.33169400 -0.16771500
333 Cr 0.42834500 -0.46706600 1.80055800
334 C 0.94009800 1.34205700 2.63371600
335 C 2.40452100 1.26619100 3.07591400
336 C 2.15854100 -1.18146300 2.70312600
337 C 2.66187700 -0.11910500 3.68673100
338 C -1.62337100 -0.88607600 3.30857800
339 C -0.62569200 -1.45200900 4.01161500
340 C -0.24940800 0.57944600 -2.72864700
341 C 1.85740000 -1.53564000 -1.21292400
342 C 2.50607900 1.34825400 -0.89137000
343 C -2.57023100 1.74492200 -0.67938400
344 C -2.49737400 -1.13483700 -0.69944400
345 C 1.32535300 -2.71780900 -0.65687600
346 C 1.66362800 -3.96429100 -1.18809100
347 C 2.52855300 -4.03250200 -2.28397900
348 C 2.71846700 -1.63321400 -2.31162000
349 C 3.05518700 -2.87412100 -2.85271400
350 O 0.45776700 -2.56707700 0.41427300
351 C 2.04330400 2.60026600 -1.32164200
352 C 2.92979200 3.64622100 -1.57674600
353 C 4.29650600 3.44821100 -1.38406400
354 C 3.88952000 1.17962700 -0.64907600
355 C 4.78048900 2.22578800 -0.91574200
356 O 4.26037400 -0.02628700 -0.14136600
357 C -2.25706200 3.05064300 -0.23219900
358 C -3.06316100 4.13470100 -0.60070200
359 C -4.17428900 3.93092800 -1.42008400
360 C -3.69123200 1.57554700 -1.50481000
361 C -4.49196400 2.65447900 -1.87951600
362 O -1.14465500 3.17420000 0.54522100
363 C -2.08380400 -2.03125500 -1.69127800
364 C -2.83270100 -3.17073700 -2.00074000
365 C -4.01415600 -3.42619500 -1.30728500
366 C -3.68677000 -1.42622800 0.00853900
367 C -4.44540600 -2.55975500 -0.29913100
368 O -4.01053000 -0.53373200 0.99175200
369 C -0.20345300 -3.74151300 0.90607900
370 C 5.63754600 -0.26902500 0.14252700
371 C -0.83105400 4.45349000 1.09385300
372 C -5.28280100 -0.63590600 1.62984800

373 H 0.72802300 2.15017600 1.92762400
374 H 3.05756300 1.39602300 2.20241300
375 H 2.66604200 2.07135300 3.78007900
376 H 2.01354600 -2.17096200 3.15864400
377 H 2.11965500 -0.19483200 4.64095700
378 H 3.72523300 -0.25652200 3.93618400
379 H 0.26320100 1.45010200 3.49643700
380 H -2.27472200 -1.46203800 2.65744100
381 H -1.86491900 0.16887100 3.40862400
382 H -0.41765300 -2.51730500 3.95750300
383 H 2.85678600 -1.29854900 1.86280300
384 H -0.01712100 -0.87851000 4.70335700
385 H 1.27068100 -4.88048000 -0.76512000
386 H 2.78755100 -5.00607400 -2.68966100
387 H 3.13252000 -0.72546800 -2.74018300
388 H 3.72347700 -2.93475200 -3.70581900
389 H 0.97629600 2.75811100 -1.43655000
390 H 2.55525600 4.60497000 -1.92106400
391 H 4.99828800 4.25274300 -1.58389000
392 H 5.84342900 2.09871800 -0.74883500
393 H -2.83133700 5.13564300 -0.25751300
394 H -4.78933000 4.78192000 -1.69860800
395 H -3.94322300 0.58164400 -1.85953100
396 H -5.35238100 2.49659700 -2.52219200
397 H -1.16354000 -1.84297900 -2.23106100
398 H -2.49890700 -3.84228500 -2.78592800
399 H -4.61041600 -4.30253200 -1.54452400
400 H -5.36387000 -2.77266000 0.23558000
401 H 0.39165200 1.39579000 -3.07254000
402 H 0.05190500 -0.33569200 -3.25084200
403 H -1.27976400 0.81829500 -2.99997100
404 H -0.76942700 -4.22455700 0.10457800
405 H 0.51756700 -4.43866200 1.34473000
406 H -0.89481600 -3.39689200 1.67426800
407 H 6.01621600 0.43518800 0.89212100
408 H 5.68093100 -1.28354000 0.53927800
409 H 6.24616400 -0.20460300 -0.76690600
410 H 0.05521000 4.30218700 1.71012700
411 H -0.60847400 5.18100200 0.30431700
412 H -1.65107700 4.82772600 1.71762100
413 H -5.36561100 -1.56165600 2.21208500
414 H -5.34780100 0.22188600 2.29999500
415 H -6.09493800 -0.58969700 0.89562000
416

417 **1TS2**

418 N -0.12169300 0.46633500 -1.29243200
419 P 1.32970500 0.04227200 -0.45808800
420 P -1.46924900 0.37479100 -0.20697700
421 Cr 0.11556400 -0.55628800 1.74835600
422 C 0.62463500 1.15925400 2.75312000
423 C 2.06088100 1.00847900 3.24597900
424 C 1.66463500 -1.47682300 3.10358000
425 C 2.23106400 -0.34277600 3.95259500
426 C -1.46141700 -1.28671600 2.96120100
427 C -0.40428500 -1.86033600 3.69330100
428 C -0.20807600 0.66492000 -2.75106700
429 C 1.91284500 -1.46561600 -1.31636900
430 C 2.54626500 1.36273900 -0.80084900
431 C -2.48580800 1.85069800 -0.62318800
432 C -2.51369100 -1.03845900 -0.76655900
433 C 1.37827800 -2.69858600 -0.88508900
434 C 1.75453900 -3.88984600 -1.51162500
435 C 2.66386900 -3.85435300 -2.57226600
436 C 2.82129300 -1.46094400 -2.38115700
437 C 3.19931200 -2.64573400 -3.01317800
438 O 0.47730700 -2.65617900 0.16638400
439 C 2.15513200 2.61718800 -1.28666400
440 C 3.08500300 3.64420800 -1.45651400
441 C 4.42023200 3.42412500 -1.12169100
442 C 3.89329100 1.17396000 -0.41540200
443 C 4.82956000 2.19753100 -0.59425800
444 O 4.17770000 -0.03739500 0.14214900
445 C -2.06055900 3.13730500 -0.21393900
446 C -2.83180000 4.26492800 -0.51976400
447 C -4.01753100 4.12446800 -1.24205100
448 C -3.67751400 1.74551200 -1.35481800
449 C -4.44304500 2.86829000 -1.66833500
450 O -0.87743700 3.20012500 0.45890600
451 C -2.14214000 -1.90902500 -1.79724600
452 C -2.92207700 -3.02239500 -2.12287100
453 C -4.08822000 -3.27845000 -1.40354700
454 C -3.69230800 -1.32452900 -0.03744100
455 C -4.47732400 -2.43717900 -0.35793300
456 O -3.97811100 -0.44735300 0.96552700
457 C -0.17356200 -3.88106400 0.53058800
458 C 5.52081200 -0.32442800 0.52753700
459 C -0.42922100 4.46504700 0.94360300
460 C -5.18282200 -0.60990900 1.71146000

461 H 0.47504300 1.99749800 2.06874600
462 H 2.75224400 1.05416000 2.39383600
463 H 2.34797700 1.82988500 3.92040400
464 H 1.82805700 -2.45716600 3.55165700
465 H 1.72111900 -0.31741300 4.92630700
466 H 3.29092100 -0.53704900 4.17601700
467 H -0.08993800 1.24513600 3.58385900
468 H -2.07242900 -1.91884900 2.31977200
469 H -1.94713200 -0.38478300 3.32451600
470 H -0.24357600 -2.93101100 3.61489900
471 H 2.15402300 -1.51821800 2.11444400
472 H -0.11766000 -1.43455300 4.64907000
473 H 1.35627500 -4.84353900 -1.18837900
474 H 2.95063100 -4.78610900 -3.05101500
475 H 3.23892500 -0.51486700 -2.71286000
476 H 3.90343200 -2.62383900 -3.83897200
477 H 1.10985400 2.79508600 -1.51247700
478 H 2.76762900 4.60563400 -1.84802900
479 H 5.15415100 4.21354100 -1.25534000
480 H 5.86671300 2.05224700 -0.31612600
481 H -2.51530300 5.25117700 -0.20281300
482 H -4.60462200 5.00892300 -1.47235700
483 H -4.01184700 0.76896500 -1.68746500
484 H -5.36025000 2.75923400 -2.23839100
485 H -1.23029600 -1.72250800 -2.35182800
486 H -2.62351200 -3.67455900 -2.93800000
487 H -4.70639600 -4.13668100 -1.65086500
488 H -5.38531500 -2.65059200 0.19397100
489 H 0.08427900 -0.23973700 -3.29593000
490 H -1.23451200 0.92394600 -3.02038400
491 H 0.44469500 1.48073400 -3.07288400
492 H -0.71824100 -4.29500200 -0.32292000
493 H 0.55050000 -4.60890300 0.91163900
494 H -0.88260800 -3.62335000 1.31578800
495 H 5.86560200 0.36555400 1.30651500
496 H 5.50446500 -1.34122300 0.92109300
497 H 6.19750100 -0.27697900 -0.33344700
498 H 0.51124900 4.26866600 1.45865100
499 H -0.25400800 5.16633700 0.11935700
500 H -1.15000300 4.89654700 1.64755900
501 H -5.18542100 -1.55893000 2.26081600
502 H -5.20687600 0.22021700 2.41790300
503 H -6.06099500 -0.55948800 1.05754600
504

505 **1INT3**

506 N 0.13589700 0.70118800 -1.44698100
507 P 1.47098500 0.45114600 -0.36544000
508 P -1.33667000 0.33300700 -0.59620700
509 Cr -0.18246600 -0.62443900 1.39451800
510 C -0.43718200 0.91683800 2.65215000
511 C 0.44228200 0.19204500 3.66382200
512 C -0.26468900 -0.37632600 4.90911500
513 C -1.59030200 -1.89522100 2.17696700
514 C -2.10506200 -1.71520600 3.61066300
515 C 0.22352700 0.69355300 -2.91865900
516 C 2.43403000 -0.97403200 -1.01180600
517 C 2.58308800 1.88653700 -0.59061100
518 C -2.22646000 1.91932000 -0.40075800
519 C -2.36137000 -0.64195200 -1.75081000
520 C 2.37302600 -2.20099100 -0.32040100
521 C 3.10820400 -3.30369200 -0.76421600
522 C 3.90577200 -3.19049700 -1.90550300
523 C 3.25568100 -0.88752400 -2.14385400
524 C 3.98462800 -1.98515900 -2.60025700
525 O 1.56513500 -2.26797600 0.81160500
526 C 2.27437200 2.99718800 -1.38436900
527 C 3.13596400 4.09354700 -1.45838200
528 C 4.31813100 4.08730600 -0.72114100
529 C 3.77372600 1.90966400 0.17208200
530 C 4.64124200 3.00302800 0.09829300
531 O 3.97960200 0.81660800 0.96137700
532 C -3.41720900 1.92714500 0.36008700
533 C -4.09899100 3.12627700 0.58891000
534 C -3.59111700 4.31860000 0.06642100
535 C -1.73548900 3.12770500 -0.90361600
536 C -2.41271000 4.32760100 -0.67804600
537 O -3.81844100 0.70982600 0.81920600
538 C -3.43724700 -0.07636800 -2.44885100
539 C -4.22613500 -0.84450800 -3.30392500
540 C -3.94163400 -2.20000400 -3.46129500
541 C -2.08132900 -2.01502100 -1.92822900
542 C -2.87587000 -2.79057900 -2.77964400
543 O -1.00717800 -2.50350800 -1.24040600
544 C 1.80445800 -3.34956600 1.72930000
545 C 5.16533500 0.75047600 1.74982500
546 C -5.02293300 0.61744900 1.57725700
547 C -0.73296800 -3.90026300 -1.32800400
548 H -0.01102400 1.85076700 2.27814400

549 H 0.97282900 -0.68617400 3.17489800
550 H 1.29207800 0.82308700 3.95071900
551 H 0.48392600 -0.53032600 5.69695500
552 H -1.47414100 1.05395200 2.96084500
553 H -1.12000900 -2.89060600 2.07000000
554 H -2.42927900 -1.86940500 1.46867800
555 H -2.80124300 -2.53662100 3.84245000
556 H 3.07293400 -4.24903300 -0.23628100
557 H 4.47151600 -4.05446200 -2.24172900
558 H 3.34185900 0.06418700 -2.66011700
559 H 4.61362400 -1.89635500 -3.48040500
560 H 1.34978100 3.00956200 -1.94967100
561 H 2.88257400 4.94200500 -2.08604400
562 H 4.99714500 4.93345700 -0.77109100
563 H 5.55824100 3.02180800 0.67524800
564 H -5.01502700 3.14047200 1.16767800
565 H -4.12635400 5.24567200 0.25033100
566 H -0.80984600 3.12714600 -1.46812100
567 H -2.02143600 5.25751500 -1.07826100
568 H -3.65935000 0.97745000 -2.31661900
569 H -5.05398200 -0.38879600 -3.83764700
570 H -4.55029700 -2.81252500 -4.12024600
571 H -2.67364500 -3.84528200 -2.92035700
572 H 1.13980200 1.19591900 -3.23704800
573 H 0.22864500 -0.32698900 -3.31795100
574 H -0.62752200 1.23119400 -3.34557900
575 H 1.21867200 -3.12707100 2.62020400
576 H 1.47001100 -4.30445500 1.31162800
577 H 2.86745600 -3.40346000 1.98275000
578 H 5.20583700 1.57147800 2.47538800
579 H 5.11720100 -0.20142000 2.28003700
580 H 6.06155000 0.77137200 1.11892100
581 H -5.13439100 -0.43784400 1.82717600
582 H -4.95729700 1.20794800 2.49868400
583 H -5.88594000 0.94841800 0.98779400
584 H 0.13640800 -4.07025600 -0.69550400
585 H -1.57925100 -4.49206200 -0.96096900
586 H -0.49345600 -4.19260200 -2.35678000
587 C -1.02393600 -1.69931200 4.70899900
588 H -1.48657200 -1.95873000 5.66962000
589 H -0.29815300 -2.50384800 4.50596000
590 H -0.95463200 0.38927500 5.28704300
591 H -2.70397200 -0.79640400 3.68107400
592

593 **1TS3**

594 N -0.01735700 0.33394300 -1.55763700
595 P 1.29266100 0.39556500 -0.43515100
596 P -1.41628000 -0.12425800 -0.64540000
597 Cr -0.09175700 -0.36058400 1.52898000
598 C -0.66279100 -2.42764200 4.68026200
599 C 1.58233600 0.01814900 2.75180400
600 C 0.55586700 -0.39138800 3.68119200
601 C 0.68367900 -1.72442800 4.43387200
602 C -1.37922500 -2.80628700 3.37006700
603 C -1.76922100 -1.60378800 2.49141500
604 C 0.03943900 0.81259600 -2.94504600
605 C 2.60173800 -0.67886300 -1.14967500
606 C 1.95318900 2.09991600 -0.55326400
607 C -2.04231300 -1.68866500 -1.37054700
608 C -2.73337000 1.11230700 -0.97507900
609 C 3.87084700 -0.75027100 -0.52910900
610 C 4.85601300 -1.60944900 -1.02970600
611 C 4.57793700 -2.41373100 -2.13683200
612 C 2.34516000 -1.51429100 -2.24432300
613 C 3.32410000 -2.37523600 -2.74449100
614 O 4.04210300 0.05493200 0.55531900
615 C 3.05903800 2.43841000 -1.34271000
616 C 3.51508800 3.75412300 -1.42349700
617 C 2.86001000 4.74913000 -0.70011000
618 C 1.29506900 3.12313500 0.16528400
619 C 1.75322300 4.44281900 0.09451200
620 O 0.20791500 2.73897600 0.90308800
621 C -3.25360800 -1.81653400 -2.06455300
622 C -3.69108400 -3.05285400 -2.54175400
623 C -2.91460900 -4.18714600 -2.31701900
624 C -1.28108500 -2.86041700 -1.12903100
625 C -1.71404900 -4.09974600 -1.60823600
626 O -0.13038600 -2.69439300 -0.40410200
627 C -3.42140500 1.71078500 0.10797100
628 C -4.41578300 2.66829700 -0.13112500
629 C -4.73409000 3.03764400 -1.43772200
630 C -3.08942500 1.49884500 -2.27879000
631 C -4.07514000 2.45524600 -2.51865400
632 O -3.07123400 1.30747900 1.36583700
633 C 5.31749000 0.10336500 1.19155000
634 C -0.51028100 3.73502300 1.62848900
635 C 0.68629700 -3.83665200 -0.13887300
636 C -3.89324400 1.70485000 2.46286900

637 H -1.31464600 -1.77633100 5.28171100
638 H 2.40374200 -0.66674800 2.54749100
639 H 1.85983000 1.06825900 2.69592500
640 H 0.12749800 0.41153000 4.29130800
641 H -0.62152900 -0.76026300 3.05490900
642 H 1.33777500 -2.39365800 3.85671700
643 H 1.19556200 -1.53763100 5.38666100
644 H -0.49321500 -3.33032300 5.27873800
645 H -2.14978400 -1.94321700 1.52551400
646 H -2.55625200 -1.00416500 2.96238400
647 H -2.27877300 -3.39298200 3.60475500
648 H -0.72349200 -3.47906600 2.79672500
649 H 5.83311300 -1.65820100 -0.56374300
650 H 5.35044100 -3.07552900 -2.51776000
651 H 1.36318200 -1.49756900 -2.70336400
652 H 3.10805300 -3.00402300 -3.60270600
653 H 3.57055800 1.65988500 -1.89999800
654 H 4.37221300 3.99705300 -2.04360100
655 H 3.20571200 5.77770200 -0.74961200
656 H 1.25853900 5.23306600 0.64621700
657 H -3.86869400 -0.93876700 -2.22702900
658 H -4.63026300 -3.12550600 -3.08087100
659 H -3.24211100 -5.15562600 -2.68384800
660 H -1.13266200 -4.99667800 -1.43209800
661 H -4.94708900 3.12733800 0.69380200
662 H -5.50795800 3.78133400 -1.60448000
663 H -2.60264200 1.02996000 -3.12617000
664 H -4.32924000 2.73242100 -3.53672700
665 H 1.07874100 0.83181600 -3.28136400
666 H -0.51508600 0.13500300 -3.60436100
667 H -0.36858600 1.82449000 -3.04062500
668 H 6.09468200 0.43547300 0.49352800
669 H 5.21682700 0.83002400 1.99810000
670 H 5.59093500 -0.87259700 1.61002500
671 H -1.33176100 3.20597400 2.10999600
672 H 0.12381300 4.20798900 2.38757900
673 H -0.91242600 4.50028600 0.95472400
674 H 1.53850400 -3.46362800 0.42948100
675 H 0.14178700 -4.58153100 0.45230000
676 H 1.04477200 -4.28666000 -1.07054000
677 H -3.49392100 1.18547800 3.33475800
678 H -3.84490200 2.78745600 2.63194400
679 H -4.93524300 1.40549900 2.30382900
680

