

Cartesian Coordinates of all the substrates from **Figure 2** in main text.

1A

H	7.164106533	0.138728010	0.158455011
H	4.144087300	-1.548703112	0.383910027
H	3.994319285	-0.228837016	1.511527109
H	2.678459195	1.083651076	-0.191270014
H	2.830539201	-0.239685017	-1.326540094
H	1.588977115	-1.741245128	0.252728018
H	1.441664102	-0.418443030	1.393978098
H	0.144359011	0.893628066	-0.292012021
H	0.284415021	-0.424189030	-1.435681102
H	-0.952814070	-1.935714142	0.097158007
H	-1.091851079	-0.662668047	1.291695095
H	-1.353095097	1.770957128	1.291546094
H	-2.816623205	1.009897071	1.937431142
H	-2.886849206	2.639014190	1.251204092
H	-3.598152257	-2.091861150	-0.128498009
H	-2.205607160	-0.541341039	-1.543785114
H	-2.314617165	1.722315124	-1.002338070
H	-4.811390347	1.718243126	-0.227941017
O	5.354649384	0.941076066	-1.021625072
O	6.382623445	-0.285587021	0.548952042
C	5.288041383	0.152161011	-0.108324008
C	4.029169290	-0.462156033	0.443037032
C	2.758494200	-0.004458000	-0.261320019
C	1.505468109	-0.651228044	0.325312023
C	0.222417016	-0.195515014	-0.366349026
C	-1.029559075	-0.850394062	0.217086015
C	-2.427490175	1.654449121	1.147732080
O	-5.786324402	-0.681985049	-0.010846001
C	-4.621303333	-0.317565023	-0.132179009
N	-3.501309253	-1.099198081	0.016098001
C	-2.310902166	-0.391197028	-0.461302033
C	-2.745795195	1.083206080	-0.232166016
N	-4.192798304	0.951255066	-0.442179032

1B

H	4.201386300	-1.563953112	0.356693026
H	4.055240292	-0.273260020	1.518005112
H	2.742230197	1.077627075	-0.148618011
H	2.886992206	-0.218423016	-1.309739092
H	1.647734121	-1.752250125	0.247097018
H	1.500147110	-0.447500032	1.407724102
H	0.206393015	0.890709066	-0.264907019

H	0.342855024	-0.415500030	-1.421542100
H	-0.897251062	-1.938963142	0.102379007
H	-1.041137076	-0.669835049	1.300476093
H	-1.301256095	1.765955128	1.303556095
H	-2.769989200	1.006654071	1.939430141
H	-2.833328203	2.636909192	1.255003093
H	-3.544079253	-2.090721149	-0.132327010
H	-2.141862156	-0.541247041	-1.539665109
H	-2.247998163	1.721832123	-0.996082073
H	-4.749763344	1.721460122	-0.236859017
O	5.368825407	0.960400069	-1.024344075
O	6.470900477	-0.245844017	0.512615037
C	5.424973389	0.139205010	-0.075057006
C	4.105095298	-0.475957034	0.442760032
C	2.823978202	-0.009711001	-0.237781017
C	1.566393111	-0.662465049	0.334760024
C	0.281883020	-0.198134014	-0.349484025
C	-0.973714068	-0.853821062	0.225408016
C	-2.374935169	1.651690117	1.153069082
O	-5.730614420	-0.676791047	-0.027852002
C	-4.564002327	-0.314667022	-0.141926010
N	-3.446484247	-1.098213081	0.012857001
C	-2.251662165	-0.392079028	-0.457461033
C	-2.685311194	1.082629076	-0.229477017
N	-4.131429296	0.953675068	-0.448978032

2A

O	4.291938307	-0.721047050	-0.422502030
P	2.769793198	-0.507006037	-0.056743004
O	2.633060190	1.076191079	0.053242004
O	2.111564150	-0.920251068	-1.432549103
O	2.278915163	-1.214109090	1.141487080
C	1.501452108	1.699766125	0.694994051
C	0.357604026	1.867900135	-0.285993021
C	-0.880868062	2.529550183	0.321089023
O	-0.068242005	0.554815040	-0.747832055
C	-1.476641104	0.401129029	-0.563923043
C	-1.808931131	1.333920095	0.602182045
N	-1.809480131	-0.980821072	-0.384163028
O	-1.455533107	3.390477243	-0.650099045
O	-3.181588228	1.672343122	0.558366042
C	-1.464636104	-1.839350134	0.653388045
C	-2.126693152	-3.008681219	0.386077028
N	-2.863996205	-2.895178207	-0.778213058
C	-2.644554189	-1.686117119	-1.217745088
N	-0.662643049	-1.432368103	1.718339124