681 1SC2

682 N 0.14355700 -0.12693000 -1.59757300
683 P 1.37901100 0.00664400 -0.37833200
684 P -1.35626300 -0.10597700 -0.74864200
685 Cr -0.28040600 0.08481200 1.48608100
686 C -1.63248200 -0.97023400 4.92617700
687 C 1.35375200 0.42274200 2.84364700
688 C 0.14851200 0.36280100 3.57055200
689 C -0.14753900 -0.75776700 4.55916000
690 C -2.39548300 -1.98266400 4.05713000
691 C -2.34455900 -1.70240600 2.55332200
692 C 0.33500400 0.07401300 -3.03935200
693 C 2.48734500 -1.42981100 -0.67578600
694 C 2.37711300 1.46234900 -0.87987600
695 C -2.44056200 -1.38003800 -1.48865300
696 C -2.19348200 1.49643600 -1.06629600
697 C 3.67779400 -1.55692600 0.07724600
698 C 4.50883200 -2.66907600 -0.09716500
699 C 4.15211300 -3.66481700 -1.00941200
700 C 2.14541600 -2.45248400 -1.56831300
701 C 2.97192400 -3.56496300 -1.74375200
702 O 3.93277300 -0.54220500 0.94825800
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704 C 4.24060100 2.46156700 -2.09438300
705 C 3.85036700 3.72341500 -1.65015300
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707 C 2.73247900 3.87463400 -0.82774600
708 O 0.87687300 2.82103600 0.34591400
709 C -3.62298800 -1.08860600 -2.18444000
710 C -4.45122200 -2.10323000 -2.66555800
711 C -4.10338800 -3.43370800 -2.44315700
712 C -2.11460300 -2.74033100 -1.25435600
713 C -2.94342100 -3.75835000 -1.73662700
714 O -0.97510800 -2.96792900 -0.54164400
715 C -2.58219500 2.27042900 0.04991200
716 C -3.20811100 3.50829200 -0.12683100
717 C -3.43286200 3.99473000 -1.41628200
718 C -2.42740300 2.01844300 -2.34861600
719 C -3.03824000 3.25875200 -2.53197800
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721 C 5.14194700 -0.56255300 1.70344000
722 C 0.50432300 4.08924600 0.87892400
723 C -0.62043700 -4.31211000 -0.21857000
724 C -2.93973900 2.37011900 2.43656800

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727 H 1.80032200 1.37733800 2.57556200
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729 H -1.33594200 -1.89235100 2.15024900
730 H 0.28957600 -1.70143800 4.19949200
731 H 0.39997700 -0.52102800 5.48407600
732 H -1.69853700 -1.30857800 5.96712800
733 H -3.01398200 -2.35854500 1.98624100
734 H -2.64565000 -0.67010400 2.32221200
735 H -3.44361300 -2.00712000 4.38148600
736 H -1.99655700 -2.98911100 4.24337500
737 H 5.42657100 -2.76621000 0.47077500
738 H 4.80531600 -4.52315300 -1.13790500
739 H 1.21439900 -2.38074100 -2.11879200
740 H 2.69623400 -4.34157600 -2.45062300
741 H 3.81168100 0.35814800 -2.03961500
742 H 5.10933000 2.34593400 -2.73482500
743 H 4.41479200 4.60461400 -1.94148600
744 H 2.44684300 4.86585100 -0.49713600
745 H -3.90799300 -0.05519000 -2.34381100
746 H -5.35894500 -1.85282200 -3.20516400
747 H -4.73886500 -4.23371800 -2.81191800
748 H -2.69691000 -4.79917200 -1.56473700
749 H -3.52012700 4.10161300 0.72403300
750 H -3.91939800 4.95777200 -1.54024400
751 H -2.13969300 1.43840500 -3.21949400
752 H -3.21132400 3.63949500 -3.53350800
753 H 1.29624700 -0.34473500 -3.34822500
754 H -0.45438200 -0.45042200 -3.58856800
755 H 0.31997900 1.13629600 -3.31031800
756 H 6.01870200 -0.55880000 1.04537000
757 H 5.13117700 0.34874800 2.30188000
758 H 5.18221900 -1.43519100 2.36621300
759 H -0.35959400 3.89838500 1.51527500
760 H 1.31325000 4.51965600 1.48059500
761 H 0.22204000 4.78807200 0.08320700
762 H 0.30903300 -4.24410800 0.34659400
763 H -1.39586200 -4.78895300 0.39236900
764 H -0.44934700 -4.90519900 -1.12418100
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769 1P
770 N -0.50955500 1.29203500 0.89594900
771 P -1.67586000 0.42760400 -0.05737100
772 P 1.10881000 0.84548100 0.40021400
773 Cr 0.21650300 -1.06048600 -1.20537200
774 C 1.19673200 -0.74944200 -3.32307500
775 C 0.72235700 -2.00993300 -3.52445600
776 C 3.02354000 -3.28576900 -3.30187400
777 C 1.51174000 -3.29965600 -3.62620700
778 C 2.87774800 -3.06347300 -0.72096600
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780 C -0.78694300 1.86123600 2.22724200
781 C -2.49728900 -0.76647900 1.08598200
782 C -3.00035000 1.64057300 -0.43109600
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786 C -2.81701600 -3.07301800 1.81522900
787 C -3.72244500 -2.64036400 2.78694000
788 C -3.42058600 -0.36724900 2.06171200
789 C -4.02900200 -1.28750200 2.91515100
790 O -1.29834200 -2.53723900 -0.00979800
791 C -2.88963900 3.01353800 -0.18192500
792 C -3.89271400 3.90476400 -0.56985100
793 C -5.02171500 3.42253300 -1.22744200
794 C -4.13938800 1.17482900 -1.12901500
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796 O -4.15401300 -0.16396800 -1.39370800
797 C 3.10742200 2.28751900 -0.92245500
798 C 3.67475700 3.39997500 -1.55009200
799 C 2.96979500 4.60654800 -1.58591500
800 C 1.14816000 3.59345600 -0.37775900
801 C 1.70777600 4.70926400 -1.00496600
802 O 3.71005400 1.06201900 -0.84099200
803 C 2.87516700 1.62574000 2.49096600
804 C 3.59925900 1.42594100 3.66651300
805 C 3.49370200 0.20750100 4.33384400
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808 O 1.12003800 -1.54191100 2.10890100
809 C -1.33463600 -3.91120700 -0.42255300
810 C -5.27333500 -0.71680100 -2.07844500
811 C 5.05192500 0.92728700 -1.30063400
812 C 0.98769600 -2.79298900 2.77491800

813 H 0.56300200 0.11494400 -3.51727200
814 H 1.77717700 -3.07012200 -0.69303300
815 H -0.32324700 -2.10613600 -3.82654500
816 H 3.42875900 -2.27285200 -3.41621200
817 H 1.37520200 -3.62520600 -4.66871200
818 H 1.01265000 -4.08384000 -3.03654900
819 H 2.24532800 -0.54102600 -3.12989000
820 H 3.21806600 -3.50380800 0.22297500
821 H 3.20525100 -2.01715200 -0.73515100
822 H 3.07112800 -4.89044400 -1.85557800
823 H 3.53462100 -3.88996400 -4.06011400
824 H 4.50631200 -3.88501200 -1.86361000
825 H -2.60077700 -4.13136600 1.72923200
826 H -4.18978300 -3.37322900 3.43822400
827 H -3.68406600 0.68384600 2.13475600
828 H -4.74051500 -0.95203000 3.66327500
829 H -2.00650300 3.39400600 0.31754000
830 H -3.78869000 4.96438100 -0.35834600
831 H -5.81040900 4.10427100 -1.53213800
832 H -6.02688400 1.70435400 -2.04009400
833 H 4.65352800 3.33796800 -2.01136900
834 H 3.41715700 5.46604100 -2.07677100
835 H 0.16153200 3.66274300 0.06654000
836 H 1.16156000 5.64682500 -1.03760200
837 H 2.95688000 2.57333200 1.96817600
838 H 4.23572400 2.21475700 4.05508400
839 H 4.05070700 0.03546400 5.25046000
840 H 2.60605800 -1.74617400 4.37344000
841 H -1.79004400 2.29397700 2.24687800
842 H -0.72038700 1.10262700 3.01580400
843 H -0.06927400 2.65541800 2.45056800
844 H -0.72527000 -3.97267800 -1.32529800
845 H -0.90965500 -4.56947500 0.34259300
846 H -2.36049300 -4.21830100 -0.64892700
847 H -5.38095800 -0.28385400 -3.08031600
848 H -5.07189700 -1.78550400 -2.16422800
849 H -6.19970200 -0.56604300 -1.51164800
850 H 5.34176800 -0.10039200 -1.07717900
851 H 5.12521100 1.10095800 -2.38134500
852 H 5.72133800 1.61714600 -0.77371300
853 H 0.29009300 -3.37494200 2.17366200
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856

857 **1INT4**
858 N -0.25646700 0.34578900 -1.37987000
859 P -1.58049300 0.09275000 -0.28447400
860 P 1.25776500 0.29864500 -0.55239200
861 Cr 0.24778900 -0.38944400 1.76074900
862 C 1.89140600 -0.27282300 2.94372200
863 C 3.08636400 -1.19001800 2.66138400
864 C 2.97984000 -2.61080500 3.23771000
865 C -0.10347900 -2.39861600 1.63895300
866 C 0.51620000 -3.33696100 2.67185400
867 C 2.02996200 -3.59576800 2.53653600
868 C -1.12128000 0.75230000 3.63018100
869 C -1.59859000 -0.50415800 3.67831800
870 C -0.36359200 0.63696100 -2.82227700
871 C -2.76714200 1.44811200 -0.67010300
872 C -2.46716600 -1.40435200 -0.87735200
873 C 1.79701400 2.05952800 -0.42106900
874 C 2.43821800 -0.44837600 -1.74614700
875 C -2.67924600 2.68135600 0.01688100
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877 C -4.54500900 3.54284200 -1.26226800
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879 C -4.65153900 2.33377300 -1.94594500
880 O -1.69672200 2.78665100 0.96505500
881 C -2.00666600 -2.20627400 -1.92690900
882 C -2.68487000 -3.37115600 -2.29599000
883 C -3.83243500 -3.74798900 -1.60162800
884 C -3.61278300 -1.82105400 -0.16272900
885 C -4.29944800 -2.98110200 -0.53078300
886 O -3.96868900 -1.02153500 0.88981200
887 C 0.98383000 3.11262300 -0.85750900
888 C 1.38065900 4.44351900 -0.71151200
889 C 2.60067300 4.73294200 -0.10258100
890 C 3.02741000 2.37236400 0.20375500
891 C 3.42500000 3.70538300 0.36034900
892 O 3.76568900 1.30442100 0.60919600
893 C 2.40270600 -1.83709800 -2.01874500
894 C 3.31784500 -2.40291000 -2.91461000
895 C 4.26116100 -1.59640200 -3.55183500
896 C 3.39212900 0.33536400 -2.41195800
897 C 4.29922700 -0.22490100 -3.30985300
898 O 1.43479200 -2.55774100 -1.38604900
899 C -1.52119200 4.03860900 1.62824800
900 C -5.21087900 -1.26682500 1.54804700

901 C 5.05826400 1.52629300 1.17079800
902 C 1.34575700 -3.96034600 -1.63731500
903 H 2.17346300 0.78617200 2.80177300
904 H 3.28232900 -1.24857400 1.58138000
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907 H -1.20090100 -2.45464200 1.65171000
908 H 0.24218600 -2.62521300 0.62455000
909 H 0.29485100 -3.00067400 3.69627500
910 H 0.00035300 -4.30701500 2.57708400
911 H 2.23724200 -4.59092000 2.95082600
912 H 2.29117800 -3.65332000 1.46925200
913 H 2.70794900 -2.54716400 4.30250900
914 H 1.56023600 -0.38834500 3.98734900
915 H -1.20795100 -1.23756900 4.37835600
916 H -2.41565100 -0.81944200 3.03447200
917 H -0.33298600 1.08659000 4.29972400
918 H -1.54795000 1.48678600 2.95101200
919 H -3.50711600 4.66790400 0.24158600
920 H -5.22702500 4.35889300 -1.48321200
921 H -3.85636700 0.35094600 -2.16423900
922 H -5.41402000 2.19405600 -2.70578300
923 H -1.10290700 -1.92318500 -2.45308700
924 H -2.32168800 -3.97266100 -3.12372500
925 H -4.37157200 -4.64784400 -1.88323600
926 H -5.18606500 -3.29589000 0.00722200
927 H 0.02626200 2.88969000 -1.31334500
928 H 0.74512500 5.24358900 -1.07887700
929 H 2.92223900 5.76367200 0.01638200
930 H 4.36954800 3.94720200 0.83314400
931 H 3.30033200 -3.46608500 -3.12082400
932 H 4.96435700 -2.05055000 -4.24404800
933 H 3.42212600 1.40353900 -2.22990800
934 H 5.02533600 0.40552600 -3.81313200
935 H 0.26977400 1.48664400 -3.09357000
936 H -0.05766000 -0.22144400 -3.42919600
937 H -1.39698100 0.89336700 -3.06680000
938 H -1.29147600 4.83576700 0.91334900
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940 H -0.67025500 3.90447400 2.29721200
941 H -5.32238300 -0.46696500 2.28121100
942 H -6.04510400 -1.23078600 0.83832000
943 H -5.20608700 -2.23579100 2.06138700
944 H 5.46180900 0.53607100 1.38054900

945 H 5.71048100 2.04814300 0.46107100

946 H 4.99228100 2.09928200 2.10305200

947 H 2.25452600 -4.47893000 -1.31164800

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949 H 1.16711400 -4.16000500 -2.70023700

950

951 **1TS4**

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953 P -1.56050500 0.11768100 -0.45058200

954 P 1.25692400 0.03525900 -0.71143900

955 Cr -0.10112400 0.05672500 1.73979300

956 C 1.53221800 0.52550200 2.90065000

957 C 2.64476900 -0.47573600 3.23474200

958 C 2.32466000 -1.58698000 4.26095100

959 C -0.24635000 -2.06265000 2.32801600

960 C 0.28653500 -3.03063100 3.38422200

961 C 1.78704900 -2.92006000 3.70133900

962 C -1.29143200 -0.74497100 3.63089100

963 C -1.63263700 0.52283800 3.12026600

964 C -0.35098000 0.37567000 -3.02102000

965 C -2.32840200 1.77230800 -0.58481100

966 C -2.78366200 -1.08006700 -1.09398400

967 C 2.12730900 1.64270500 -0.95351100

968 C 2.21643400 -1.16067300 -1.72831600

969 C -1.74877200 2.80666100 0.18185500

970 C -2.26042100 4.10564700 0.11341600

971 C -3.35084000 4.37634600 -0.71804200

972 C -3.42181800 2.07245600 -1.40506400

973 C -3.93651700 3.36700600 -1.47902800

974 O -0.66522700 2.47020700 0.97962000

975 C -2.47670600 -1.98211000 -2.12071400

976 C -3.39736300 -2.94741200 -2.53268000

977 C -4.63906200 -3.02365500 -1.90470600

978 C -4.03050200 -1.20219500 -0.43663000

979 C -4.95941800 -2.16043900 -0.85427900

980 O -4.23146200 -0.34617100 0.60735000

981 C 1.50179500 2.77450000 -1.49060700

982 C 2.16082700 4.00483500 -1.55884400

983 C 3.46190200 4.11493400 -1.07056700

984 C 3.43503300 1.78325900 -0.43293900

985 C 4.10191800 3.01155700 -0.50175400

986 O 3.96239200 0.65707100 0.12388600

987 C 1.90412900 -2.53591300 -1.63147700

988 C 2.60332900 -3.47589300 -2.39617100

989 C 3.61107500 -3.05133100 -3.26471300

990 C 3.22600000 -0.76585400 -2.61468900

991 C 3.92407300 -1.69875200 -3.38217000

992 O 0.89114800 -2.86349600 -0.77349000

993 C -0.02725000 3.53488200 1.70398200

994 C -5.50092500 -0.33674200 1.25823300

995 C 5.29902100 0.68745000 0.61915000

996 C 0.50838700 -4.23198200 -0.65967800

997 H 1.96645400 1.33409700 2.28846000

998 H 3.02137600 -0.93740000 2.31142000

999 H 3.49444100 0.09933300 3.63637200

1000 H 3.25949300 -1.82481200 4.78362400

1001 H -1.15020700 -2.43065100 1.83469600

1002 H 0.52985600 -1.96978800 1.54574500

1003 H -0.29324400 -2.96077900 4.31483100

1004 H 0.10494000 -4.05135600 3.01555100

1005 H 2.01315000 -3.71171500 4.42727800

1006 H 2.36060600 -3.17314300 2.79710000

1007 H 1.65052200 -1.19914400 5.03935100

1008 H 1.15068600 0.98664900 3.82572800

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1011 H -1.21717400 1.40904500 3.59498600

1012 H -2.57296700 0.65419900 2.59110400

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1014 H -3.73925800 5.38966500 -0.76222600

1015 H -3.87762300 1.27671300 -1.98725300

1016 H -4.78340000 3.58300200 -2.12280700

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1018 H -3.14626400 -3.62796300 -3.34025300

1019 H -5.36720300 -3.76490500 -2.22097600

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1021 H 0.48187000 2.70156000 -1.85124600

1022 H 1.66220800 4.86407700 -1.99702400

1023 H 3.98817700 5.06366800 -1.12357400

1024 H 5.10882900 3.11512800 -0.11483800

1025 H 2.37250800 -4.53188100 -2.32305200

1026 H 4.14820700 -3.79017900 -3.85257000

1027 H 3.46606600 0.28799300 -2.70806300

1028 H 4.70194100 -1.36980300 -4.06408200

1029 H 0.30316900 1.18781600 -3.34924700

1030 H -0.06798500 -0.52825800 -3.57061900

1031 H -1.37852700 0.63998300 -3.28224900

1032 H 0.36605000 4.28238400 1.00921400

1033	H	-0.72690100	3.99651100	2.40833300	1077	C	3.34916300	-1.97074200	-4.05597000
1034	H	0.79468600	3.07838500	2.25115400	1078	C	3.29423600	-0.73725400	-1.97939100
1035	H	-5.44197300	0.44880400	2.01236000	1079	C	3.91517400	-1.02265600	-3.19942400
1036	H	-6.30504600	-0.10383500	0.55089900	1080	O	3.75470500	0.16452400	-1.06905400
1037	H	-5.70579900	-1.29751400	1.74531800	1081	C	2.09680700	-1.33169800	2.61713800
1038	H	5.50046900	-0.31863200	0.98752800	1082	C	2.91969100	-1.83693000	3.62981800
1039	H	6.00909800	0.93504400	-0.17847100	1083	C	3.98870000	-2.67251800	3.30171900
1040	H	5.40228000	1.40536500	1.44135200	1084	C	3.43149100	-2.49897800	0.96719900
1041	H	1.33465400	-4.84723400	-0.28444700	1085	C	4.24792100	-3.01087800	1.97456700
1042	H	-0.31470400	-4.25160700	0.05512500	1086	O	1.01641800	-0.52945500	2.84846300
1043	H	0.16332700	-4.62806400	-1.62187500	1087	C	-5.10655500	1.33171700	-1.29552900
1044					1088	C	-1.58732500	2.72974300	2.58971700
1045	1INT5				1089	C	4.97505900	0.85337500	-1.33470200
1046	N	-0.20735200	-1.80582600	0.01805300	1090	C	0.74631900	-0.13944700	4.19341900
1047	P	-1.50566400	-0.66677500	-0.15384000	1091	H	1.97360600	5.25041800	1.39399500
1048	P	1.29785900	-0.93549500	-0.04029800	1092	H	-0.08245700	4.50501000	0.22533600
1049	Cr	0.22561600	1.32382500	0.06911100	1093	H	0.29599300	6.17990800	-0.07941100
1050	C	2.01828500	4.94469600	0.33882800	1094	H	0.65121700	5.86048600	-2.34968400
1051	C	0.63375700	5.15792000	-0.29238100	1095	H	1.21931400	2.19226800	-2.17251100
1052	C	0.58042800	4.90478700	-1.81676100	1096	H	0.01157600	0.92430400	-2.57236000
1053	C	0.25324500	1.75689300	-1.90983300	1097	H	-1.82341800	2.32954000	-2.06673200
1054	C	-0.87777700	2.75612800	-1.71606200	1098	H	-1.07564100	2.90932600	-0.61337900
1055	C	-0.68174300	4.17249800	-2.29993600	1099	H	-0.65067500	4.08345000	-3.39312500
1056	C	2.57385700	3.50881400	0.27186700	1100	H	-1.57041800	4.77325400	-2.06025900
1057	C	1.73134200	2.42549700	0.96857300	1101	H	1.46090800	4.33238300	-2.12990700
1058	C	-0.32478600	-3.14249800	0.62859200	1102	H	2.73868800	5.62150000	-0.14185700
1059	C	-2.66439900	-1.40270400	-1.36544500	1103	H	2.39410800	1.61362800	1.29979100
1060	C	-2.44818900	-0.66068800	1.42254200	1104	H	1.26955600	2.83175300	1.88682800
1061	C	2.10628400	-1.40871400	-1.61174600	1105	H	3.57159000	3.53865600	0.73724300
1062	C	2.35204900	-1.65571200	1.26587500	1106	H	2.75918100	3.22822200	-0.77409500
1063	C	-3.81591900	-0.65380600	-1.70212300	1107	H	-5.60469500	-0.56314500	-2.91324400
1064	C	-4.71712700	-1.12992900	-2.65847100	1108	H	-5.17132900	-2.70690300	-4.04301000
1065	C	-4.46672700	-2.34561700	-3.29969900	1109	H	-1.53608600	-3.17819600	-1.81883000
1066	C	-2.42890800	-2.60563500	-2.04111900	1110	H	-3.12584900	-4.02281500	-3.50740700
1067	C	-3.32360200	-3.08341600	-3.00083000	1111	H	-3.46418800	-2.52786500	1.10894200
1068	O	-3.95252100	0.53313300	-1.04258000	1112	H	-4.71295100	-2.46089200	3.24661700
1069	C	-3.32478900	-1.69137700	1.78756500	1113	H	-4.44754400	-0.49692800	4.75850000
1070	C	-4.04088700	-1.65027600	2.98319300	1114	H	-2.95419900	1.34904600	4.15051600
1071	C	-3.89290200	-0.55097600	3.82628700	1115	H	0.63343800	-2.84644400	-2.22066200
1072	C	-2.31840800	0.44693900	2.28618100	1116	H	1.73671200	-3.36713900	-4.38153400
1073	C	-3.04045000	0.50099500	3.48233300	1117	H	3.83743100	-2.18512600	-5.00221700
1074	O	-1.45908200	1.47227200	1.90294900	1118	H	4.82881000	-0.51643000	-3.48817400
1075	C	1.55626700	-2.34569400	-2.49147700	1119	H	2.73697600	-1.58992300	4.66844100
1076	C	2.17280600	-2.63381200	-3.71055300	1120	H	4.61927900	-3.05911300	4.09720300

1121 H 3.63359900 -2.75604400 -0.06709000
1122 H 5.07730200 -3.66431900 1.72362300
1123 H -1.28637200 -3.58651800 0.36203900
1124 H 0.46945700 -3.79520500 0.25544500
1125 H -0.25500500 -3.09488300 1.72112000
1126 H -6.02454000 0.79329800 -1.03320900
1127 H -5.00545400 2.21013400 -0.65708900
1128 H -5.14983300 1.64591300 -2.34497200
1129 H -0.96542800 3.43792300 2.04480700
1130 H -2.62942600 3.06312500 2.58084200
1131 H -1.22533200 2.65499200 3.61997600
1132 H 5.14120400 1.50186400 -0.47459000
1133 H 5.81008300 0.14994400 -1.43301600
1134 H 4.89598900 1.46280100 -2.24243300
1135 H -0.14771500 0.47992800 4.14794800
1136 H 0.54712000 -1.01260300 4.82523100
1137 H 1.57869600 0.43836300 4.61138700
1138
1139 **1TS5**
1140 N 0.28283800 -1.55100400 0.88543700
1141 P 1.54637300 -0.46118800 0.46704800
1142 P -1.24110300 -0.84197500 0.39316600
1143 Cr 0.08346100 1.30943500 -0.53899100
1144 C -3.06495500 4.02864800 -1.72561800
1145 C -1.99441000 5.12147800 -1.57070100
1146 C -1.27972000 5.19995700 -0.19565500
1147 C 0.29575200 2.56921900 1.08768100
1148 C 0.64927400 3.36449200 -0.08663200
1149 C 0.21975000 4.83929300 -0.22746800
1150 C -2.62094600 2.59661200 -1.38094700
1151 C -1.29399200 2.16425500 -2.03389900
1152 C 0.45145200 -2.99835700 1.10434600
1153 C 2.70981600 -0.42155800 1.87562500
1154 C 2.50582500 -1.20489400 -0.91013800
1155 C -2.18428000 -0.65693100 1.96035200
1156 C -2.11307800 -2.19798100 -0.48752400
1157 C 3.86144700 0.38969900 1.74992300
1158 C 4.76713100 0.50289300 2.80863600
1159 C 4.51968300 -0.17485000 4.00465100
1160 C 2.47519800 -1.06797900 3.09507300
1161 C 3.37469000 -0.95412600 4.15664500
1162 O 3.99340200 1.03476100 0.55503400
1163 C 3.33186700 -2.32554500 -0.75224500
1164 C 4.03557700 -2.86477300 -1.82905200

1165 C 3.92664600 -2.26607600 -3.08292700
1166 C 2.41882000 -0.60812400 -2.18291100
1167 C 3.12632600 -1.13569400 -3.26601100
1168 O 1.61610500 0.51945000 -2.30524200
1169 C -1.61243000 -0.89925700 3.21305000
1170 C -2.32369800 -0.66272600 4.39146100
1171 C -3.62347600 -0.16668700 4.31795000
1172 C -3.49799700 -0.13914400 1.90467000
1173 C -4.21621000 0.09829200 3.08046500
1174 O -3.97812300 0.09422000 0.64962200
1175 C -1.87273500 -2.40076300 -1.86522300
1176 C -2.53544300 -3.42338500 -2.55397400
1177 C -3.43557100 -4.24781600 -1.87652000
1178 C -3.02305800 -3.04198200 0.16357400
1179 C -3.68362600 -4.06370600 -0.51772000
1180 O -0.97116000 -1.55823200 -2.45609400
1181 C 5.14566600 1.84490300 0.33417800
1182 C 1.84395300 1.37438700 -3.43712700
1183 C -5.32171800 0.54388100 0.49862500
1184 C -0.72718900 -1.70574000 -3.85178000
1185 H -3.42294900 4.04949400 -2.76436600
1186 H -1.23914900 5.00330900 -2.35979500
1187 H -2.47596300 6.08332200 -1.78303000
1188 H -1.35159500 6.22805600 0.17647100
1189 H -0.64261800 2.80819100 1.59227900
1190 H 1.08421300 2.25915900 1.77061100
1191 H 1.71259100 3.27551800 -0.34244300
1192 H -0.21708100 2.83646200 -1.23328100
1193 H 0.72213800 5.36013000 0.59930000
1194 H 0.65763000 5.25090900 -1.14724500
1195 H -1.80073600 4.58703800 0.55151400
1196 H -3.93206300 4.28051000 -1.09966600
1197 H -1.35119800 1.13436800 -2.41377000
1198 H -1.04534000 2.79075500 -2.89830900
1199 H -3.41617400 1.90412300 -1.68428600
1200 H -2.55860800 2.49058800 -0.28987600
1201 H 5.65463000 1.11718600 2.71418500
1202 H 5.22771300 -0.07982800 4.82268800
1203 H 1.57999700 -1.66592700 3.22004800
1204 H 3.17929200 -1.46964900 5.09152900
1205 H 3.44176700 -2.76847700 0.23336700
1206 H 4.66822300 -3.73532800 -1.68750600
1207 H 4.47177500 -2.67006400 -3.93100300
1208 H 3.06678100 -0.68092500 -4.24768200

1209	H	-0.59413100	-1.26802400	3.26252500	1253	C	-2.84402500	2.95176200	2.25385800
1210	H	-1.86401800	-0.86245100	5.35433900	1254	O	-1.06980200	2.48272900	0.65072600
1211	H	-4.18811100	0.02331700	5.22618200	1255	C	0.71673100	-3.46488200	-0.90422200
1212	H	-5.22644400	0.48875800	3.04248100	1256	C	1.23226400	-4.46222000	-1.73465700
1213	H	-2.35799400	-3.58669200	-3.61001000	1257	C	2.56041800	-4.38908400	-2.14986100
1214	H	-3.94270600	-5.03769000	-2.42324200	1258	C	2.85054100	-2.32857100	-0.92214200
1215	H	-3.21956700	-2.89117400	1.22034600	1259	C	3.37523000	-3.32731300	-1.74759500
1216	H	-4.38333300	-4.70584900	0.00789800	1260	O	3.55816600	-1.24640700	-0.48129800
1217	H	1.40031900	-3.19076100	1.61027600	1261	C	1.56049400	-0.22621200	3.15754200
1218	H	-0.35575200	-3.37233400	1.74023000	1262	C	2.24124400	-0.35398300	4.37443400
1219	H	0.43857000	-3.55625800	0.16130500	1263	C	3.05604700	-1.46345000	4.60359800
1220	H	6.06526000	1.25331700	0.41023700	1264	C	2.52557200	-2.31739100	2.41790500
1221	H	5.04658900	2.23212900	-0.68060200	1265	C	3.19795000	-2.45191900	3.63189200
1222	H	5.18450000	2.68110300	1.04219800	1266	O	0.72278400	0.81124100	2.86956100
1223	H	1.28541200	2.28858100	-3.24226700	1267	C	-5.02493600	1.52430400	-2.22743300
1224	H	2.91011800	1.60090000	-3.53473900	1268	C	-0.66270800	3.85294400	0.71657700
1225	H	1.47537200	0.91557600	-4.36044900	1269	C	4.97425400	-1.23977200	-0.65178300
1226	H	-5.48930400	0.62354200	-0.57593800	1270	C	0.49679300	1.79151800	3.87911400
1227	H	-6.02933200	-0.17595400	0.92641600	1271	H	-5.92891100	-0.79155600	-2.72818000
1228	H	-5.46845500	1.52536000	0.96525400	1272	H	-5.97337600	-3.24932600	-2.60646900
1229	H	-0.01173400	-0.92566600	-4.10930700	1273	H	-2.40440700	-3.22249500	-0.23036700
1230	H	-0.29231300	-2.68607000	-4.07866900	1274	H	-4.20336700	-4.48133200	-1.35908100
1231	H	-1.64604600	-1.56563500	-4.43324600	1275	H	-4.16708900	-0.64615800	1.70173000
1232					1276	H	-5.30493400	0.84444500	3.31955500
1233	1SC3				1277	H	-4.46357600	3.16750500	3.64545300
1234	N	-0.81968600	-1.42125900	0.85057800	1278	H	-2.50588600	3.97010700	2.40348700
1235	P	-1.79053100	-0.30362700	-0.04212000	1279	H	-0.31701000	-3.51118400	-0.58237200
1236	P	0.85027400	-1.01203500	0.54108400	1280	H	0.60174300	-5.28755400	-2.05010000
1237	Cr	0.12465600	0.86969000	-1.05298900	1281	H	2.97460700	-5.15909900	-2.79423300
1238	C	-1.26169400	-2.17594700	2.03594400	1282	H	4.40538600	-3.28457400	-2.08176500
1239	C	-3.13558500	-1.28336500	-0.80601600	1283	H	2.14193400	0.40022700	5.14538200
1240	C	-2.65251500	0.78070700	1.16329000	1284	H	3.57712000	-1.54974900	5.55279600
1241	C	1.51050900	-2.39546500	-0.47835400	1285	H	2.63532800	-3.08798400	1.66278700
1242	C	1.70648000	-1.21050200	2.15348000	1286	H	3.82358400	-3.31999300	3.81391700
1243	C	-4.13740400	-0.59962500	-1.53456200	1287	H	-2.29741800	-2.49766300	1.90350400
1244	C	-5.15710900	-1.31176200	-2.17351800	1288	H	-0.63963900	-3.06611200	2.16336400
1245	C	-5.17795400	-2.70634900	-2.10442500	1289	H	-1.19926800	-1.56946600	2.94641100
1246	C	-3.17447000	-2.68251100	-0.76837400	1290	H	-6.01131200	1.35580500	-1.78027800
1247	C	-4.18898600	-3.39716300	-1.40774200	1291	H	-4.73737400	2.56748700	-2.09270100
1248	O	-4.02239600	0.75813600	-1.56163400	1292	H	-5.05817500	1.28926200	-3.29762400
1249	C	-3.78093600	0.35429100	1.87486000	1293	H	0.18413100	3.94583200	0.03717200
1250	C	-4.43312400	1.19548000	2.77657900	1294	H	-1.47049800	4.51716800	0.39054800
1251	C	-3.96114700	2.49372600	2.95739700	1295	H	-0.34585800	4.12415200	1.72925300
1252	C	-2.18362000	2.09669800	1.36494900	1296	H	5.33184100	-0.34918900	-0.13363800

1297 H 5.42676900 -2.13227700 -0.20425000
1298 H 5.25075900 -1.18023100 -1.71093000
1299 H -0.25219200 2.46972300 3.47292600
1300 H 0.10446300 1.33424800 4.79490500
1301 H 1.41521200 2.34475000 4.10944600
1302 C -0.81279900 1.21435300 -2.94026000
1303 C -0.04314200 2.33927300 -2.57321600
1304 C 1.37095300 2.58387600 -3.08597100
1305 C 2.38945700 1.58290900 -2.50479200
1306 C 3.84350500 1.79675400 -2.97012400
1307 C 4.52079900 3.13367600 -2.61220400
1308 C 4.78646100 3.39430300 -1.11380200
1309 C 3.64178600 4.06392800 -0.33957500
1310 H -1.89579300 1.24447000 -2.87592700
1311 H -0.41699900 0.47775600 -3.64329500
1312 H 2.74060000 3.44052600 -0.30140100
1313 H -0.58276300 3.21480000 -2.20981300
1314 H 1.67662900 3.60144900 -2.81948600
1315 H 1.40796400 2.52720500 -4.18449000
1316 H 2.10226600 0.55922700 -2.79407400
1317 H 2.37396300 1.61710300 -1.39536500
1318 H 3.85580400 1.68595500 -4.06331100
1319 H 4.45761600 0.97768200 -2.57429000
1320 H 3.95430500 3.97404700 -3.03593900
1321 H 5.48438900 3.13935700 -3.13742000
1322 H 5.66792700 4.04199200 -1.02854200
1323 H 5.06316400 2.45044000 -0.62114000
1324 H 3.36605300 5.02005900 -0.80125900
1325 H 3.94017400 4.27066000 0.69472800
1326
1327 **1P'**
1328 N 1.14277500 1.41830100 0.65063700
1329 P 1.98786200 0.10606800 -0.11548000
1330 P -0.54989000 1.38393900 0.21984100
1331 Cr -0.31688200 -0.88711200 -1.07882600
1332 C -4.47509700 -3.69222700 -0.53852100
1333 C -3.10209800 -3.35640500 -1.15103400
1334 C -3.07672900 -3.38729600 -2.68778400
1335 C -1.60244200 -0.70250800 -3.05017000
1336 C -1.01169800 -1.90235100 -3.31089600
1337 C -1.68081200 -3.25992600 -3.31845200
1338 C -5.61335600 -2.70464600 -0.84875500
1339 C -5.41063600 -1.30309300 -0.26042700
1340 C 1.60982300 2.09855200 1.87279900

1341 C 3.60270800 0.80918900 -0.63213900
1342 C 2.43489800 -1.06451600 1.23849800
1343 C -0.87453600 3.02813700 -0.53329700
1344 C -1.45373800 1.45040900 1.81687800
1345 C 4.57161200 -0.07391300 -1.16308400
1346 C 5.79162900 0.41367400 -1.64025900
1347 C 6.04584700 1.78711800 -1.61679100
1348 C 3.87509300 2.18205700 -0.64948900
1349 C 5.08938500 2.67557000 -1.13163400
1350 O 4.21455500 -1.39102600 -1.18178200
1351 C 3.38429800 -0.76766900 2.22674500
1352 C 3.68345400 -1.66958400 3.24763300
1353 C 3.03325400 -2.90196600 3.28199300
1354 C 1.80018100 -2.32115100 1.28604900
1355 C 2.09624800 -3.23422400 2.30170000
1356 O 0.88026000 -2.62736600 0.28624500
1357 C 0.13447700 3.96732100 -0.76885400
1358 C -0.13616400 5.17427200 -1.41753100
1359 C -1.43392300 5.44446600 -1.84592800
1360 C -2.18120700 3.31002000 -0.99265000
1361 C -2.45946600 4.51789300 -1.63953700
1362 O -3.10617000 2.33372100 -0.75895600
1363 C -1.79321200 0.24110400 2.46417500
1364 C -2.48618100 0.26207500 3.67985100
1365 C -2.84435000 1.48325800 4.25461600
1366 C -1.83506100 2.65853500 2.41513700
1367 C -2.52408100 2.68553500 3.62741900
1368 O -1.40999500 -0.91872000 1.84001100
1369 C 5.14387300 -2.34698500 -1.68138800
1370 C 0.73372300 -4.01481000 -0.04864500
1371 C -4.46663100 2.58471700 -1.10038400
1372 C -1.73208100 -2.15718900 2.46659000
1373 H -4.36320900 -3.76727400 0.55278200
1374 H -2.76172100 -2.37667600 -0.78118600
1375 H -2.37498700 -4.09270800 -0.77811600
1376 H -3.50096400 -4.34418200 -3.01861900
1377 H -2.64150200 -0.62595900 -2.74070800
1378 H -1.11106600 0.23104500 -3.31937100
1379 H -0.00595700 -1.89007600 -3.73646200
1380 H -4.52017000 -0.80802600 -0.66743300
1381 H -1.74920400 -3.54573200 -4.38016400
1382 H -1.00503100 -4.00798100 -2.87923800
1383 H -3.73594800 -2.61316600 -3.09951500
1384 H -4.77095000 -4.69343200 -0.88123900