H	4.861905348	-0.827393061	0.351370025
H	1.200382084	-0.557743041	-1.477613107
H	1.198193084	1.110481082	1.561468111
H	1.845197135	2.677807190	1.026803072
H	0.695646050	2.437083174	-1.152694085
H	-0.642901049	3.081329222	1.235201090
H	-2.010875144	0.741418051	-1.454431106
H	-1.536591113	0.853121061	1.541076112
H	-2.401001170	3.451744247	-0.447604032
H	-3.493666251	1.851484131	1.452600105
H	-2.107085151	-3.914959282	0.969475067
H	-3.041902220	-1.246225090	-2.118747154
H	0.312873023	-1.281247093	1.462149103
H	-0.695529049	-2.109302150	2.469041178

2B

O	4.181013299	-0.024843002	1.035986075
P	3.193180232	-0.578705043	-0.146103011
O	2.416484172	0.774083057	-0.615886042
O	4.041513291	-0.977394073	-1.300068092
O	2.215080157	-1.524640110	0.484348035
C	1.488767105	1.411442101	0.258241019
C	0.228157016	1.751364124	-0.511652037
C	-0.824287060	2.465549179	0.339181025
O	-0.389463028	0.533492039	-0.996534070
C	-1.733975126	0.467306033	-0.556035042
C	-1.781725129	1.323249093	0.711359053
N	-2.140227152	-0.903257065	-0.391184028
O	-1.491483108	3.432059245	-0.463823033
O	-3.110909225	1.753608126	0.949347070
C	-1.626287117	-1.862888134	0.468318034
C	-2.432746175	-2.961352214	0.303388022
N	-3.421162247	-2.702274193	-0.628567045
C	-3.212151231	-1.476592107	-1.029822076
N	-0.562452041	-1.600724115	1.324990097
H	3.793029272	-0.186552013	1.904047138
H	1.242489088	0.765518053	1.104130082
H	1.934302138	2.334649170	0.640530044
H	0.484849035	2.369706173	-1.374591097
H	-0.387069028	2.938697210	1.223509088
H	-2.412629174	0.901607064	-1.297795096
H	-1.383587100	0.752658057	1.550286109
H	-2.380613172	3.537045254	-0.094090007
H	-3.229356233	1.908148140	1.893339136
H	-2.347606170	-3.912394281	0.804100060

H	-3.778445274	-0.937321067	-1.772526128
H	0.331349024	-1.419304103	0.858129062
H	-0.429928031	-2.367477172	1.970985144

2C

O	4.034347290	0.006212000	1.170831085
P	3.255605234	-0.512115037	-0.030805002
O	2.390202171	0.815538056	-0.618300043
O	4.093582295	-0.894464065	-1.237783088
O	2.183972155	-1.543238114	0.342037024
C	1.456239104	1.426529103	0.240636017
C	0.199631014	1.792445127	-0.531153038
C	-0.863335060	2.468479175	0.332279024
O	-0.423102031	0.597538044	-1.072822077
C	-1.731254123	0.449775033	-0.558328041
C	-1.770054130	1.291954095	0.718763053
N	-2.059084150	-0.943932068	-0.386771028
O	-1.583619116	3.410701244	-0.457465033
O	-3.108889223	1.672785123	0.997073074
C	-1.491473106	-1.879362136	0.468915034
C	-2.244210164	-3.016583216	0.300825021
N	-3.248065231	-2.806305201	-0.626491045
C	-3.102199221	-1.569543113	-1.023116072
N	-0.438509031	-1.572377111	1.322310094
H	1.189170088	0.766092057	1.070755079
H	1.872757136	2.349684169	0.667374047
H	0.462543033	2.438311177	-1.372072097
H	-0.429626031	2.958339211	1.209221085
H	-2.472518179	0.848407060	-1.259434090
H	-1.330610096	0.728638050	1.541311109
H	-2.470645177	3.475058252	-0.073904006
H	-3.201193229	1.829584131	1.943550140
H	-2.110303152	-3.963296285	0.799555057
H	-3.698133265	-1.057682078	-1.762212125
H	0.476746034	-1.419618101	0.856017063
H	-0.314675023	-2.316238167	1.997091146