1385	H	-6.27371200	-0.66250600	-0.47515900	1429	C	-0.70903200	-2.95723500	3.07986600
1386	H	-5.29380500	-1.34404300	0.82994900	1430	C	0.62561600	-3.02749000	2.90183900
1387	H	-6.54582800	-3.12398600	-0.45037500	1431	C	0.01251400	0.04150700	-2.03877600
1388	H	-5.76124500	-2.63131300	-1.93425600	1432	C	2.58261800	-1.40441100	-0.27115600
1389	H	6.53989000	-0.26227700	-2.03690200	1433	C	2.28417100	1.46264900	-0.01535700
1390	H	6.99573500	2.15666000	-1.99201400	1434	C	-2.18200700	1.54004500	0.03346000
1391	H	3.12685100	2.87656600	-0.28616800	1435	C	-2.57617600	-1.31642800	-0.28975000
1392	H	5.28146700	3.74392600	-1.12675300	1436	C	3.94639600	-1.37187200	0.08885300
1393	H	3.91768700	0.17703900	2.17905100	1437	C	4.80672100	-2.39524700	-0.27613700
1394	H	4.42289100	-1.41588300	4.00089400	1438	C	4.33199500	-3.49459100	-1.01484500
1395	H	3.25538800	-3.61780700	4.06807600	1439	C	2.12041300	-2.51028400	-0.99590000
1396	H	1.60744500	-4.20113200	2.33787900	1440	C	2.97867200	-3.54613600	-1.37516700
1397	H	1.14482600	3.74527900	-0.44456800	1441	O	5.25362800	-4.43613800	-1.32297600
1398	H	0.66010400	5.89287700	-1.58465400	1442	C	2.02539600	2.57483600	0.81104100
1399	H	-1.65933100	6.37921700	-2.35112700	1443	C	2.58825700	3.81330900	0.54895700
1400	H	-3.46118700	4.74207400	-1.98679100	1444	C	3.44086400	3.97883100	-0.55758600
1401	H	-2.75040400	-0.65862900	4.18564900	1445	C	3.13693700	1.64339900	-1.11548900
1402	H	-3.38075700	1.48485100	5.19923000	1446	C	3.71400100	2.88235400	-1.39085000
1403	H	-1.59137300	3.59211900	1.91697600	1447	O	3.94612100	5.22053000	-0.72605500
1404	H	-2.80619700	3.63373900	4.07419200	1448	C	-2.11095800	2.54652700	1.01684900
1405	H	2.68973700	2.25678100	1.82327200	1449	C	-2.63035200	3.81203700	0.79372000
1406	H	1.12909900	3.07690000	1.95827700	1450	C	-3.23956500	4.11546000	-0.43677400
1407	H	1.38106700	1.51945800	2.77469100	1451	C	-2.79914500	1.85719900	-1.18807500
1408	H	6.06801300	-2.34918900	-1.09128900	1452	C	-3.32249300	3.12615300	-1.43035500
1409	H	4.65315500	-3.31684400	-1.58771400	1453	O	-3.71405900	5.37411000	-0.56036800
1410	H	5.38149400	-2.15873100	-2.73537700	1454	C	-3.96203800	-1.10279700	-0.29796400
1411	H	0.21417500	-4.04349200	-1.00646300	1455	C	-4.85193600	-2.10497100	-0.68988900
1412	H	1.71426400	-4.49163200	-0.14360300	1456	C	-4.36252700	-3.35819800	-1.08336900
1413	H	0.13575900	-4.54751300	0.69890200	1457	C	-2.10314300	-2.58946900	-0.66916500
1414	H	-5.01974300	1.69919600	-0.78644800	1458	C	-2.97523500	-3.59066400	-1.06830800
1415	H	-4.85097400	3.46378700	-0.56986900	1459	O	-5.12749300	-4.39829600	-1.48694300
1416	H	-4.58690600	2.72784100	-2.18131600	1460	C	4.84608800	-5.58010000	-2.06710900
1417	H	-1.34571900	-2.92986100	1.80327900	1461	C	4.83265000	5.46444600	-1.81542400
1418	H	-1.24995400	-2.24252500	3.44721800	1462	C	-4.35108300	5.75879300	-1.77636500
1419	H	-2.81624800	-2.27783900	2.57577900	1463	C	-6.54305500	-4.23868200	-1.52086500
1420					1464	H	1.40064000	-0.44359200	5.06470100
1421					1465	H	-1.08979500	-0.34114800	5.20834600
1422	2R				1466	H	-1.06350500	1.35320600	4.47128700
1423	N	0.01684500	-0.23837300	-0.59267400	1467	H	-1.14627600	-2.86600000	4.07165500
1424	P	1.45480000	-0.11611200	0.37788000	1468	H	1.31503500	-2.99393300	3.74245900
1425	P	-1.41339800	-0.07674900	0.39195600	1469	H	1.06650000	-3.20168900	1.92264900
1426	Cr	0.03440000	-0.49221900	2.53886400	1470	H	1.42850100	1.25011800	4.32455300
1427	C	0.84202100	0.39893900	4.66352200	1471	H	-1.40437100	-3.07350100	2.25135300
1428	C	-0.51358700	0.45517000	4.74363600	1472	H	4.34222600	-0.53163600	0.65315900

1473	H	5.85740700	-2.36966900	-0.00549500	1517	C	3.21514700	-1.68722800	-1.28037400
1474	H	1.07681800	-2.56665800	-1.28922100	1518	C	3.86571300	-2.86668400	-1.64083300
1475	H	2.58577200	-4.37703400	-1.94962800	1519	C	1.82995400	2.46472000	-0.60912200
1476	H	1.37079800	2.46461500	1.67292300	1520	C	2.59452900	3.60175200	-0.81831800
1477	H	2.39497900	4.67078900	1.18537900	1521	C	3.97892800	3.58347800	-0.56856600
1478	H	3.37218100	0.80469200	-1.76395800	1522	C	3.80012500	1.26286800	0.09656400
1479	H	4.37144200	2.98366600	-2.24649200	1523	C	4.57900100	2.40328400	-0.10525400
1480	H	-1.64508900	2.32800000	1.97520500	1524	C	-2.01555600	2.77507500	0.59202100
1481	H	-2.58410200	4.58660200	1.55239200	1525	C	-2.60001400	3.98757000	0.26241800
1482	H	-2.89065300	1.10156000	-1.96258200	1526	C	-3.43461200	4.08396800	-0.86640600
1483	H	-3.79250600	3.33391100	-2.38446700	1527	C	-3.07595500	1.73104600	-1.30802800
1484	H	-4.36648100	-0.14034100	-0.00028900	1528	C	-3.66971900	2.94399600	-1.65275100
1485	H	-5.91559800	-1.89734100	-0.68778500	1529	C	-1.96960700	-2.51623100	-0.61742700
1486	H	-1.03650800	-2.79340200	-0.65927500	1530	C	-2.79884300	-3.60428500	-0.83991300
1487	H	-2.61193400	-4.56640200	-1.37502700	1531	C	-4.18415400	-3.49976200	-0.61710200
1488	H	0.92699700	-0.35157300	-2.49088700	1532	C	-3.87593600	-1.19202700	0.04539300
1489	H	-0.83926900	-0.46366500	-2.50453700	1533	C	-4.71940400	-2.28302700	-0.16902600
1490	H	-0.04998700	1.11629400	-2.24538800	1534	H	2.57405900	-4.93647500	0.73164600
1491	H	5.74291900	-6.18824000	-2.18925400	1535	H	3.42051200	-0.78466700	-1.84817400
1492	H	4.08524000	-6.15685500	-1.52665200	1536	H	4.54988700	-2.86006900	-2.48120600
1493	H	4.46020400	-5.29728300	-3.05433500	1537	H	0.76154500	2.50732200	-0.80015300
1494	H	5.10676600	6.51724500	-1.74211200	1538	H	2.14663900	4.52305900	-1.17665000
1495	H	5.73510600	4.84589500	-1.73971000	1539	H	5.64279200	2.36018400	0.09666400
1496	H	4.34022500	5.28145300	-2.77819600	1540	H	-2.43536800	4.87712700	0.86163200
1497	H	-4.64215500	6.80058900	-1.63927200	1541	H	-3.27967200	0.85893800	-1.92230700
1498	H	-3.66406100	5.68059400	-2.62762600	1542	H	-4.31003700	2.99276200	-2.52566500
1499	H	-5.24485300	5.15232000	-1.96655400	1543	H	-0.90238500	-2.62172100	-0.79089600
1500	H	-6.93955200	-5.19264600	-1.86981300	1544	H	-2.40210600	-4.55246300	-1.18831700
1501	H	-6.94331600	-4.02000400	-0.52327700	1545	H	-5.78238800	-2.17359100	0.01084600
1502	H	-6.83783100	-3.44426400	-2.21745500	1546	H	0.09937800	0.92628200	-2.66521500
1503					1547	H	0.82529300	-0.70099400	-2.62983700
1504	2SC1				1548	H	-0.93463800	-0.52605600	-2.62946400
1505	N	-0.00303600	-0.09398700	-0.79409400	1549	C	2.09930400	-0.03799100	3.18061000
1506	P	1.36529400	-0.16475000	0.25269200	1550	H	2.58589400	-0.96173000	2.87621600
1507	P	-1.36261000	0.08276900	0.25038300	1551	H	2.53917700	0.87687800	2.78975800
1508	Cr	0.00002100	-0.05967300	2.36062000	1552	C	1.30123000	-0.00611800	4.30765600
1509	C	-0.00268200	-0.08742300	-2.26177500	1553	H	1.15252200	-0.89951000	4.90489700
1510	C	2.32158400	-1.64743700	-0.19736500	1554	H	1.10653900	0.93397900	4.81426200
1511	C	2.42029200	1.26583300	-0.15966300	1555	C	-1.30626100	-0.14624600	4.30423900
1512	C	-2.24021800	1.61946200	-0.18475200	1556	H	-1.11174900	-1.09403300	4.79631900
1513	C	-2.49408500	-1.28176400	-0.18195000	1557	H	-1.15923700	0.73780200	4.91566300
1514	C	2.09780400	-2.83997000	0.52242200	1558	C	-2.10165500	-0.09758400	3.17606200
1515	C	2.73774900	-4.01881600	0.17613000	1559	H	-2.58870100	0.83029900	2.88499600
1516	C	3.62989800	-4.04376500	-0.91230900	1560	H	-2.53976500	-1.00617800	2.76923800

1561 H -1.37454100 2.72352100 1.46955000
1562 H 4.28856300 0.35937300 0.44982900
1563 H -4.31422500 -0.25832700 0.38543200
1564 H 1.41328300 -2.84334000 1.36807500
1565 O -3.95808600 5.30479100 -1.10321300
1566 O 4.63258600 4.74257500 -0.80474700
1567 O 4.20469400 -5.23712400 -1.16855600
1568 O -4.90314800 -4.61719500 -0.86309900
1569 C 6.03723300 4.80303800 -0.56978100
1570 H 6.57812500 4.09330000 -1.20753200
1571 H 6.33534000 5.82032000 -0.82495400
1572 H 6.27341700 4.60647500 0.48308900
1573 C -4.82322100 5.48421400 -2.22320900
1574 H -5.11627900 6.53409200 -2.20277200
1575 H -4.30421700 5.26778200 -3.16464700
1576 H -5.71635600 4.85356900 -2.13966600
1577 C -6.31307500 -4.59075600 -0.65468900
1578 H -6.79748500 -3.85208200 -1.30485300
1579 H -6.66791400 -5.58903500 -0.91229200
1580 H -6.55641300 -4.37558100 0.39287500
1581 C 5.12871400 -5.34474600 -2.25011700
1582 H 5.45473600 -6.38503600 -2.25554800
1583 H 4.64913900 -5.10682300 -3.20713500
1584 H 5.99550400 -4.69062900 -2.09784400
1585

1586 **2TS1**

1587 N -0.00281300 -0.09150800 -0.83476600
1588 P 1.36795600 -0.16040300 0.21083900
1589 P -1.36508800 0.08092000 0.20909900
1590 Cr 0.00071800 -0.06135700 2.30894600
1591 C -0.00481100 -0.08651500 -2.30299700
1592 C 2.35035000 -1.61629600 -0.26044200
1593 C 2.40397900 1.29501700 -0.15241100
1594 C -2.27044700 1.59244100 -0.24743400
1595 C -2.47739100 -1.31106100 -0.17580000
1596 C 2.12453000 -2.83476900 0.41374700
1597 C 2.78949900 -3.99229800 0.04424500
1598 C 3.70957100 -3.96849300 -1.02086700
1599 C 3.27204700 -1.60665400 -1.32021200
1600 C 3.94807800 -2.76442800 -1.70292500
1601 C 1.81375700 2.48281500 -0.62883700
1602 C 2.56708500 3.63408100 -0.79906200
1603 C 3.93725600 3.64018700 -0.48112700
1604 C 3.76900800 1.31580300 0.17270500

1605 C 4.53548700 2.47012900 0.01068200
1606 C -2.03751200 2.77586900 0.48363800
1607 C -2.64644300 3.96914300 0.12989100
1608 C -3.51476500 4.01715000 -0.97648100
1609 C -3.14004200 1.65502700 -1.34852200
1610 C -3.75885100 2.84838900 -1.71638600
1611 C -1.94765600 -2.53474400 -0.63306500
1612 C -2.76477900 -3.63909900 -0.81852200
1613 C -4.14034100 -3.56106300 -0.53458700
1614 C -3.84905700 -1.24721600 0.11335400
1615 C -4.67919600 -2.35436700 -0.06310300
1616 H 2.62520200 -4.93032900 0.56441800
1617 H 3.47900900 -0.68227300 -1.85110200
1618 H 4.65374600 -2.72024600 -2.52413900
1619 H 0.75539600 2.50609400 -0.87157400
1620 H 2.12083800 4.54768600 -1.17851600
1621 H 5.58848000 2.44666300 0.26552800
1622 H -2.47627700 4.88051200 0.69373100
1623 H -3.35042200 0.75971700 -1.92601000
1624 H -4.42510800 2.85981600 -2.57097700
1625 H -0.88710200 -2.61971100 -0.85229700
1626 H -2.36550200 -4.57972400 -1.18405300
1627 H -5.73501800 -2.26609800 0.16431400
1628 H 0.83662500 -0.68145200 -2.67100200
1629 H -0.92726100 -0.54607900 -2.66928800
1630 H 0.07355500 0.92869200 -2.70782900
1631 C 1.79531500 -0.24004600 3.29920500
1632 H 2.34899700 -1.12689000 2.99221800
1633 H 2.38830000 0.67461700 3.23551400
1634 C 0.91613700 -0.38271700 4.45700700
1635 H 0.78105500 -1.41396000 4.78242100
1636 H 1.13639300 0.26710300 5.30131800
1637 C -0.92027800 0.21053200 4.46215300
1638 H -1.14310700 -0.46018200 5.28929400
1639 H -0.78539800 1.23320900 4.81358400
1640 C -1.79612100 0.09726100 3.29876400
1641 H -2.34772000 0.99209400 3.01162300
1642 H -2.39026300 -0.81454600 3.21060200
1643 H 4.25435500 0.42077000 0.55123500
1644 H -1.37249400 2.76076100 1.34392500
1645 H -4.28880300 -0.32206100 0.47449600
1646 H 1.42064600 -2.87456200 1.24183100
1647 O 4.58096300 4.81136300 -0.68350300
1648 O -4.06011300 5.22304900 -1.23890200

1649 O -4.84801200 -4.69248000 -0.74820400
1650 O 4.30717200 -5.14487700 -1.30204500
1651 C 5.97091100 4.89646800 -0.37950400
1652 H 6.55530600 4.19755200 -0.99026800
1653 H 6.26301600 5.91932900 -0.61889000
1654 H 6.15845000 4.70242700 0.68358900
1655 C -4.95993100 5.35392200 -2.33807600
1656 H -5.26503700 6.40054500 -2.34494400
1657 H -4.46623900 5.11077100 -3.28657400
1658 H -5.84245700 4.71660300 -2.20634800
1659 C -6.24751400 -4.69286000 -0.47773200
1660 H -6.77430800 -3.96411000 -1.10577200
1661 H -6.59422200 -5.69795500 -0.71946800
1662 H -6.44851900 -4.48156700 0.57957000
1663 C 5.26023600 -5.20362800 -2.36194100
1664 H 5.60036500 -6.23891000 -2.39410900
1665 H 4.80239800 -4.93910900 -3.32261300
1666 H 6.11381000 -4.54415600 -2.16476700
1667

1668 **2INT1**

1669 N -0.15196500 -0.36722900 -0.70002300
1670 P 1.32147000 0.02080400 0.10734400
1671 P -1.48322400 -0.35403700 0.43580200
1672 Cr 0.40994200 -0.48096400 2.34301600
1673 C 1.91619600 -0.17041200 3.67547800
1674 C 2.53257900 -1.54266100 3.97890300
1675 C 0.73663300 -2.49233700 2.52575300
1676 C 1.42643700 -2.60890600 3.88799100
1677 C -0.33317400 -0.20578400 -2.15340000
1678 C 2.60364600 -1.01254900 -0.65457100
1679 C 1.80401200 1.74420200 -0.20109900
1680 C -2.46848900 1.15440200 0.16020400
1681 C -2.54101000 -1.74199600 -0.09776600
1682 C 3.94660800 -0.60369900 -0.64285100
1683 C 4.95905200 -1.43319000 -1.12265100
1684 C 4.63948900 -2.70361300 -1.62666700
1685 C 2.29966400 -2.29772000 -1.14914700
1686 C 3.29655100 -3.12601300 -1.63712000
1687 C 1.68711500 2.68437100 0.83303900
1688 C 1.99543400 4.02942300 0.63500400
1689 C 2.42734600 4.45924300 -0.62920000
1690 C 2.24946100 2.19150300 -1.46445700
1691 C 2.55189200 3.52540200 -1.67695400
1692 C -2.44916300 2.15502600 1.15252400

1693 C -3.13578100 3.34761000 0.98787500
1694 C -3.86642700 3.58178200 -0.19072800
1695 C -3.21132400 1.39944700 -1.00743700
1696 C -3.90179900 2.59568400 -1.19103300
1697 C -1.95416400 -2.97075100 -0.46505200
1698 C -2.73446000 -4.07545500 -0.76370700
1699 C -4.13720500 -3.99623000 -0.68199300
1700 C -3.93929500 -1.67947900 -0.00759800
1701 C -4.73600700 -2.78866900 -0.29608600
1702 H 2.65268200 0.61305000 3.46241000
1703 H 3.30621800 -1.76784400 3.23190000
1704 H 3.02678500 -1.56913700 4.96066200
1705 H -0.22451400 -3.01713400 2.44323600
1706 H 0.69670600 -2.44405800 4.69631900
1707 H 1.82306300 -3.62351800 4.04471400
1708 H 1.29850000 0.17433600 4.53428700
1709 H 1.39574400 -2.78374600 1.69868800
1710 H 5.98405200 -1.08251600 -1.10336600
1711 H 1.27081100 -2.64276800 -1.16604000
1712 H 3.06787100 -4.10997600 -2.03337400
1713 H 1.36684800 2.36770700 1.82341100
1714 H 1.90415600 4.72534200 1.46039900
1715 H 2.89559400 3.87882100 -2.64369700
1716 H -3.13115400 4.11510600 1.75494800
1717 H -3.26964300 0.64229500 -1.78373100
1718 H -4.46420200 2.75007100 -2.10441300
1719 H -0.87360300 -3.05931400 -0.52130700
1720 H -2.28676100 -5.01885600 -1.05917700
1721 H -5.81326500 -2.69974100 -0.21951100
1722 H 0.56826100 -0.54090500 -2.67389300
1723 H -1.16676000 -0.83296200 -2.48171100
1724 H -0.53744500 0.83698100 -2.42333700
1725 H -4.42652200 -0.75574700 0.28797400
1726 H -1.89612500 1.99256500 2.07558200
1727 H 2.37318300 1.48594400 -2.28063800
1728 H 4.21582900 0.37678800 -0.26209400
1729 O -4.80629900 -5.12897900 -0.99025700
1730 O -4.49798100 4.77271500 -0.26086200
1731 O 2.75237200 5.73020400 -0.94140800
1732 O 5.53291400 -3.58539200 -2.12048200
1733 C -5.27422700 5.07967300 -1.41756200
1734 H -5.68226000 6.07533000 -1.24200900
1735 H -4.65289200 5.09327100 -2.32109300
1736 H -6.09632300 4.36531800 -1.54497600

1737 C -6.22978000 -5.13138700 -0.91565300
1738 H -6.53813900 -6.13811100 -1.19894700
1739 H -6.57487600 -4.91654000 0.10296900
1740 H -6.66586900 -4.40601700 -1.61332400
1741 C 2.66966800 6.73604800 0.06706800
1742 H 3.34468400 6.51588000 0.90263100
1743 H 2.97941400 7.66282100 -0.41624000
1744 H 1.64319400 6.84202100 0.43805500
1745 C 6.91608800 -3.23606900 -2.13636800
1746 H 7.43091500 -4.09427400 -2.56871700
1747 H 7.09445900 -2.35093600 -2.75862100
1748 H 7.29140500 -3.05708100 -1.12175600
1749

1750 2INT2

1751 N 0.09350600 -0.05758100 -0.89945800
1752 P -1.29863500 0.23930800 0.07324100
1753 P 1.49169600 -0.30260800 0.09749500
1754 Cr -0.07615200 -0.01131500 2.26697700
1755 C -0.71295800 -1.93147800 2.65692300
1756 C -2.08152300 -1.82987300 3.32942100
1757 C -1.60656600 0.61606600 3.53319100
1758 C -2.07643700 -0.63344700 4.29383900
1759 C 2.21223200 0.01020800 3.51382800
1760 C 1.33606600 0.52041400 4.40032100
1761 C 0.11475500 0.04765200 -2.36704400
1762 C -1.97485300 1.87818400 -0.33924400
1763 C -2.54727100 -0.96965500 -0.46586400
1764 C 2.34423600 -1.78854700 -0.51849200
1765 C 2.62057200 1.09365800 -0.25763200
1766 C -1.70614000 2.96277500 0.52176400
1767 C -2.13838200 4.24389500 0.21827100
1768 C -2.85947600 4.48292800 -0.96614300
1769 C -2.70199400 2.13067300 -1.51442700
1770 C -3.14153700 3.41390000 -1.83306700
1771 C -2.15023400 -2.23111300 -0.95375000
1772 C -3.09075200 -3.19821400 -1.27092200
1773 C -4.46244100 -2.94187400 -1.09088100
1774 C -3.91725600 -0.72675300 -0.28263400
1775 C -4.87154000 -1.69632600 -0.59060700
1776 C 2.15288800 -3.00048500 0.16398000
1777 C 2.73308800 -4.18815500 -0.28055300
1778 C 3.52788600 -4.17948500 -1.43712600
1779 C 3.15323800 -1.79715400 -1.67644400
1780 C 3.73285000 -2.97055400 -2.12988600