3

H	4.078032295	1.229412086	-0.789810057
H	-5.685570429	-0.118520008	-0.071679005
H	-4.822523347	-1.215583087	1.032662075
H	-4.752072340	-1.508656111	-0.697005052
H	-2.219694160	-1.192557087	-0.953678068
H	-2.226090161	-1.304825094	0.780477058
H	-1.034888075	0.917649067	0.928222065

H	-1.031657072	1.025479076	-0.816692060
H	0.336683024	-1.074003079	-0.946710068
H	0.332448024	-1.184290084	0.802375058
H	1.521032111	1.015397074	0.944910067
H	1.524179107	1.127394079	-0.804378058
H	2.889023209	-0.969077068	-0.936892068
H	2.885054205	-1.082977078	0.812167060
O	-3.630337261	1.358708096	-0.041024003
C	5.407475402	-0.279322020	-0.009475001
C	4.104203296	0.515979037	0.040877003
C	-4.788861345	-0.720905051	0.058111004
C	-3.554869256	0.145217011	-0.013817001
C	-2.228006158	-0.581363042	-0.042799003
C	-0.999595074	0.316462023	0.014985001
C	0.307823022	-0.472595034	-0.030806002
C	1.549800113	0.415009030	0.028283002
C	2.859916206	-0.369209027	-0.019646001
H	4.075114295	1.113961078	0.958093068
H	6.279549454	0.376487027	0.035884003
H	5.471651373	-0.978888072	0.828166062
H	5.475107377	-0.861700061	-0.932198065

4

C	3.077506699	0.810721057	-0.297544120
C	1.889614855	0.022465309	0.201208853
O	1.684062991	-0.150521408	1.398713960
N	1.054193805	-0.474716120	-0.747392283
C	-0.088525377	-1.297115987	-0.414119170
C	-1.383150201	-0.559636670	-0.067391765
O	-2.353229281	-1.201604706	0.332396228
N	-1.392979213	0.769386148	-0.232194622
C	-2.562195254	1.580274033	0.059275855
H	3.138908654	0.867954211	-1.383173251
H	0.150193926	-1.922798163	0.445314668
H	-0.309939315	-1.954598345	-1.254361915
H	1.282368901	-0.339804404	-1.718274289
H	-3.390496336	1.325684652	-0.604314783
H	-0.557783841	1.214750389	-0.574506106
H	-2.304291678	2.627153550	-0.079614670
H	-2.888291653	1.426042123	1.088576573
H	3.986406863	0.349376846	0.089518831
H	3.018248315	1.820311347	0.110483826

5

C	2.915059233	2.099921821	-0.154532395
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N	1.935948223	1.339692567	-0.387340579
C	1.689403855	0.232618446	0.523332606
C	2.004628620	-1.159391109	-0.122024574
O	2.432179394	-1.191415980	-1.296969823
C	0.237555620	0.286644898	1.022398047
C	-0.806480061	0.090959393	-0.075611122
C	-2.234873720	0.158997452	0.465908232
C	-3.247309111	0.002734860	-0.653591752
N	-4.659658206	0.065541841	-0.126071641
O	1.804838204	-2.137134428	0.639410056
H	3.593753016	1.965832344	0.698020098
H	2.349156675	0.301307216	1.401732302
H	0.070769376	1.249471354	1.516256165
H	-0.670744112	0.852911009	-0.846477516
H	-0.649684805	-0.878195045	-0.558402888
H	-2.393345023	1.117767551	0.969255723
H	-2.386752406	-0.626451315	1.212442986
H	-3.160100753	0.798923108	-1.390243922
H	-3.151176179	-0.955980799	-1.159705245
H	-5.345652577	-0.002015509	-0.879835447
H	-4.846306399	-0.695543189	0.529014667
H	-4.831510105	0.943078246	0.367731635
H	0.122852951	-0.491361673	1.779259448
H	3.120662856	2.937104556	-0.819958560

6A

C	-2.240055916	2.302617303	0.266977763
N	-1.537035601	1.297382168	0.563079058
C	-1.215202645	0.364161729	-0.503495945
C	-1.657279928	-1.058927766	-0.195087519
O	-2.062764016	-1.262935761	1.065894427
C	0.304491836	0.372988425	-0.790324830
C	1.173496831	-0.093423496	0.370759009
O	-1.630828490	-1.937548344	-1.025720396
H	-2.636528941	2.489257489	-0.738092003
H	-1.732323268	0.622820915	-1.438098987
H	0.576586345	1.390309545	-1.071900806
H	0.949931382	0.491940676	1.266232948
H	0.950732784	-1.132442213	0.629734637
H	0.479295256	-0.254622629	-1.665525123
H	-2.475108025	3.035318070	1.035988441
C	2.697227461	0.007510497	0.128802054
O	3.094576735	0.631982106	-0.886021804
O	3.421028328	-0.543197520	0.998494777
H	-2.305502685	-2.200221045	1.153148283

6B

C	-2.566327795	2.095281673	0.157309417
N	-1.616153272	1.313279330	0.433160617
C	-1.280483543	0.266939527	-0.519217138
C	-1.681410162	-1.162567940	-0.013104064
O	-2.300054138	-1.261825108	1.068734225
C	0.217632169	0.334802073	-0.847033940
C	1.104515651	0.023064841	0.351851373
O	-1.345533837	-2.093944971	-0.784473320
H	-3.157179314	2.024588090	-0.765135098
H	-1.835390031	0.406268844	-1.459390375
H	0.456770261	1.329545572	-1.230126984
H	0.893867487	0.700206696	1.182950525
H	0.910465184	-0.983891332	0.731563612
H	0.419283309	-0.378284631	-1.645333148
H	-2.834949174	2.887407763	0.854517194
C	2.574876156	0.112944902	0.053189660
O	3.072629146	0.425320518	-1.003711766
O	3.321583149	-0.203576620	1.133490291
H	4.258395714	-0.129377358	0.888542694

6C

C	-2.268654141	2.267814316	0.158952902
N	-1.524383486	1.303941225	0.489102329
C	-1.210894428	0.305147134	-0.524109045
C	-1.701546462	-1.079244199	-0.102471484
O	-2.858400870	-1.030136121	0.572290415
C	0.289978207	0.300191116	-0.835782716
C	1.167052003	0.018467043	0.378179877
O	-1.147978751	-2.113059324	-0.389859660
H	-2.707846127	2.378470920	-0.838778770
H	-1.749923275	0.506696015	-1.463761565
H	0.544963479	1.272831455	-1.257934264
H	0.986814899	0.744786460	1.173196878
H	0.945072995	-0.961138234	0.808154568
H	0.477504642	-0.444311529	-1.608856870
H	-2.497194936	3.038794150	0.891217489
C	2.636470166	0.047019495	0.056939779
O	3.123030702	0.276677871	-1.025347205
O	3.385135596	-0.219824627	1.146279457
H	4.321415866	-0.189186963	0.889775116
H	-3.138848545	-1.940162665	0.766111187

6D

C	-2.523088706	2.111018076	-0.178070057
N	-1.609324182	1.360076316	0.259769268
C	-1.228979484	0.200868038	-0.533969161
C	-1.638728143	-1.150035488	0.140454676
O	-2.214488918	-1.119817351	1.251904474
C	0.280124145	0.239040735	-0.826214827
C	1.168843046	0.095266551	0.404504291
O	-1.357066398	-2.171263905	-0.534517626
H	-3.050628178	1.930426814	-1.124362867
H	-1.758607745	0.211849505	-1.499836387
H	0.510883529	1.179627017	-1.336893214
H	0.948725847	0.876693240	1.132577629
H	0.947721496	-0.855519435	0.904307461
H	0.501494683	-0.563618591	-1.527077115
H	-2.823996866	2.988990941	0.392084389
C	2.688290890	0.099922682	0.129450542
O	3.086067660	-0.262885394	-1.007154281
O	3.424350911	0.445783244	1.092752739