1781 C 2.09438300 2.36978800 -0.54584700
1782 C 2.92506600 3.47133000 -0.68396800
1783 C 4.31600900 3.33803700 -0.52153100
1784 C 4.00862000 0.97606000 -0.08688000
1785 C 4.85451900 2.07919800 -0.21751500
1786 H -0.70253500 -2.54796900 1.75093400
1787 H -2.85170200 -1.67177800 2.56266000
1788 H -2.34563000 -2.76525100 3.84632100
1789 H -1.33503100 1.44598200 4.19984100
1790 H -1.39298000 -0.85142900 5.12805000
1791 H -3.06827400 -0.48957100 4.74705700
1792 H 0.06721100 -2.28721700 3.34998400
1793 H 2.81207100 0.65067800 2.87166300
1794 H 2.40921500 -1.05780600 3.45786500
1795 H 1.19173900 1.59276600 4.50366100
1796 H -2.40895500 0.98112700 2.87496300
1797 H 0.78683500 -0.11126500 5.09194400
1798 H -1.94264700 5.07943800 0.88234700
1799 H -2.94307200 1.31549600 -2.19025300
1800 H -3.70067300 3.57200400 -2.74776300
1801 H -1.09589200 -2.45059000 -1.09507500
1802 H -2.79350700 -4.16623800 -1.66113700
1803 H -5.92116700 -1.47240600 -0.44138100
1804 H 2.56694500 -5.10322600 0.27556600
1805 H 3.34156200 -0.87387800 -2.21600700
1806 H 4.35557500 -2.98506200 -3.01858300
1807 H 1.02351900 2.50228700 -0.67266500
1808 H 2.52448500 4.45166600 -0.92158500
1809 H 5.92219700 1.94547300 -0.08858100
1810 H -0.85932200 -0.24395300 -2.76911700
1811 H 0.34933200 1.06522800 -2.69879700
1812 H 0.86202300 -0.64063400 -2.77180600
1813 H 1.54017300 -3.02441000 1.06108300
1814 H 4.45107700 0.00983300 0.13868000
1815 H -1.16541800 2.79828900 1.45090300
1816 H -4.25619800 0.23219200 0.09827000
1817 O 4.13965600 -5.26211900 -1.96099100
1818 O -5.29571200 -3.95043900 -1.42812500
1819 O -3.23628900 5.76167900 -1.17272100
1820 O 5.03654000 4.47137900 -0.67808100
1821 C 3.98870300 -6.52456200 -1.31467400
1822 H 4.56354200 -7.23182900 -1.91293500
1823 H 4.38930700 -6.49844700 -0.29421200
1824 H 2.93728300 -6.83531500 -1.29121300

1825 C -6.70043800 -3.76989900 -1.26492400
1826 H -7.07000200 -2.94455400 -1.88553800
1827 H -7.15761900 -4.70372600 -1.59320200
1828 H -6.95830900 -3.58600500 -0.21495500
1829 C -3.98342700 6.08547000 -2.34418000
1830 H -4.16937000 7.15815200 -2.28670800
1831 H -3.41297600 5.86144700 -3.25350800
1832 H -4.93961900 5.54923300 -2.36558000
1833 C 6.45336000 4.41268400 -0.53496100
1834 H 6.90067700 3.73968300 -1.27656900
1835 H 6.80952400 5.42900500 -0.70562700
1836 H 6.73876900 4.09061700 0.47401200

1837
1838 **2TS2**
1839 N 0.06826100 -0.20991400 -0.84492600
1840 P -1.39385000 -0.09466200 0.06492600
1841 P 1.45254700 -0.08307000 0.19448900
1842 Cr -0.26642700 -0.04272000 2.35590700
1843 C -1.95415900 0.29918000 3.48943600
1844 C -1.62425600 1.53394400 4.33450200
1845 C 0.78150900 0.92250900 3.96753400
1846 C -0.24945000 1.36051100 4.99793400
1847 C 0.90396600 -1.39930400 3.93613100
1848 C 0.12628600 -2.06491600 2.98951600
1849 C 0.13859500 -0.24338400 -2.31404900
1850 C -2.17519000 1.50110300 -0.35894800
1851 C -2.52507800 -1.38290600 -0.54035100
1852 C 2.43080200 -1.59261600 -0.14525200
1853 C 2.48377200 1.29162600 -0.42246200
1854 C -3.54836800 1.71885900 -0.11914100
1855 C -4.11679400 2.96690900 -0.31953000
1856 C -3.32810400 4.04466000 -0.76224800
1857 C -1.39614700 2.58680900 -0.78318400
1858 C -1.95893000 3.84684500 -0.99311800
1859 O -3.98063000 5.21654300 -0.93291000
1860 C -2.54840300 -2.62703400 0.12362900
1861 C -3.35357800 -3.66174600 -0.32313600
1862 C -4.17029800 -3.48287500 -1.45530300
1863 C -3.34739000 -1.21654600 -1.66695800
1864 C -4.16338400 -2.24935900 -2.12639700
1865 O -4.92069600 -4.54763400 -1.80768200
1866 C 1.80448600 -2.77902200 -0.55338300
1867 C 2.52191100 -3.96835400 -0.69989600
1868 C 3.89546800 -3.99124400 -0.41854500

1869 C 3.81070500 -1.63517900 0.14379700
1870 C 4.53171200 -2.81155600 0.00885300
1871 O 4.69020100 -5.08053200 -0.52527200
1872 C 2.43087800 2.52938300 0.25150900
1873 C 3.15382400 3.62463100 -0.19516700
1874 C 3.96306900 3.51510300 -1.34034100
1875 C 3.30114400 1.19727600 -1.56111500
1876 C 4.03406200 2.28922300 -2.02243200
1877 O 4.62958700 4.63430900 -1.69549700
1878 C -3.24926100 6.35475100 -1.37881100
1879 C -5.79231500 -4.44108100 -2.93179600
1880 C 4.11801300 -6.31065400 -0.95969800
1881 C 5.49044700 4.59667700 -2.83210100
1882 H -2.84074800 0.44557300 2.86074800
1883 H -1.60058700 2.43135700 3.69658300
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1885 H 1.79751200 0.83678100 4.35446100
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1887 H 0.07664000 2.29303600 5.48264900
1888 H -2.12457200 -0.58185700 4.12360200
1889 H 0.60912700 -2.51651800 2.12496600
1890 H -0.84876200 -2.45534300 3.26898100
1891 H 1.97659900 -1.32734400 3.79016400
1892 H 0.83116800 1.65245900 3.12095800
1893 H 0.55865800 -1.28899300 4.95808500
1894 H -4.18086400 0.90262500 0.21796500
1895 H -5.17387500 3.13806500 -0.14354600
1896 H -0.33242500 2.45788300 -0.96055800
1897 H -1.32782000 4.65877000 -1.33514500
1898 H -1.93286500 -2.77952000 1.00567200
1899 H -3.38279600 -4.61821300 0.18864500
1900 H -3.36778800 -0.26491400 -2.18980300
1901 H -4.78831500 -2.08543500 -2.99641300
1902 H 0.74044100 -2.78162000 -0.77440800
1903 H 2.00628300 -4.86110500 -1.03423100
1904 H 4.32978900 -0.73655300 0.46556000
1905 H 5.59524300 -2.84660400 0.22220900
1906 H 1.81885800 2.63528400 1.14413100
1907 H 3.12151600 4.57554900 0.32671300
1908 H 3.38387000 0.25443800 -2.09365000
1909 H 4.65530500 2.17807700 -2.90356400
1910 H 0.25115700 0.75981400 -2.74030900
1911 H 0.98643900 -0.85942900 -2.62706200
1912 H -0.77234300 -0.69859500 -2.71257900

1913	H	-3.97541600	7.16563500	-1.44312900
1914	H	-2.46133500	6.62654100	-0.66556000
1915	H	-2.80675600	6.18172700	-2.36753900
1916	H	-6.28798800	-5.40880000	-3.01210900
1917	H	-6.54352800	-3.65717200	-2.77837200
1918	H	-5.23107300	-4.24035600	-3.85230900
1919	H	4.93718200	-7.03027000	-0.96980000
1920	H	3.33914700	-6.65436300	-0.26785500
1921	H	3.69921800	-6.22030600	-1.96955000
1922	H	5.91618700	5.59721600	-2.91188600
1923	H	6.29664500	3.86614600	-2.69526100
1924	H	4.93178300	4.36314100	-3.74648600
1925				
1926	2INT3			
1927	N	-0.06662900	0.22666400	-0.87403000
1928	P	1.08551100	1.01418500	0.16329600
1929	P	-1.13435200	-0.80538800	0.00609500
1930	Cr	-0.18322400	-0.12946500	2.23188900
1931	C	-1.53346300	-0.10903300	3.72056200
1932	C	-0.40001400	0.44434900	4.56276400
1933	C	0.54796900	-1.88856400	5.23106500
1934	C	0.16353900	-0.46350800	5.66743100
1935	C	0.75073000	-1.89607700	2.65290800
1936	C	1.47118200	-1.96987300	3.99948300
1937	C	-0.08326500	0.37573600	-2.33871600
1938	C	2.75811700	0.66959000	-0.47137800
1939	C	0.81957600	2.80108100	-0.12534000
1940	C	-2.83290000	-0.40512400	-0.50089100
1941	C	-0.82569900	-2.51028600	-0.55338200
1942	C	3.27044000	1.24547400	-1.64635900
1943	C	4.54235100	0.92460500	-2.11601000
1944	C	5.33850600	0.01185400	-1.40367800
1945	C	3.57395600	-0.23966600	0.23311200
1946	C	4.84224900	-0.56594000	-0.22132800
1947	O	6.58328600	-0.36750800	-1.76258900
1948	C	1.85499600	3.73166500	0.09881000
1949	C	1.62002800	5.09466200	0.00571900
1950	C	0.33708000	5.57560300	-0.31238000
1951	C	-0.45917000	3.29295900	-0.42518400
1952	C	-0.70565600	4.66293500	-0.52894300
1953	O	0.21648800	6.92064400	-0.38573000
1954	C	-3.56338200	0.53764800	0.25249700
1955	C	-4.83747500	0.92518700	-0.12836300
1956	C	-5.42810300	0.37531900	-1.28198700

1957	C	-3.43598400	-0.94979000	-1.64656800
1958	C	-4.71794800	-0.56962500	-2.04002200
1959	O	-6.67156800	0.81356100	-1.56728700
1960	C	-1.78570400	-3.52205300	-0.34340900
1961	C	-1.50657600	-4.84226700	-0.65924400
1962	C	-0.25286300	-5.19606500	-1.19119300
1963	C	0.42591800	-2.87667100	-1.06662000
1964	C	0.71571100	-4.20167800	-1.39360500
1965	O	-0.08458400	-6.50754500	-1.47047300
1966	C	7.16967400	0.19547800	-2.93450800
1967	C	-1.05377700	7.48246300	-0.70164300
1968	C	-7.34818300	0.28759500	-2.70825000
1969	C	1.16264100	-6.94541700	-2.00285900
1970	H	-2.34517200	0.60449400	3.54145900
1971	H	0.50475900	0.70112000	3.89826600
1972	H	-0.63350300	1.43821700	4.96214500
1973	H	-0.35550100	-2.48131400	5.03552400
1974	H	-0.58526500	-0.52342300	6.46706400
1975	H	1.04397700	0.02826700	6.10196100
1976	H	-1.92583500	-1.07649300	4.03555900
1977	H	1.44224300	-2.01913400	1.80745100
1978	H	-0.03068500	-2.66274400	2.57162600
1979	H	2.25529100	-1.19931200	4.06793800
1980	H	1.04142200	-2.36852900	6.08437700
1981	H	2.00823100	-2.93061400	4.03828600
1982	H	2.67990000	1.96930500	-2.20045500
1983	H	4.90645900	1.39016000	-3.02441100
1984	H	3.21343500	-0.68764700	1.15492400
1985	H	5.47725500	-1.25785600	0.32235500
1986	H	2.85674300	3.38747900	0.33892400
1987	H	2.41545300	5.81436800	0.17020600
1988	H	-1.28071900	2.60247000	-0.59649500
1989	H	-1.70313900	5.00473100	-0.77947200
1990	H	-3.13080900	0.96212600	1.15497200
1991	H	-5.40830000	1.64249500	0.45232000
1992	H	-2.90858400	-1.69319000	-2.23664600
1993	H	-5.15378300	-1.01303200	-2.92746700
1994	H	-2.76232900	-3.27518500	0.06328400
1995	H	-2.24269100	-5.62479400	-0.50640900
1996	H	1.19364900	-2.12334800	-1.21781300
1997	H	1.68999400	-4.44677600	-1.79993400
1998	H	0.63476000	-0.29530800	-2.82270700
1999	H	-1.08479400	0.15847000	-2.71996200
2000	H	0.15825400	1.40881200	-2.60375900

2001	H	8.16212700	-0.24960800	-3.00949900	2045	C	-3.70249900	0.35463800	-1.46412800
2002	H	6.58825600	-0.05500400	-3.83003000	2046	C	-4.76404600	1.17795900	-1.83762600
2003	H	7.26318100	1.28455600	-2.84757800	2047	O	-5.95545800	3.27282600	-1.45264600
2004	H	-0.90656400	8.56288800	-0.70413100	2048	C	-3.05558500	-2.53567500	0.05933800
2005	H	-1.39771000	7.15893600	-1.69185600	2049	C	-3.35295000	-3.87618600	-0.12802000
2006	H	-1.80492800	7.21834600	0.05295600	2050	C	-2.41643400	-4.73431100	-0.73365500
2007	H	-8.32083400	0.77968300	-2.72558800	2051	C	-0.88429500	-2.87251500	-0.94017500
2008	H	-6.80529600	0.51761600	-3.63285400	2052	C	-1.17526900	-4.22314900	-1.13967600
2009	H	-7.48807300	-0.79637900	-2.62114200	2053	O	-2.80834200	-6.02027500	-0.87650000
2010	H	1.06233700	-8.02224300	-2.14162500	2054	C	6.46844400	-2.95756200	-3.02703400
2011	H	1.37166100	-6.47062400	-2.96932600	2055	C	2.17408400	7.16320300	-1.06245600
2012	H	1.98555700	-6.74203400	-1.30673600	2056	C	-6.89484100	2.95308200	-2.47755200
2013					2057	C	-1.91652000	-6.95013700	-1.48475600
2014	2TS3				2058	H	-2.65287800	0.42488300	2.84961000
2015	N	-0.08039200	0.17636400	-1.02593900	2059	H	0.39229700	0.39101400	3.69215500
2016	P	1.29986300	0.43511700	-0.02220200	2060	H	-1.07464700	1.34325600	4.41898200
2017	P	-1.37175900	-0.27657800	0.02673600	2061	H	0.72525600	-2.15370500	4.51681000
2018	Cr	-0.06142600	0.05452300	2.11645400	2062	H	-1.30544000	-1.27988600	5.61527900
2019	C	-1.84150700	-0.21961200	3.18041600	2063	H	-0.41641200	0.09596800	6.25603600
2020	C	-0.91588100	0.28956900	4.17202500	2064	H	-2.11341800	-1.27634200	3.22593900
2021	C	0.83540400	-1.33155700	5.24223500	2065	H	2.42052200	0.90168600	3.06937300
2022	C	-0.49901000	-0.57258100	5.39079300	2066	H	2.18684600	-0.81584100	2.68034600
2023	C	1.83938200	0.00856900	3.31747800	2067	H	2.00434700	0.47814600	5.44051600
2024	C	1.98477700	-0.41074800	4.79444000	2068	H	1.07548100	-1.80222000	6.20221200
2025	C	-0.11440900	0.23523100	-2.49337500	2069	H	2.94806600	-0.91700000	4.93760400
2026	C	2.65636800	-0.62003400	-0.62793500	2070	H	3.39413500	0.73379800	-2.14272800
2027	C	1.83656100	2.15412400	-0.32615000	2071	H	5.11750300	-0.78260200	-2.98633000
2028	C	-2.82050700	0.72254900	-0.43560000	2072	H	2.19826300	-2.22054000	0.76343200
2029	C	-1.81585500	-2.00477400	-0.35447200	2073	H	3.95555600	-3.74395300	-0.08465400
2030	C	3.49834300	-0.24642000	-1.68762300	2074	H	3.87740300	1.84835100	0.34966300
2031	C	4.48477800	-1.10582900	-2.16806200	2075	H	4.51725100	4.22829600	0.15157000
2032	C	4.64771900	-2.37405600	-1.58729500	2076	H	-0.09941000	2.83692900	-0.99882800
2033	C	2.83373000	-1.89814000	-0.05764500	2077	H	0.55065500	5.18656300	-1.21648800
2034	C	3.80992000	-2.76319600	-0.52565600	2078	H	-2.37404800	2.26442800	1.02230800
2035	O	5.56931600	-3.28338800	-1.96843000	2079	H	-4.26219400	3.72659000	0.36075200
2036	C	3.14149300	2.57173300	0.01014100	2080	H	-3.57226700	-0.59351800	-1.97701400
2037	C	3.51275100	3.90264400	-0.09866300	2081	H	-5.42732400	0.86048400	-2.63357100
2038	C	2.58792700	4.86492700	-0.54378100	2082	H	-3.79884800	-1.89265600	0.52246000
2039	C	0.91825000	3.12489700	-0.75026900	2083	H	-4.30765400	-4.28921900	0.18124900
2040	C	1.28319400	4.46678700	-0.87013900	2084	H	0.08648100	-2.49835300	-1.25135400
2041	O	3.05271400	6.13204400	-0.62124500	2085	H	-0.43587800	-4.86131800	-1.60921700
2042	C	-3.03620000	1.95412400	0.21749900	2086	H	0.17326700	-0.71966500	-2.94726900
2043	C	-4.08632900	2.78213200	-0.14391500	2087	H	-1.12466500	0.49450300	-2.82404300
2044	C	-4.96260500	2.40116700	-1.17776200	2088	H	0.56694700	1.01455700	-2.84627500

2089 H 7.11197300 -3.82967800 -3.14491100
2090 H 5.92888100 -2.77212400 -3.96351300
2091 H 7.07996600 -2.08350500 -2.77338100
2092 H 2.76285200 8.08076300 -1.04361100
2093 H 1.82210800 6.97619700 -2.08442600
2094 H 1.31372200 7.26784500 -0.39008700
2095 H -7.59079800 3.79163000 -2.51031200
2096 H -6.40044800 2.84979500 -3.45094600
2097 H -7.44202100 2.03272900 -2.24113700
2098 H -2.44437800 -7.90421300 -1.49121400
2099 H -1.67809100 -6.65803700 -2.51486100
2100 H -0.98969200 -7.05000200 -0.90655500
2101