7A

C	0.821801060	-0.917176067	-0.043828003
C	0.408103030	0.403842029	-0.135357010
C	1.371529098	1.434111102	-0.099521007
N	-0.101921007	-1.911278139	-0.031738002
C	-1.513275108	-1.643800116	-0.230687016
C	-1.845178132	-0.259915019	0.334614024
N	-0.964795071	0.727823054	-0.280418020
C	-3.305940236	0.081065006	0.105977008
O	-3.538502254	1.395231100	0.243612018
O	-4.171379299	-0.726466053	-0.127270009
O	1.146966080	2.654633190	-0.142674010
N	4.343415315	-0.659954045	0.215792016
H	-1.717024124	-0.299864022	1.429012104
H	3.408390248	1.686764123	0.039136003
H	0.230448017	-2.860707204	-0.019069001
H	-2.098895149	-2.401641173	0.285912021
H	-1.783028127	-1.671419121	-1.290477093
H	-1.145270083	1.670213120	0.042934003
H	4.574420330	-1.629330119	0.068886005
H	5.042352361	-0.000649000	-0.086162006
N	2.127302151	-1.294540095	0.047285003
C	3.026463220	-0.344676025	0.067574005
N	2.695699192	0.971780068	-0.003368000
H	-4.486992321	1.561920113	0.114982008

7B

C	0.769091053	-0.907498066	-0.105890007
C	0.378493027	0.426457031	-0.159611011
C	1.360182098	1.433959101	-0.067399005
N	-0.167873012	-1.883552135	-0.188978014
C	-1.594334114	-1.592602117	-0.289769021
C	-1.884758135	-0.212137015	0.295818021
N	-0.983049072	0.746097052	-0.334438024
C	-3.368220244	0.214733016	0.153746011
O	-3.584985258	1.442821106	0.020926002
O	-4.219514304	-0.702776052	0.235016017
O	1.169108084	2.663455194	-0.086294006
N	4.290203309	-0.723565050	0.281337020
H	-1.693100121	-0.273455019	1.381620100
H	3.397988242	1.641806118	0.137322010
H	0.147245010	-2.835936206	-0.113119008
H	-2.152981154	-2.348437169	0.257771019
H	-1.922647136	-1.621075118	-1.333188095
H	-1.203680086	1.697630122	-0.073309005
H	4.503245323	-1.690730121	0.094795007
H	5.002451359	-0.073766005	-0.012067001
N	2.066812148	-1.312150092	0.015881001
C	2.979670214	-0.380654027	0.094036007
N	2.674460192	0.942085070	0.051542004

8A

O	-2.810001202	-1.368372100	1.810407128
O	-4.598584330	1.650776117	-0.763775055
C	-1.342806097	1.108367082	-0.845632060
C	-0.750514053	1.256649088	0.571576041
C	0.736728054	1.517262110	0.530331041
C	3.931612284	-0.394724029	-0.108704008
C	2.099847149	-1.957246142	-0.247128018
O	1.180190082	2.636770188	0.723555054
H	-5.660932413	-0.211772015	-1.151180083
O	5.738938431	1.127671082	0.025380002
O	-5.298836371	-1.003068070	-0.725824050
H	-2.975085216	0.244899018	-1.926195137
C	1.661676121	0.375466027	0.228438016
O	6.218123459	-1.017978073	-0.416376030
C	3.032067217	0.632031044	0.158421011
C	3.459196248	-1.695248120	-0.311775022
H	-3.552114254	-2.536550182	0.267868020
H	-3.420078244	1.239895088	0.897205066
H	-5.063996367	-0.485904035	1.275652092