2102 **2SC2**

2103 N -0.17798800 0.21980000 -0.97603300
2104 P 1.20080700 0.62413000 -0.01523800
2105 P -1.37518100 -0.41620200 0.10074400
2106 Cr -0.02961700 -0.06708100 2.08982500
2107 C -1.77834200 -0.68672300 3.23394500
2108 C -0.68406800 -0.45882300 4.08222600
2109 C 1.61569200 -1.65132500 4.51598700
2110 C 0.08957700 -1.58669800 4.75205700
2111 C 2.38074300 0.66150600 3.68847600
2112 C 2.39835500 -0.36271200 4.82876700
2113 C -0.26994400 0.32706600 -2.43794400
2114 C 2.65108500 -0.25437700 -0.68167900
2115 C 1.51713600 2.39810700 -0.31730800
2116 C -2.93488600 0.44756200 -0.26158000
2117 C -1.64332100 -2.16075100 -0.36330700
2118 C 3.33874700 0.15751800 -1.83517700
2119 C 4.40520000 -0.58011000 -2.34623100
2120 C 4.80897200 -1.76075800 -1.70092000
2121 C 3.07249400 -1.44132200 -0.04694900
2122 C 4.13153200 -2.18488400 -0.54310000
2123 O 5.82692100 -2.55021500 -2.10375700
2124 C 2.79619500 2.95508800 -0.11162400
2125 C 3.00275000 4.32178100 -0.21706300
2126 C 1.93340500 5.18076100 -0.52915400
2127 C 0.45603300 3.26577400 -0.61359800
2128 C 0.65365900 4.64244500 -0.72912900
2129 O 2.24229400 6.49434100 -0.61325400
2130 C -3.25681600 1.60549100 0.47660700
2131 C -4.39776600 2.33945700 0.19595400
2132 C -5.26183000 1.93359200 -0.83865100

2133 C -3.80608000 0.05323400 -1.28939800
2134 C -4.95871200 0.78163300 -1.58155800
2135 O -6.34827100 2.71099700 -1.03160700
2136 C -2.82268900 -2.83696500 0.01388200
2137 C -2.97483400 -4.19285100 -0.23034400
2138 C -1.94766500 -4.92217700 -0.85666800
2139 C -0.62017800 -2.90170500 -0.97101600
2140 C -0.76430100 -4.26640900 -1.22651300
2141 O -2.19883300 -6.23600300 -1.05439400
2142 C 6.57867800 -2.17922500 -3.25796900
2143 C 1.21044500 7.42692200 -0.92271200
2144 C -7.28193500 2.35601500 -2.04996100
2145 C -1.20470300 -7.04071500 -1.68164100
2146 H -2.56326100 0.05882600 3.12355100
2147 H 1.35937200 1.04208500 3.49188300
2148 H -0.64368600 0.50946900 4.58961700
2149 H 1.81980000 -1.94740700 3.47171100
2150 H -0.34512200 -2.54551700 4.44091000
2151 H -0.08158600 -1.51452400 5.83628200
2152 H -2.07730600 -1.70562000 2.98990500
2153 H 2.97145000 1.55504600 3.91858800
2154 H 2.79231900 0.23054700 2.76764400
2155 H 2.01280600 0.09246300 5.75066400
2156 H 2.00809200 -2.47134300 5.12979100
2157 H 3.44553100 -0.61876100 5.03082600
2158 H 3.05099000 1.07472800 -2.34073000
2159 H 4.91435700 -0.23118100 -3.23701600
2160 H 2.56500000 -1.78654800 0.85135500
2161 H 4.46402400 -3.09437300 -0.05332500
2162 H 3.64103500 2.31396900 0.12280800
2163 H 3.98640300 4.75490300 -0.06685600
2164 H -0.54351100 2.86785000 -0.76564700
2165 H -0.18756300 5.28048800 -0.97370900
2166 H -2.60581200 1.93017400 1.28503000
2167 H -4.65525300 3.22609300 0.76625600
2168 H -3.59527100 -0.84259400 -1.86581700
2169 H -5.61056200 0.44552200 -2.37927700
2170 H -3.63417900 -2.29662300 0.49294600
2171 H -3.88300400 -4.71627200 0.05066700
2172 H 0.30839900 -2.41535600 -1.25589900
2173 H 0.04302300 -4.80347900 -1.71066500
2174 H 0.15100300 -0.55202400 -2.93902200
2175 H -1.31903100 0.43270600 -2.72909400
2176 H 0.26489800 1.21929800 -2.77676600

2177	H	7.33636400	-2.95410300	-3.37675200	2221	C	4.09177200	-0.67224300	-0.75810900
2178	H	5.94466500	-2.14786200	-4.15220100	2222	C	5.11122900	-1.59513600	-0.98908900
2179	H	7.06795400	-1.20805200	-3.11747700	2223	O	6.04693000	-3.78302300	-0.44334300
2180	H	1.69053600	8.40587500	-0.93236800	2224	C	3.56914300	2.25370800	0.71039400
2181	H	0.77355600	7.22501100	-1.90841800	2225	C	4.01659600	3.56234300	0.61293200
2182	H	0.42146100	7.41475900	-0.16079400	2226	C	3.22615300	4.53848300	-0.01973200
2183	H	-8.06239100	3.11628800	-2.01129300	2227	C	1.53459800	2.85815400	-0.43506700
2184	H	-6.81154400	2.36481800	-3.04055500	2228	C	1.97688800	4.17790800	-0.54433800
2185	H	-7.72200100	1.37007300	-1.85862200	2229	O	3.75726700	5.78243700	-0.06807000
2186	H	-1.62675100	-8.04479200	-1.73324200	2230	C	-4.93076600	3.95472200	-4.05520200
2187	H	-0.98533500	-6.68435400	-2.69563800	2231	C	-2.22796400	-6.76144700	-2.15584100
2188	H	-0.28018500	-7.06327300	-1.09156200	2232	C	7.13301700	-3.56711900	-1.34197700
2189					2233	C	3.01464700	6.82328700	-0.69469200
2190	2P				2234	H	0.68613900	-1.20095000	4.56143500
2191	N	0.50528500	-0.09578200	-0.81200100	2235	H	-3.82571700	-1.96831100	4.49922100
2192	P	-1.10743300	-0.27439800	-0.20425800	2236	H	-1.73157000	-1.41196100	4.26224100
2193	P	1.65748100	0.19005700	0.45355700	2237	H	-3.09755000	0.74404800	2.67627300
2194	Cr	-0.21753300	-0.13921200	2.24631200	2238	H	-1.70996000	1.64249100	4.75903300
2195	C	0.05159500	-0.31568500	4.54765800	2239	H	-2.68812200	0.53698700	5.70364900
2196	C	-1.30628300	-0.42046400	4.41876900	2240	H	0.51982300	0.62097800	4.84916000
2197	C	-3.45669300	0.87544200	3.70915400	2241	H	-5.43187000	-2.06009700	3.78825000
2198	C	-2.27633400	0.70428800	4.69556200	2242	H	-4.03648600	-1.74136000	2.75043100
2199	C	-4.47572700	-1.52871300	3.73397200	2243	H	-5.06282600	0.15354200	4.95903300
2200	C	-4.68425600	-0.02332600	3.94276100	2244	H	-3.79026100	1.91828000	3.78051100
2201	C	0.83078900	-0.06225100	-2.24739800	2245	H	-5.47646200	0.31823300	3.26411800
2202	C	-2.15736300	0.96883600	-1.02990600	2246	H	-2.43270800	-0.07999300	-2.90050500
2203	C	-1.68081800	-1.89016300	-0.84319200	2247	H	-3.74430400	1.68781300	-3.96524100
2204	C	3.05662700	-0.93892700	0.15286000	2248	H	-2.11826200	2.29114400	0.68650900
2205	C	2.32126400	1.87213100	0.17584600	2249	H	-3.45743600	4.07587100	-0.39453700
2206	C	-2.63576900	0.82940700	-2.34276800	2250	H	-3.79208500	-1.38891700	-0.80243500
2207	C	-3.38930100	1.83165200	-2.95147000	2251	H	-4.55375300	-3.65663600	-1.42941100
2208	C	-3.68168800	3.00993300	-2.24524200	2252	H	0.29659300	-2.75067200	-0.95992900
2209	C	-2.46509600	2.15697200	-0.33572100	2253	H	-0.46501400	-4.98697900	-1.60216000
2210	C	-3.21217800	3.16326600	-0.92809300	2254	H	2.29883500	-2.40105100	1.56161900
2211	O	-4.40267500	4.04243800	-2.73336700	2255	H	4.10902100	-4.04448700	1.14970000
2212	C	-3.05679400	-2.17075800	-0.97035200	2256	H	4.11753700	0.27585600	-1.28701900
2213	C	-3.49614800	-3.43774600	-1.32278400	2257	H	5.89575900	-1.35369800	-1.69663300
2214	C	-2.57149700	-4.47126000	-1.55715900	2258	H	4.20216200	1.51894900	1.20006100
2215	C	-0.76971000	-2.93260600	-1.06306300	2259	H	4.97966000	3.85866800	1.01604800
2216	C	-1.20000500	-4.21035700	-1.42531000	2260	H	0.55916200	2.60299500	-0.83948000
2217	O	-3.10312500	-5.66705800	-1.90141200	2261	H	1.34631400	4.90918600	-1.03653600
2218	C	3.07882000	-2.17091600	0.83879700	2262	H	0.72445500	0.94421100	-2.66712800
2219	C	4.08399100	-3.09864800	0.61824600	2263	H	1.85899100	-0.40270000	-2.39835000
2220	C	5.11188900	-2.81915000	-0.30123700	2264	H	0.17013600	-0.74508900	-2.78879400

2265 H -5.47085800 4.88762300 -4.21879400
2266 H -4.12960600 3.86122600 -4.79827000
2267 H -5.62330200 3.10991700 -4.15097600
2268 H -2.87309900 -7.60257900 -2.41161700
2269 H -1.55648100 -6.54798100 -2.99669800
2270 H -1.63554300 -7.01327100 -1.26748600
2271 H 7.74812600 -4.46528400 -1.28128100
2272 H 6.77758900 -3.43648300 -2.37123000
2273 H 7.72809600 -2.69573900 -1.04356400
2274 H 3.63360100 7.71754400 -0.61486800
2275 H 2.83051500 6.60054200 -1.75303500
2276 H 2.05888800 6.99474400 -0.18400000
2277

2278 **2INT4**

2279 N 0.18686800 -0.06533000 -0.99884900
2280 P 1.48916600 -0.38561900 0.10988000
2281 P -1.27780600 0.29158600 -0.16202300
2282 Cr -0.43671500 -0.28883700 2.11316500
2283 C 0.34703100 0.08598600 -2.45416700
2284 C 2.39800300 -1.83039000 -0.53996500
2285 C 2.66708200 1.00675600 -0.10145800
2286 C -2.53995600 -0.80790600 -0.88329900
2287 C -1.81503200 1.97972300 -0.59516000
2288 C 2.22791800 -3.08103400 0.08884600
2289 C 2.86675100 -4.21726700 -0.38273900
2290 C 3.70454300 -4.13987600 -1.50957000
2291 C 3.25212300 -1.76663800 -1.65470000
2292 C 3.89761900 -2.90138900 -2.14320800
2293 O 4.27888900 -5.29996000 -1.89343000
2294 C 2.21037800 2.29236200 -0.45573700
2295 C 3.07672000 3.37598900 -0.49351300
2296 C 4.43346300 3.21314300 -0.16230900
2297 C 4.02173900 0.86059400 0.23437800
2298 C 4.90211500 1.94360500 0.20600900
2299 O 5.19366400 4.33040600 -0.23068300
2300 C -2.17714400 -2.06126900 -1.41490500
2301 C -3.14112300 -2.94671600 -1.87090600
2302 C -4.50572500 -2.61483000 -1.78990200
2303 C -3.90373600 -0.48910700 -0.80194900
2304 C -4.88315100 -1.37712800 -1.24786400
2305 O -5.36467900 -3.54788000 -2.25852000
2306 C -1.58898900 3.03067700 0.31672100
2307 C -1.92838600 4.33802100 0.00586700
2308 C -2.50890700 4.63885500 -1.23967100

2309 C -2.40293800 2.29446100 -1.83173700
2310 C -2.74635400 3.60450000 -2.15988500
2311 O -2.80328200 5.93927700 -1.44919700
2312 C 5.14772000 -5.30251600 -3.02408900
2313 C 6.57919500 4.24031900 0.08874400
2314 C -6.76446700 -3.28716900 -2.20121000
2315 C -3.40672300 6.32396500 -2.68305300
2316 H 1.59434600 -3.16270500 0.96668500
2317 H 2.74209400 -5.17927900 0.10368700
2318 H 3.43710300 -0.81438900 -2.14283900
2319 H 4.54827900 -2.81253000 -3.00532000
2320 H 1.16659200 2.44817000 -0.71306400
2321 H 2.72979800 4.36339600 -0.78126500
2322 H 4.41207800 -0.11476200 0.51189600
2323 H 5.94274400 1.78687000 0.46504200
2324 H -1.12927500 -2.33939300 -1.47812700
2325 H -2.86756800 -3.90769000 -2.29457200
2326 H -4.21834900 0.46663900 -0.39281200
2327 H -5.92688000 -1.09555400 -1.17306400
2328 H -1.15060300 2.81750800 1.28710200
2329 H -1.76460200 5.14827000 0.70894600
2330 H -2.61224100 1.50747900 -2.55000100
2331 H -3.19863400 3.80952300 -3.12311100
2332 H -0.60945900 -0.10165600 -2.94905900
2333 H 0.69871800 1.08761300 -2.72620300
2334 H 1.06233600 -0.65469000 -2.82200800
2335 H 5.47998400 -6.33474200 -3.13742500
2336 H 4.61968300 -4.98683700 -3.93194900
2337 H 6.01723600 -4.65501300 -2.85866400
2338 H 6.97737600 5.24768500 -0.03661900
2339 H 6.72903200 3.91531200 1.12570500
2340 H 7.10092300 3.55475300 -0.59028600
2341 H -7.24643200 -4.16911000 -2.62413800
2342 H -7.10142300 -3.14757200 -1.16678000
2343 H -7.03003800 -2.40526600 -2.79694400
2344 H -3.54896400 7.40286200 -2.61689100
2345 H -2.75428100 6.09277400 -3.53362800
2346 H -4.37864500 5.83479200 -2.81907200
2347 C -1.02136200 -2.22948100 1.99213900
2348 C -0.38236300 -2.40299300 3.34894400
2349 C -1.31695900 -2.68659800 4.53774000
2350 C -2.53712300 -1.75700500 4.66918600
2351 C -2.24044900 -0.24668900 4.59361100
2352 C -2.09603800 0.30920500 3.16768400

2353	H	-2.10572300	-2.32824100	1.96403800	2397	C	-3.45890300	-2.16613100	-2.03820700
2354	H	-0.55384400	-2.78764900	1.18041400	2398	C	-4.74657500	-1.59880500	-2.06138200
2355	H	0.43990900	-3.12880400	3.32349900	2399	C	-3.87590000	0.35297400	-0.92345900
2356	H	0.18696200	-1.45208900	3.64053400	2400	C	-4.94970300	-0.33283100	-1.49440700
2357	H	-1.66585500	-3.72357600	4.45428100	2401	O	-5.70704300	-2.34963200	-2.64553000
2358	H	-0.72337400	-2.63384800	5.46047100	2402	C	2.70084200	2.18153700	0.55170400
2359	H	-3.01298700	-1.98347200	5.63108100	2403	C	3.67825000	3.15584200	0.43623900
2360	H	-3.28341200	-2.00631900	3.90292600	2404	C	4.84441800	2.90255100	-0.30994900
2361	H	-3.06673500	0.28293700	5.09160400	2405	C	4.00481900	0.69145100	-0.82587800
2362	H	-1.34813100	-0.01513700	5.19796600	2406	C	5.00183500	1.66095400	-0.94275600
2363	H	-2.97942300	0.04111600	2.57157600	2407	O	5.74123600	3.91265200	-0.35390600
2364	H	-2.04602700	1.40893200	3.18922900	2408	C	3.22486600	-2.47776600	0.04556800
2365	C	1.46368600	0.84140100	3.79581000	2409	C	3.70167200	-3.70577000	-0.38673100
2366	C	0.90507900	1.87199100	3.13865800	2410	C	3.10687900	-4.35043100	-1.48734000
2367	H	2.32127500	0.30895900	3.39102300	2411	C	1.55772100	-2.50007200	-1.69294000
2368	H	1.12573300	0.54802800	4.78654300	2412	C	2.02787300	-3.73844800	-2.13919800
2369	H	1.29834700	2.21431700	2.18432600	2413	O	3.64461500	-5.54378500	-1.82914800
2370	H	0.09284600	2.44422400	3.57799600	2414	C	-2.48470900	7.22923800	-1.33889600
2371					2415	C	-7.03989000	-1.84663100	-2.69501400
2372	2TS4				2416	C	6.94953200	3.73138800	-1.08779600
2373	N	0.20987600	0.22726300	-0.94366100	2417	C	3.09825200	-6.25192100	-2.93806500
2374	P	-1.20539200	0.60601500	-0.01835600	2418	H	1.66649400	-2.12135000	2.84274800
2375	P	1.48759800	-0.28919200	0.10936900	2419	H	-0.72633400	-2.38819100	1.35970200
2376	Cr	-0.39352900	-0.53333800	2.12351800	2420	H	0.48292700	-3.57849200	1.59464200
2377	C	0.62924500	-2.16829500	3.17688700	2421	H	-1.46308200	-4.74123600	2.14128300
2378	C	-0.22882300	-2.98226900	2.17789200	2422	H	-2.40892800	0.26018500	3.54376900
2379	C	-1.31422400	-3.87883900	2.80271000	2423	H	-2.98502300	-0.60581900	2.11709100
2380	C	-2.28540800	-0.66461300	2.96382100	2424	H	-1.96635900	-1.97733800	4.68568100
2381	C	-2.64278100	-1.88510200	3.82256500	2425	H	-3.64128400	-1.72157100	4.25570500
2382	C	-2.67758200	-3.21505700	3.04921700	2426	H	-3.30185600	-3.93691800	3.58994400
2383	C	0.60879000	-0.37674000	4.24536000	2427	H	-3.17695300	-3.04593700	2.08380900
2384	C	0.35737000	0.82073300	3.51202900	2428	H	-0.92368900	-4.28416700	3.74543100
2385	C	0.43077800	0.72957600	-2.31092400	2429	H	0.58181600	-2.64967700	4.15087500
2386	C	-1.52559500	2.39529100	-0.12641200	2430	H	1.63454000	-0.62694500	4.49836500
2387	C	-2.58546300	-0.19553700	-0.90644800	2431	H	-0.11647800	-0.66825800	4.99852100
2388	C	2.84198000	0.92647300	-0.07876100	2432	H	1.21584400	1.35467600	3.10918900
2389	C	2.14516500	-1.84284800	-0.60566000	2433	H	-0.47855000	1.44154000	3.82447700
2390	C	-1.28211000	3.20189800	1.00357300	2434	H	-0.95554200	2.74270600	1.93159900
2391	C	-1.46320800	4.57529600	0.95704300	2435	H	-1.28639700	5.19917700	1.82719000
2392	C	-1.89284400	5.19091200	-0.23228500	2436	H	-2.17709700	2.43056800	-2.19016700
2393	C	-1.96091100	3.02299400	-1.30600300	2437	H	-2.47900000	4.85372700	-2.29488800
2394	C	-2.14230000	4.40328400	-1.36850600	2438	H	-1.41994100	-1.94023400	-1.44472700
2395	O	-2.03943100	6.53159900	-0.17750500	2439	H	-3.31987500	-3.14814100	-2.47910900
2396	C	-2.40306900	-1.47893500	-1.46121400	2440	H	-4.05818600	1.33264200	-0.49284200

2441 H -5.93101900 0.12692600 -1.49302000
2442 H 1.80519400 2.40630200 1.12476600
2443 H 3.57137700 4.12342200 0.91595700
2444 H 4.14669200 -0.26129100 -1.32576600
2445 H 5.88792500 1.44156700 -1.52692200
2446 H 3.71045200 -1.99873600 0.89313400
2447 H 4.53662900 -4.19151500 0.10803000
2448 H 0.72003500 -2.04756800 -2.21355900
2449 H 1.55120300 -4.20967600 -2.99087500
2450 H 1.31876700 0.25612200 -2.73605200
2451 H -0.42950500 0.47781100 -2.93979200
2452 H 0.57836000 1.81539700 -2.32098500
2453 H -2.52905100 8.28005100 -1.05165200
2454 H -1.78036200 7.10724100 -2.17057500
2455 H -3.48190300 6.89233100 -1.64661400
2456 H -7.62615900 -2.61414700 -3.20110800
2457 H -7.44181100 -1.68498800 -1.68742500
2458 H -7.09143800 -0.91183500 -3.26638200
2459 H 7.50522100 4.66282600 -0.97558000
2460 H 7.54109000 2.90197400 -0.68160700
2461 H 6.74652400 3.55309300 -2.15081800
2462 H 3.68610700 -7.16631200 -3.02326900
2463 H 2.04568000 -6.50957300 -2.76680000
2464 H 3.18867700 -5.67224400 -3.86491400
2465