H	-5.116122368	2.190983156	-0.154926011
H	-2.077329149	-1.985591145	1.926533139
C	5.397147397	-0.157073012	-0.186734013
C	1.202096089	-0.929647066	0.021793002
H	-1.548198113	2.094054151	-1.267916092
H	-1.210066086	2.094214153	1.093417079
H	-0.622665046	0.630407047	-1.512476109
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H	3.382222242	1.640884117	0.317411023
H	4.166623298	-2.486220181	-0.519219038
H	1.734635127	-2.962954213	-0.406404029
H	0.145087010	-1.154248083	0.059426004
O	-2.347444167	-1.068728076	-0.464621034
C	-3.780446273	0.762059054	-0.014786001
C	-4.489322320	-0.554442039	0.348927025
C	-3.303434237	-1.498131108	0.495262036
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8B

O	-2.809391204	-1.415174103	1.783939127
O	-4.556803326	1.679471119	-0.731203052
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C	-0.711358053	1.203895085	0.580509040
C	0.773732054	1.491625107	0.534773039
C	4.016280289	-0.349990025	-0.107901008
C	2.195549156	-1.942964140	-0.258549019
O	1.184809085	2.626137191	0.728463051
H	-5.651639425	-0.153558011	-1.141899081
O	5.843077444	1.170913087	0.000267000
O	-5.306292373	-0.959239070	-0.729735051
H	-2.962327212	0.266679019	-1.922959139
C	1.717143125	0.373549027	0.229792017
O	6.288205471	-0.995620069	-0.387048028
C	3.087082220	0.648070047	0.160370012
C	3.553866254	-1.651704119	-0.316830023
H	-3.581080258	-2.541352185	0.224688016
H	-3.378027242	1.222503090	0.917670065
H	-5.048088362	-0.480916035	1.278351091
H	-5.061782363	2.219186160	-0.111514008
H	-2.072407150	-2.031389145	1.876216135
C	5.515870376	-0.029228002	-0.170796012
C	1.275654092	-0.938461068	0.015308001
H	-1.497810110	2.075033150	-1.247623092
H	-1.180840087	2.022769144	1.123432081
H	-0.598173046	0.596240041	-1.506316110

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H	3.435815245	1.657666121	0.321587023
H	4.276913309	-2.428514175	-0.525867038
H	1.850362132	-2.955648212	-0.425801031
H	0.222823016	-1.182282084	0.050832004
O	-2.353243167	-1.083721080	-0.487843035
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C	-4.480869322	-0.544223039	0.346611025
C	-3.311506238	-1.511727111	0.468668034
C	-2.600995186	0.279481020	-0.889757065

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H	2.024976146	-0.542639037	-1.814223131
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H	1.236544088	-2.572068183	1.315656092
H	2.834745202	-2.076105152	1.876885136
H	1.501940110	-0.898521066	1.801510129
C	2.387785170	-1.499326107	-0.111036008
H	-0.672869050	-1.049050075	0.749399055
H	0.339083024	0.803195055	-1.428267101
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H	-0.763629055	-1.423191101	-0.970606067
O	3.336444240	-2.107234151	-0.604293044
C	0.836613059	1.224659090	0.600367041
C	0.526476038	0.214504016	-0.528377038
N	1.693338124	-0.604794043	-0.863064063
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O	0.231245017	1.193591083	1.670075122
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C	-2.004751145	0.229530016	-0.359246026
H	-1.982453140	1.056353076	0.350232025
H	-2.102787152	0.638675045	-1.367431096
S	-3.472679251	-0.796382057	-0.005996000
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H	-4.760892343	0.855072063	-1.230991088
C	2.606359186	2.304032165	-0.841069060
H	3.417936245	1.576202115	-0.884733062
H	2.002997145	2.212023159	-1.743280126
H	3.032301220	3.304599237	-0.827180062