2466 **2INT5**

2467 N -0.09879900 -0.05940500 -1.08807700
2468 P 1.23723300 -0.69042300 -0.16796000
2469 P -1.31026800 0.62876300 -0.07735700
2470 Cr -0.22945100 -0.12143300 2.06713500
2471 C -0.14143600 -0.04462700 -2.56048000
2472 C 1.31314300 -2.46458300 -0.61489000
2473 C 2.75597000 0.04307500 -0.86147600
2474 C -2.91599200 -0.01070700 -0.64177800
2475 C -1.34514400 2.42365300 -0.37923400
2476 C 2.50247900 -3.19872000 -0.42532200
2477 C 2.53380400 -4.56978400 -0.62694000
2478 C 1.37189700 -5.25754800 -1.02204200
2479 C 0.15818200 -3.16359200 -0.99248400
2480 C 0.17908700 -4.54374100 -1.20496400
2481 O 1.51152600 -6.59161300 -1.19764700
2482 C 3.32787500 1.15374500 -0.20667600
2483 C 4.45392000 1.78282500 -0.71431500
2484 C 5.04984800 1.31573400 -1.89987800

2485 C 3.36303600 -0.41387500 -2.04261200
2486 C 4.49630200 0.20835200 -2.56330700
2487 O 6.14380800 1.99234300 -2.31078300
2488 C -3.38600300 -1.23534700 -0.12174600
2489 C -4.57176800 -1.79382900 -0.56806100
2490 C -5.33468300 -1.13983300 -1.55421800
2491 C -3.68642300 0.63111900 -1.62509800
2492 C -4.88328500 0.08047200 -2.08134100
2493 O -6.47501000 -1.76199800 -1.91757000
2494 C -2.43720800 3.19999400 0.06276800
2495 C -2.42439700 4.57952800 -0.06367000
2496 C -1.31343900 5.23096000 -0.63166700
2497 C -0.23636500 3.08361800 -0.92560000
2498 C -0.21513800 4.47240400 -1.06262600
2499 O -1.40443400 6.57646500 -0.71481600
2500 C 0.37826800 -7.35553700 -1.59856300
2501 C 6.81864000 1.56661400 -3.49282700
2502 C -7.31438600 -1.15527700 -2.89901100
2503 C -0.31691700 7.30916800 -1.27284200
2504 H 3.41609100 -2.69190500 -0.12710800
2505 H 3.44860300 -5.13734900 -0.48980300
2506 H -0.77682400 -2.62921500 -1.13731600
2507 H -0.73030600 -5.04673500 -1.51265500
2508 H 2.88804800 1.52387400 0.71505100
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2510 H 2.95830900 -1.27732900 -2.56207300
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2514 H -3.35873700 1.57997200 -2.03826800
2515 H -5.45324300 0.60491500 -2.83918000
2516 H -3.30846200 2.72143500 0.50154500
2517 H -3.26322100 5.18270400 0.26812700
2518 H 0.62935200 2.51505600 -1.25200400
2519 H 0.65360100 4.94850200 -1.50187400
2520 H 0.46376200 0.76916200 -2.97445300
2521 H 0.23160000 -0.99674700 -2.94859700
2522 H -1.17485600 0.07460200 -2.89688900
2523 H 0.72810400 -8.38550900 -1.67476200
2524 H -0.42527900 -7.29747200 -0.85392300
2525 H 0.00000100 -7.02569200 -2.57405400
2526 H 7.66001000 2.24948400 -3.61335200
2527 H 7.19236800 0.54094700 -3.38915900
2528 H 6.16455900 1.63425900 -4.37054500

2529	H	-8.16300400	-1.82939600	-3.01700200	2573	C	2.47570100	-1.18449000	-1.56012200
2530	H	-7.67046400	-0.17391100	-2.56392700	2574	C	3.62997900	-1.81108400	-2.03189400
2531	H	-6.79295900	-1.05220300	-3.85815400	2575	O	6.05796500	-1.70229500	-2.27694100
2532	H	-0.61644800	8.35682400	-1.23390300	2576	C	0.53216700	3.47099900	0.42153600
2533	H	0.59937900	7.16926800	-0.68639100	2577	C	0.53976400	4.84125400	0.21365000
2534	H	-0.13530600	7.01976100	-2.31513700	2578	C	1.17171300	5.37873600	-0.92273200
2535	C	-1.86415100	-0.40829300	3.23201700	2579	C	1.77514700	3.14103800	-1.62091000
2536	C	-1.53511500	-0.49468700	4.72876800	2580	C	1.79096200	4.51687500	-1.84279700
2537	C	-0.53881000	-1.61415300	5.07231100	2581	O	1.12946300	6.72322400	-1.03420700
2538	C	0.87169500	-1.51410500	4.46034200	2582	C	-0.97328400	-3.33070200	-0.27372300
2539	C	1.88242700	-0.56761400	5.13002600	2583	C	-1.18212500	-4.59247100	-0.80615700
2540	C	1.69558200	0.95534600	5.00146600	2584	C	-2.18858200	-4.79540600	-1.76902100
2541	C	1.82408500	1.53593700	3.57561200	2585	C	-2.75619100	-2.44608500	-1.64058800
2542	C	0.54327900	1.63709000	2.74153200	2586	C	-2.97751500	-3.71094500	-2.18433100
2543	H	-2.61861500	0.36284000	3.03141400	2587	O	-2.31592500	-6.06008100	-2.22292000
2544	H	-2.27579300	-1.37178000	2.87582600	2588	C	-4.13366600	-0.23548600	0.41212000
2545	H	-1.16619400	0.47290200	5.08771200	2589	C	-5.29764600	0.51071800	0.51017200
2546	H	-2.45981600	-0.68410200	5.29539300	2590	C	-5.29795200	1.87587700	0.16996800
2547	H	-0.42359300	-1.68496800	6.16204700	2591	C	-2.94026800	1.71789000	-0.35304700
2548	H	-0.98158800	-2.56829000	4.75370600	2592	C	-4.10757500	2.47773800	-0.26360900
2549	H	1.31526400	-2.51771800	4.45863600	2593	O	-6.48547400	2.51001200	0.29368900
2550	H	0.82563900	-1.28948600	3.36352900	2594	C	6.06899200	-2.96262100	-2.94127800
2551	H	1.90510700	-0.82700400	6.19728700	2595	C	1.76653400	7.34738700	-2.14749600
2552	H	2.88041500	-0.81566200	4.74227300	2596	C	-3.32535500	-6.35207800	-3.18765400
2553	H	0.74559300	1.27454400	5.44648200	2597	C	-6.56496400	3.89496000	-0.03109300
2554	H	2.47744800	1.41180100	5.62088100	2598	H	3.87307300	1.63792500	-0.26647700
2555	H	2.22405600	2.55828300	3.66963400	2599	H	5.91847800	0.52050200	-1.09066900
2556	H	2.60049900	0.97843500	3.02740600	2600	H	1.51976000	-1.68305100	-1.69432400
2557	H	-0.27362400	2.11474600	3.29863800	2601	H	3.54745400	-2.77155900	-2.52710000
2558	H	0.71311100	2.21333500	1.82199700	2602	H	0.04021400	3.07795700	1.30815700
2559					2603	H	0.07391600	5.52302200	0.91775400
2560	2TS5				2604	H	2.26846000	2.49278300	-2.33890200
2561	N	-0.29283900	0.18235400	-1.12774200	2605	H	2.28484500	4.90671200	-2.72512600
2562	P	1.02350900	0.79493800	-0.19530300	2606	H	-0.19501600	-3.19734500	0.47361900
2563	P	-1.36430100	-0.58198000	-0.01298700	2607	H	-0.58939200	-5.44514800	-0.49111800
2564	Cr	0.04766200	-0.18259400	1.99606300	2608	H	-3.38562100	-1.62259100	-1.96434200
2565	C	-0.50665600	0.37818100	-2.56731300	2609	H	-3.76119500	-3.84219300	-2.92116000
2566	C	2.52924400	0.06792300	-0.93126900	2610	H	-4.16279300	-1.28913600	0.67450900
2567	C	1.14988300	2.58953600	-0.49068100	2611	H	-6.22700800	0.06130500	0.84486000
2568	C	-1.75510500	-2.22917100	-0.68001200	2612	H	-2.02698900	2.20644100	-0.68006500
2569	C	-2.93127700	0.35299300	-0.03298800	2613	H	-4.07895100	3.52714500	-0.53271000
2570	C	3.79173600	0.67246500	-0.75710700	2614	H	-1.02388600	1.32073500	-2.77893900
2571	C	4.94567000	0.05608300	-1.21569000	2615	H	0.45697400	0.37808900	-3.08455600
2572	C	4.87702100	-1.19151900	-1.86174300	2616	H	-1.10225200	-0.44989800	-2.96309400

2617	H	7.11445500	-3.16223500	-3.17812800	2661	C	1.08225900	0.38835900	4.49812400
2618	H	5.68356300	-3.75846100	-2.29212300	2662	C	4.77834000	0.87987000	3.14937900
2619	H	5.48459300	-2.92902500	-3.86896100	2663	C	3.58421100	0.91006100	4.11832400
2620	H	1.60851800	8.41788500	-2.01441600	2664	C	2.33190600	0.17516200	3.61889300
2621	H	2.84224300	7.13523600	-2.15915100	2665	C	5.29181900	-0.51610200	2.75047300
2622	H	1.31623900	7.02642100	-3.09452400	2666	C	5.76736900	-1.37942000	3.92501900
2623	H	-3.23819300	-7.41974300	-3.39041800	2667	C	-1.11733200	-0.14261300	-2.49821400
2624	H	-4.32533800	-6.13513800	-2.79358300	2668	C	-2.40924700	1.83241700	0.11814300
2625	H	-3.16332000	-5.78941500	-4.11488300	2669	C	-3.15280400	-0.98136600	0.12980200
2626	H	-7.60287500	4.17991500	0.14344200	2670	C	1.95824200	0.96162500	-1.34217700
2627	H	-5.90899800	4.49329000	0.61311700	2671	C	1.51078800	-1.89646500	-1.06183000
2628	H	-6.30963100	4.07260000	-1.08300300	2672	C	-3.57829900	2.21568600	0.80740200
2629	C	-1.39212600	-1.33156300	2.99008100	2673	C	-4.02744000	3.52641800	0.77153700
2630	C	-0.42803500	-1.01876400	4.02267600	2674	C	-3.31733500	4.50189000	0.04781700
2631	C	0.46877300	-2.14338500	4.56375100	2675	C	-1.70109700	2.81622900	-0.58615400
2632	C	1.51712100	-2.66298200	3.54503700	2676	C	-2.14665700	4.13809200	-0.63360700
2633	C	2.98124400	-2.34489900	3.89748700	2677	O	-3.84302300	5.74754600	0.07262700
2634	C	3.34606000	-0.87698100	4.18931000	2678	C	-3.10757300	-2.22501000	0.79326900
2635	C	3.05960500	0.15697800	3.07701200	2679	C	-4.13806500	-3.14228700	0.66622400
2636	C	1.69216000	0.85570000	3.16982100	2680	C	-5.25688900	-2.84088100	-0.13284400
2637	H	-2.35392200	-0.81952400	3.01173700	2681	C	-4.27537200	-0.69303500	-0.66314700
2638	H	-1.45014800	-2.35706900	2.62601000	2682	C	-5.31996400	-1.60640500	-0.79911500
2639	H	0.57990600	-0.12460300	3.60524000	2683	O	-6.20950700	-3.79552300	-0.18836100
2640	H	-0.79425700	-0.32939000	4.79005400	2684	C	2.27909400	2.16072100	-0.67289900
2641	H	0.98049900	-1.78864900	5.46521800	2685	C	3.03462500	3.14618100	-1.28867900
2642	H	-0.18112100	-2.96435800	4.88866900	2686	C	3.49670300	2.96118000	-2.60479500
2643	H	1.42515000	-3.74959000	3.43190100	2687	C	2.42820400	0.79013000	-2.65444600
2644	H	1.29312400	-2.26009200	2.54013200	2688	C	3.18757400	1.77252300	-3.28669800
2645	H	3.25594700	-2.93932400	4.77956000	2689	O	4.22681500	3.97454800	-3.11647700
2646	H	3.61680800	-2.71037400	3.07897300	2690	C	2.89071800	-2.16433000	-1.17318900
2647	H	2.86007600	-0.54407900	5.11734200	2691	C	3.34603900	-3.43904600	-1.47251500
2648	H	4.42088400	-0.86169200	4.40758700	2692	C	2.43439900	-4.49256200	-1.66746900
2649	H	3.82850600	0.94040600	3.14313800	2693	C	0.61210100	-2.95752400	-1.24328200
2650	H	3.20234600	-0.30741700	2.09134400	2694	C	1.05890100	-4.24312400	-1.55226200
2651	H	1.55202800	1.24148900	4.18966800	2695	O	2.98107000	-5.69413900	-1.95981800
2652	H	1.65558200	1.73955900	2.52556800	2696	C	-3.18150100	6.78991900	-0.63804500
2653					2697	C	-7.38463300	-3.55748000	-0.96095300
2654	2SC3				2698	C	4.74999600	3.85433100	-4.43830100
2655	N	-0.70899400	-0.13171500	-1.08688900	2699	C	2.12099700	-6.81095700	-2.16703300
2656	P	-1.73344700	0.14504300	0.28395700	2700	H	-1.48267500	1.25919900	3.67202100
2657	P	0.91075100	-0.26445800	-0.49750100	2701	H	4.94791100	-1.63733200	4.60640100
2658	Cr	0.07396400	-0.10131000	1.87526400	2702	H	-0.08002400	-1.47065700	4.12611000
2659	C	-1.31349900	0.18861500	3.55318500	2703	H	0.84108000	1.45934200	4.54185700
2660	C	-0.10371600	-0.38959400	3.95612400	2704	H	5.60321600	1.44329700	3.60588200

2705	H	4.50574500	1.42990400	2.23617900	2749	N	1.01138300	0.12448500	-0.81367300
2706	H	3.86801400	0.47540900	5.08567700	2750	P	1.82146200	-0.61937000	0.52756100
2707	H	3.32237700	1.95730700	4.32145000	2751	P	-0.55157700	0.73386100	-0.38049900
2708	H	2.14008100	0.53670900	2.57959000	2752	Cr	-0.14460600	0.06611600	2.11358800
2709	H	2.53681400	-0.90070900	3.53123700	2753	C	-0.17018800	-0.12097900	4.42720900
2710	H	1.30710300	0.08156600	5.52949900	2754	C	-1.44213700	0.31902200	4.18510400
2711	H	-2.21505200	-0.41206800	3.47095400	2755	C	-2.66901100	-0.55730300	4.16101100
2712	H	6.20263600	-2.31965400	3.56905400	2756	C	-5.93679200	-0.87129200	1.96856800
2713	H	6.53473600	-0.86054800	4.51214000	2757	C	-4.93756700	-1.10643900	3.11540000
2714	H	4.51509900	-1.05625400	2.18996100	2758	C	-3.68050900	-0.22750000	3.04905600
2715	H	6.12350800	-0.38066200	2.04698400	2759	C	-6.58702000	0.52332100	1.91712900
2716	H	-4.14826500	1.48037200	1.36825800	2760	C	-7.44815300	0.86559100	3.13893300
2717	H	-4.93032100	3.82597200	1.29382300	2761	C	1.53175100	0.13343200	-2.19111900
2718	H	-0.78689900	2.55667800	-1.11213500	2762	C	1.99575200	-2.39125100	0.10531300
2719	H	-1.58086900	4.86880500	-1.19963900	2763	C	3.51861100	0.04462900	0.54898500
2720	H	-2.25550700	-2.47264900	1.42226200	2764	C	-1.76990500	-0.01620000	-1.51349100
2721	H	-4.11329500	-4.09685400	1.18178900	2765	C	-0.51228900	2.50961500	-0.81912000
2722	H	-4.34812400	0.26291000	-1.17312200	2766	C	2.97216700	-3.19158800	0.73348500
2723	H	-6.17275700	-1.34933500	-1.41635900	2767	C	3.02115100	-4.55979200	0.51481400
2724	H	1.93466900	2.32205600	0.34615800	2768	C	2.08833100	-5.17727300	-0.33760800
2725	H	3.29155100	4.06686500	-0.77497700	2769	C	1.06065500	-3.02114600	-0.72721900
2726	H	2.21413200	-0.12904900	-3.19191900	2770	C	1.10307400	-4.39729900	-0.95948300
2727	H	3.53546900	1.60521000	-4.29929800	2771	O	2.22684700	-6.51530000	-0.48733700
2728	H	3.61585200	-1.36753500	-1.03415200	2772	C	3.79174200	1.14694500	1.38505900
2729	H	4.40652100	-3.64945800	-1.56637800	2773	C	5.04545200	1.73613600	1.41109100
2730	H	-0.45674300	-2.78361200	-1.15406400	2774	C	6.07744200	1.23359400	0.59699400
2731	H	0.33409600	-5.03495300	-1.70129300	2775	C	4.55954400	-0.44871600	-0.25432100
2732	H	-0.44560000	-0.78915200	-3.06999500	2776	C	5.82695300	0.13257200	-0.23747600
2733	H	-2.12901500	-0.55111100	-2.58238200	2777	O	7.26341400	1.87189300	0.69607500
2734	H	-1.10348300	0.86212400	-2.93569900	2778	C	-2.48812600	-1.14715700	-1.07358700
2735	H	-3.78064900	7.68594500	-0.47321500	2779	C	-3.38857800	-1.79569700	-1.90446100
2736	H	-2.16737300	6.95352000	-0.25310000	2780	C	-3.60392100	-1.32592600	-3.21309700
2737	H	-3.13685600	6.57367400	-1.71258500	2781	C	-1.99638700	0.44075700	-2.82143700
2738	H	-7.99791100	-4.45157000	-0.84644500	2782	C	-2.90070100	-0.19884600	-3.66807300
2739	H	-7.93526700	-2.68601800	-0.58718800	2783	O	-4.50294700	-2.02105700	-3.94298800
2740	H	-7.14120500	-3.41431700	-2.02058400	2784	C	-1.70713400	3.22710400	-1.03291200
2741	H	5.30065500	4.77726400	-4.62154200	2785	C	-1.68850400	4.59875600	-1.23358200
2742	H	5.43195600	2.99948700	-4.51877900	2786	C	-0.47055100	5.30225900	-1.22262900
2743	H	3.94527600	3.75596500	-5.17676800	2787	C	0.69347000	3.22396100	-0.79383800
2744	H	2.77839000	-7.65422500	-2.38080000	2788	C	0.72517400	4.60436700	-1.00100700
2745	H	1.52805300	-7.02879300	-1.27021400	2789	O	-0.56154400	6.63580900	-1.43385600
2746	H	1.45120000	-6.64510100	-3.01974000	2790	C	1.31752000	-7.21013600	-1.33446200
2747					2791	C	8.36545600	1.40943900	-0.08189900
2748	2P'				2792	C	-4.79152900	-1.59690600	-5.27363600

2793 C 0.63074100 7.41475900 -1.43443400
2794 H 0.03596400 -1.17463800 4.61323600
2795 H -6.85644100 0.91896300 4.06035400
2796 H -1.62216300 1.39644900 4.15926600
2797 H -2.37201800 -1.61347500 4.10786300
2798 H -6.73164600 -1.62570800 2.04551500
2799 H -5.42828000 -1.06147900 1.01199300
2800 H -5.43339000 -0.95273400 4.08328900
2801 H -4.63078800 -2.16200200 3.09999600
2802 H -3.20046900 -0.35439900 2.06569100
2803 H -3.95505000 0.83348700 3.11845700
2804 H -3.17108800 -0.43249400 5.13359600
2805 H 0.63429800 0.57795500 4.65282300
2806 H -7.94065500 1.83583200 3.01163200
2807 H -8.23147900 0.11329300 3.29263400
2808 H -5.81474400 1.29399200 1.78404900
2809 H -7.21221600 0.57228200 1.01606600
2810 H 3.70742400 -2.74040800 1.39398900
2811 H 3.77563100 -5.17841300 0.99008900
2812 H 0.28323200 -2.43679100 -1.21127900
2813 H 0.37178400 -4.84610200 -1.62163800
2814 H 3.00911000 1.54322700 2.02857300
2815 H 5.26206700 2.57972900 2.05848100
2816 H 4.38935700 -1.30981900 -0.89368600
2817 H 6.60723000 -0.27661100 -0.86842100
2818 H -2.34002800 -1.52255800 -0.06353000
2819 H -3.94714100 -2.66305400 -1.56768500
2820 H -1.47124900 1.31786200 -3.18762300
2821 H -3.05198300 0.18427300 -4.67043100
2822 H -2.66099300 2.70736800 -1.05187800
2823 H -2.60475700 5.15431400 -1.40574600
2824 H 1.62928800 2.70085500 -0.61673500
2825 H 1.67802800 5.12067900 -0.98924800
2826 H 1.19596600 1.03841400 -2.70507100
2827 H 2.62503100 0.14774100 -2.16997700
2828 H 1.19906200 -0.74255900 -2.75884700
2829 H 1.62040600 -8.25709200 -1.29802600
2830 H 0.28555400 -7.11637200 -0.97394300
2831 H 1.37940700 -6.84852500 -2.36839900
2832 H 9.19874100 2.06651700 0.16836800
2833 H 8.62567900 0.37534000 0.17384100
2834 H 8.15241800 1.48186600 -1.15524300
2835 H -5.53749300 -2.29716900 -5.65041000
2836 H -5.20465300 -0.58120300 -5.28590700

2837 H -3.89762500 -1.63931300 -5.90761000
2838 H 0.31325600 8.44118800 -1.62091400
2839 H 1.14215400 7.36140100 -0.46533000
2840 H 1.31580900 7.09470500 -2.22928100
2841

2842 **2INT6**

2843 N 0.47491700 -0.05744800 -1.02738200
2844 P -0.95436300 0.64176200 -0.36163100
2845 P 1.53543500 -0.67656500 0.19887000
2846 Cr -0.48065000 -0.06534000 2.09842100
2847 C -1.60305000 1.43874800 2.92666900
2848 C -3.07508800 1.72795400 2.60690000
2849 C -4.07407300 1.12423800 3.61316400
2850 C -3.86690700 -0.36934700 3.90179500
2851 C -3.93289400 -1.26244400 2.65608100
2852 C -3.36059800 -2.67117500 2.86390700
2853 C -1.85955200 -2.71286600 3.19879600
2854 C -0.92833500 -2.09380500 2.15242600
2855 C 0.59198500 -0.56153400 4.55056700
2856 C 1.37011700 0.33655700 3.92079200
2857 C 0.84853600 0.04024900 -2.44868100
2858 C -0.81654100 2.45226700 -0.58977600
2859 C -2.33384300 0.12408400 -1.43437600
2860 C 3.15409400 0.15011700 -0.02807700
2861 C 1.84289400 -2.41571300 -0.28098800
2862 C 0.44116300 3.06275700 -0.69059500
2863 C 0.57433200 4.45062500 -0.76249800
2864 C -0.56853400 5.26196600 -0.72022100
2865 C -1.95579800 3.28325400 -0.53764000
2866 C -1.83614500 4.66233900 -0.60440200
2867 O -0.56284700 6.61237400 -0.78544400
2868 C -2.69837100 0.83109400 -2.59245100
2869 C -3.71199400 0.37369000 -3.43321200
2870 C -4.38846400 -0.81735800 -3.12592100
2871 C -3.02494200 -1.07026300 -1.14156000
2872 C -4.03359400 -1.53581300 -1.96916400
2873 O -5.38383400 -1.35086900 -3.86463200
2874 C 3.45336800 1.27801300 0.76475400
2875 C 4.64568200 1.96998400 0.61660700
2876 C 5.59093100 1.54888500 -0.33611300
2877 C 4.10878500 -0.25564200 -0.97480300
2878 C 5.31383400 0.42719100 -1.13391000
2879 O 6.72289600 2.28258700 -0.40109100
2880 C 2.95581300 -3.10919500 0.23868100

2881 C 3.13240200 -4.46220800 -0.00601400
2882 C 2.19626300 -5.17208800 -0.77941100
2883 C 0.90879600 -3.13840300 -1.03517400
2884 C 1.07987500 -4.49964200 -1.29591400
2885 O 2.46432100 -6.48577500 -0.96334400
2886 C 0.68387400 7.29129500 -0.90437500
2887 C -5.80912700 -0.67420500 -5.04622800
2888 C 7.74073900 1.90536700 -1.32634500
2889 C 1.55918700 -7.27169200 -1.73218600
2890 H -1.43024800 1.45164600 4.01241200
2891 H -3.23661600 2.81603400 2.58790300
2892 H -3.32243000 1.38415700 1.59339900
2893 H -3.99769900 1.67702500 4.55952700
2894 H -5.09342700 1.29497000 3.24066200
2895 H -2.89287000 -0.49269200 4.39212800
2896 H -1.57484900 -3.77024700 3.32068300
2897 H -1.68381700 -2.26149000 4.18486300
2898 H -3.53141000 -3.26528300 1.95459000
2899 H -3.91251400 -3.17981400 3.66614500
2900 H -4.61270000 -0.70739700 4.63357400
2901 H -0.95338400 2.22594200 2.48970100
2902 H 0.83183400 -1.62089700 4.54624300
2903 H -0.27650600 -0.26052400 5.12894800
2904 H -3.38314100 -0.78582000 1.83439900
2905 H -4.97449200 -1.33584000 2.31505000
2906 H -1.24022800 -2.34826900 1.13031700
2907 H 0.09870400 -2.46818300 2.27578100
2908 H 2.27689900 0.03712000 3.40284600
2909 H 1.16788600 1.40399900 3.98249700
2910 H 1.34016100 2.45526700 -0.72062800
2911 H 1.56363900 4.88334100 -0.85567400
2912 H -2.94727700 2.84879300 -0.45404800
2913 H -2.71062700 5.30427100 -0.57335000
2914 H -2.19423600 1.75859100 -2.84498400
2915 H -3.96636400 0.94740600 -4.31659800
2916 H -2.77480500 -1.63702200 -0.25092700
2917 H -4.57248000 -2.45007200 -1.74263300
2918 H 2.73876700 1.62267000 1.50827200
2919 H 4.87964000 2.83381600 1.23058300
2920 H 3.92084400 -1.12755700 -1.59385600
2921 H 6.02641800 0.08075000 -1.87329000
2922 H 3.69993100 -2.58392000 0.83142000
2923 H 3.99091900 -4.99770100 0.38641500
2924 H 0.03236800 -2.63658700 -1.43586000

2925 H 0.34365200 -5.02127300 -1.89625000
2926 H 1.40805200 -0.85238200 -2.74122200
2927 H -0.05435500 0.08849300 -3.06333600
2928 H 1.46222300 0.92568100 -2.64870700
2929 H 0.43962700 8.35341800 -0.93887300
2930 H 1.32914300 7.09306200 -0.03969300
2931 H 1.20612700 7.00678400 -1.82611000
2932 H -6.61277200 -1.28330800 -5.46068200
2933 H -6.19132900 0.32701200 -4.81420700
2934 H -4.99397300 -0.59872700 -5.77593100
2935 H 8.54525500 2.62842500 -1.18956700
2936 H 8.11570700 0.89692000 -1.11456700
2937 H 7.37720200 1.95447600 -2.35990000
2938 H 1.97495500 -8.27979100 -1.73861700
2939 H 0.56158600 -7.29164100 -1.27614500
2940 H 1.48489900 -6.90152900 -2.76224300
2941

2942 **2TS6**

2943 N 0.51911000 0.05694600 -1.15478800
2944 P 0.32345200 1.43870300 -0.13809200
2945 P 0.18198200 -1.40917900 -0.29288200
2946 Cr -0.31777100 0.06138100 1.97748800
2947 C -1.28113100 1.53107000 3.03312700
2948 C -2.71276300 1.43323800 2.48529100
2949 C -3.86323400 1.45794400 3.52219500
2950 C -3.83758600 0.36302100 4.60405200
2951 C -3.91668600 -1.09177500 4.07485400
2952 C -2.93998400 -2.08095000 4.74346500
2953 C -1.44540300 -1.69705100 4.64205000
2954 C -0.90576200 -1.61540100 3.21470800
2955 C 1.12611100 -0.74292000 3.70886200
2956 C 1.60686700 0.27490200 2.87935400
2957 C 0.92732500 0.10332300 -2.56845000
2958 C 1.95893600 2.24340800 0.00343000
2959 C -0.70646300 2.61963800 -1.07486900
2960 C 1.57746000 -2.54647200 -0.60319700
2961 C -1.23088600 -2.17529600 -1.17424500
2962 C 3.14107500 1.55352300 -0.29262800
2963 C 4.39466200 2.12916000 -0.07104500
2964 C 4.48221000 3.41796500 0.47339500
2965 C 2.06359500 3.53435200 0.56292900
2966 C 3.30158700 4.11457100 0.79122000
2967 O 5.63672100 4.07405200 0.73076100
2968 C -0.17079000 3.63885400 -1.87740400

2969	C	-0.99257400	4.48697900	-2.62016000	3013	H	3.38685000	5.11018800	1.21459800
2970	C	-2.38527400	4.32336900	-2.57591200	3014	H	0.90350500	3.78569300	-1.92377400
2971	C	-2.10912200	2.46859700	-1.04532200	3015	H	-0.54191800	5.26496600	-3.22517600
2972	C	-2.93662300	3.30038600	-1.78163400	3016	H	-2.55797500	1.69001300	-0.43577600
2973	O	-3.27424600	5.08524400	-3.24834000	3017	H	-4.01605700	3.19122100	-1.75585100
2974	C	2.56561300	-2.70134900	0.39013600	3018	H	2.46369200	-2.18234400	1.33899600
2975	C	3.66895800	-3.51600500	0.18839300	3019	H	4.42711000	-3.64336400	0.95440400
2976	C	3.81971100	-4.21013900	-1.02560500	3020	H	0.98620400	-3.17454300	-2.58571500
2977	C	1.73896900	-3.25190000	-1.80696300	3021	H	2.93235700	-4.60396900	-2.96682700
2978	C	2.84303400	-4.07391300	-2.02574200	3022	H	-0.79932500	-4.19299700	-0.49977800
2979	O	4.92506000	-4.97925300	-1.12699500	3023	H	-2.83416100	-5.18364900	-1.49375900
2980	C	-1.49506900	-3.55366900	-1.03628200	3024	H	-1.99091400	-0.32569000	-1.99090900
2981	C	-2.63138500	-4.12196400	-1.59148400	3025	H	-3.98894900	-1.31914000	-2.99282200
2982	C	-3.54713600	-3.32806600	-2.30510600	3026	H	0.28757800	-0.55471500	-3.16436500
2983	C	-2.15905100	-1.39253800	-1.87386500	3027	H	0.81283900	1.12130100	-2.94942900
2984	C	-3.30319800	-1.95450200	-2.44436800	3028	H	1.96997500	-0.20728900	-2.69730200
2985	O	-4.61803900	-3.98055100	-2.81416200	3029	H	7.65045700	4.14066100	0.72617200
2986	C	6.87388900	3.43080800	0.43971300	3030	H	6.99003000	2.50844700	1.02220500
2987	C	-2.79308700	6.15312200	-4.06227000	3031	H	6.96348900	3.20403300	-0.62981800
2988	C	5.13981300	-5.72919900	-2.32087200	3032	H	-3.68062300	6.62117100	-4.48876500
2989	C	-5.58482500	-3.24209600	-3.55433300	3033	H	-2.24215000	6.88959900	-3.46520800
2990	H	-1.20774000	1.29212200	4.09954400	3034	H	-2.15274300	5.77922700	-4.87026000
2991	H	-2.88155700	2.24824900	1.77277000	3035	H	6.07564300	-6.26685000	-2.16627800
2992	H	-2.84369900	0.51204600	1.87398700	3036	H	4.32903600	-6.44792800	-2.48992400
2993	H	-3.85093700	2.43747600	4.01757700	3037	H	5.23655200	-5.07035300	-3.19227400
2994	H	-4.81359900	1.40089500	2.97288200	3038	H	-6.33861900	-3.96737200	-3.86240000
2995	H	-2.93823300	0.49661100	5.21607600	3039	H	-6.05531700	-2.46807900	-2.93530800
2996	H	-0.85580800	-2.42533700	5.21191800	3040	H	-5.13842200	-2.77999000	-4.44357100
2997	H	-1.30891600	-0.73700500	5.15362000	3041				
2998	H	-3.09274600	-3.08003700	4.31416100	3042		2INT7		
2999	H	-3.18667600	-2.16426600	5.81051500	3043	N	-0.48698100	-0.00850900	-1.20574700
3000	H	-4.67483200	0.54621600	5.28808600	3044	P	-1.28065200	-0.92180800	0.01968200
3001	H	-0.83370600	2.51657400	2.86818100	3045	P	0.81498300	0.95614900	-0.56902300
3002	H	1.59063600	1.30534100	3.22526900	3046	Cr	0.27265200	-0.22431800	1.85009000
3003	H	2.32553700	0.05026600	2.09491300	3047	C	0.55343600	-1.89159200	2.97223800
3004	H	-3.75639500	-1.10680000	2.98845700	3048	C	2.00692800	-2.17929400	2.55390200
3005	H	-4.93424000	-1.47707100	4.21022200	3049	C	3.02302000	-2.43079200	3.69659000
3006	H	-1.73983300	-1.36061700	2.51976400	3050	C	3.21331600	-1.26775800	4.68684900
3007	H	-0.50298600	-2.56569100	2.85566200	3051	C	3.91627300	-0.02720300	4.09762300
3008	H	0.74365900	-0.49314300	4.69126600	3052	C	3.64189800	1.29795300	4.84204500
3009	H	1.49750000	-1.75706700	3.60171400	3053	C	2.15034700	1.63275400	5.05682800
3010	H	3.09582700	0.54821100	-0.70088800	3054	C	1.27525900	1.53962700	3.79483300
3011	H	5.28714900	1.56900400	-0.32470000	3055	C	-0.24083300	1.42524600	4.07324800
3012	H	1.16801000	4.09705900	0.81372900	3056	C	-1.02998700	0.99867100	2.83082400

3057	C	-0.90052100	0.00766800	-2.61944100	3101	H	-0.13436500	-2.71275600	2.75279800
3058	C	-2.98667700	-0.30477400	0.16292300	3102	H	-1.96991800	0.48906900	3.06264100
3059	C	-1.41462100	-2.63468700	-0.57904500	3103	H	-1.23700500	1.83053400	2.14361600
3060	C	0.53694700	2.67262000	-1.12143800	3104	H	3.63614000	0.09636100	3.04265400
3061	C	2.29267600	0.40234400	-1.49931100	3105	H	4.99957900	-0.20085400	4.08099800
3062	C	-3.32375500	0.98587300	-0.26552700	3106	H	1.62864000	0.63303700	3.25593000
3063	C	-4.60480600	1.50325800	-0.06866000	3107	H	1.48181700	2.37724400	3.11504000
3064	C	-5.57401400	0.73008300	0.58710300	3108	H	-0.38981400	0.68169700	4.86584400
3065	C	-3.96621600	-1.06506400	0.83606800	3109	H	-0.60318100	2.38223000	4.47676800
3066	C	-5.23928400	-0.55899000	1.04229600	3110	H	-2.58233800	1.60597000	-0.76068800
3067	O	-6.84353800	1.12401800	0.83056500	3111	H	-4.83450300	2.50046000	-0.42528100
3068	C	-2.50776600	-3.09662100	-1.32985300	3112	H	-3.73445700	-2.06398800	1.19524700
3069	C	-2.54915200	-4.40011600	-1.82346800	3113	H	-5.99993600	-1.14052600	1.55299000
3070	C	-1.48098900	-5.27512900	-1.57064000	3114	H	-3.34779600	-2.43798000	-1.52719500
3071	C	-0.35018100	-3.52791200	-0.33511400	3115	H	-3.41018300	-4.72328300	-2.39659300
3072	C	-0.37792500	-4.82424500	-0.82110300	3116	H	0.50787100	-3.20433200	0.24678900
3073	O	-1.41502300	-6.55480700	-1.99274700	3117	H	0.43390700	-5.51821500	-0.62876000
3074	C	0.05079300	3.61510600	-0.19227500	3118	H	-0.10860900	3.32190800	0.84156200
3075	C	-0.21881200	4.92178200	-0.56938400	3119	H	-0.58516200	5.65257000	0.14434000
3076	C	-0.00902100	5.32985800	-1.89887200	3120	H	1.14451300	2.40300400	-3.17925900
3077	C	0.74873800	3.09699100	-2.44377000	3121	H	0.65717200	4.69904500	-3.86606200
3078	C	0.47991500	4.40635400	-2.83777200	3122	H	3.36161900	2.28153700	-1.30888300
3079	O	-0.30026400	6.62073200	-2.16809200	3123	H	5.44044300	1.44279700	-2.35153600
3080	C	3.40985400	1.24999100	-1.64596300	3124	H	1.56590300	-1.60401300	-1.83571400
3081	C	4.58065800	0.79172900	-2.23039000	3125	H	3.61990300	-2.41900700	-2.88753200
3082	C	4.67539200	-0.53470600	-2.68796200	3126	H	-0.01568600	-0.01247200	-3.26231100
3083	C	2.40545500	-0.92239600	-1.94338200	3127	H	-1.49635500	-0.88239000	-2.83851000
3084	C	3.57621500	-1.39295400	-2.54109200	3128	H	-1.49235200	0.89833800	-2.85685200
3085	O	5.85732400	-0.87856300	-3.24990500	3129	H	-8.30263700	2.50795600	0.70611300
3086	C	-7.25862100	2.41887100	0.40448500	3130	H	-6.66949500	3.20582500	0.89104900
3087	C	-2.50211000	-7.09556600	-2.74193600	3131	H	-7.18319700	2.52249100	-0.68493800
3088	C	-0.09370600	7.11707100	-3.48899600	3132	H	-2.22708500	-8.12885700	-2.95465000
3089	C	6.02649000	-2.20488800	-3.74013600	3133	H	-3.43188900	-7.07650000	-2.16115900
3090	H	0.44792100	-1.61238600	4.02685700	3134	H	-2.64318900	-6.55332600	-3.68456900
3091	H	2.03214500	-3.04178300	1.87661700	3135	H	-0.38594500	8.16701500	-3.45770300
3092	H	2.42134700	-1.34854300	1.92906200	3136	H	0.96005700	7.03971900	-3.78223100
3093	H	2.68839800	-3.31701500	4.25039500	3137	H	-0.71925500	6.58538100	-4.21621500
3094	H	3.99100500	-2.69044000	3.24607700	3138	H	7.03987600	-2.24488100	-4.14084000
3095	H	2.23220800	-0.99520200	5.09311700	3139	H	5.92314100	-2.94376800	-2.93577000
3096	H	2.06234100	2.64372100	5.47488500	3140	H	5.30925900	-2.42916500	-4.53940000
3097	H	1.73235600	0.96038900	5.81611600	3141				
3098	H	4.12624700	2.11201300	4.28628200	3142				
3099	H	4.12588900	1.27352800	5.82693500					
3100	H	3.78924800	-1.63009500	5.54758900	3143				