10A

C	-2.220407162	1.021785074	-0.369193027
C	-2.882556208	-0.131807009	0.358278026

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C	-1.237194087	0.434069031	-1.421090103
C	-0.105081008	-0.361377026	-0.846429059
C	-0.105732008	-1.710012123	-0.596916043
C	1.180822084	0.124084009	-0.422345030
N	1.093335077	-2.089797153	-0.038776003
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C	1.796226130	1.384064100	-0.426029031
C	3.206011229	-0.871991061	0.570707042
C	3.087382221	1.504590108	0.059885004
C	3.785101270	0.387015028	0.555862038
O	-3.591540261	-0.949963069	-0.184338013
H	-0.847013059	1.271749092	-2.003505145
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H	-0.880742065	-2.436876176	-0.777707059
H	1.268297089	2.251718162	-0.800925060
H	3.571501255	2.473197177	0.061602005
H	3.741337269	-1.733517124	0.949525069
H	4.792729345	0.513437037	0.931356065
H	-3.030878220	1.492665110	-0.933110065
H	1.340801098	-3.030047216	0.216981015
C	-1.575259116	2.062036149	0.542285038
H	-0.747429055	1.635618115	1.106950078
H	-1.188578087	2.885425206	-0.059816004
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H	-3.048561217	-0.967792072	2.042536147

10B

C	-2.241450160	1.012796073	-0.294324021
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O	-2.867096205	-0.269832020	1.657936118
C	-1.251012091	0.453675033	-1.346301096
C	-0.119373009	-0.352712025	-0.782551057
C	-0.132024010	-1.692814122	-0.495585035
C	1.185523083	0.121160009	-0.406242029
N	1.079334079	-2.079213147	0.039076003
C	1.911089138	-0.989967070	0.102949008
C	1.815710130	1.372778099	-0.454267032
C	3.225427230	-0.876272063	0.556612041
C	3.121300223	1.489530105	-0.005956000
C	3.819674277	0.374920027	0.496021036
O	-3.656971266	-0.908885066	-0.339656025
H	-0.841825058	1.291431094	-1.919449138
H	-1.822915132	-0.160867011	-2.042727148
H	-0.927553069	-2.408027173	-0.624337045
H	1.285358091	2.237758159	-0.832511062

H	3.616092260	2.452372179	-0.038529003
H	3.761081269	-1.735047123	0.941727066
H	4.838860351	0.497086036	0.840845059
H	-3.012219218	1.547612113	-0.861204063
H	1.318817096	-3.015437219	0.315547022
C	-1.577689114	1.997189144	0.663643045
H	-0.789965058	1.513706107	1.241597091
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11A

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C	1.180713084	0.124002009	-0.422393030
N	1.093509076	-2.089889150	-0.038811003
C	1.906382138	-0.989888069	0.077804005
C	1.795981127	1.384046098	-0.426103031
C	3.205980230	-0.871804060	0.570808041
C	3.087097222	1.504737109	0.059878004
C	3.784923271	0.387269028	0.555954041
O	-3.591391260	-0.950141069	-0.183870013
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H	-1.813116129	-0.189414014	-2.106769153
H	-0.880518065	-2.437239175	-0.777734057
H	1.267999093	2.251640161	-0.801063058
H	3.571104256	2.473400180	0.061552004
H	3.741383271	-1.733270125	0.949648066
H	4.792508345	0.513839037	0.931513066
H	-3.030850216	1.492386106	-0.933409066
H	1.340977097	-3.030050216	0.217272016
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C	1.038357075	-1.247160088	-0.096428007
C	0.018485001	-0.148774010	0.006887000

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C	-3.402901245	1.097676077	0.034661002
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H	1.085776077	-1.592518115	-1.133546082
H	1.131544083	1.753243126	0.211513015
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H	-4.239774305	-2.185811157	-0.295640021
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H	-5.262402380	0.052280004	-0.110292008
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H	-1.130033080	2.846577204	0.265208019
C	2.560239182	-0.590793044	1.846214134
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H	3.596812258	-0.445589032	2.152781157

12A

O	-0.932575892	0.824957285	1.637376344
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C	-0.291942978	0.005413121	-0.550242816
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H	-3.056170172	0.030554562	0.687587273
C	1.994040016	-1.062154319	-0.073722782
N	1.072079049	-0.431228127	-0.851724837
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H	1.378022092	-0.302469166	-1.805003906
H	-0.634039923	0.506849212	-1.455914882
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H	-1.056564291	-1.616968872	0.680521270
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12B

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13A

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O 2.375541172 2.841724204 0.518495037
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C	-2.329875165	-0.078551006	-1.429846103
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H	2.158173156	-0.700507051	-1.550031109
H	2.618647190	0.324008023	1.291388093
H	2.043857148	1.854981135	-1.273621094
H	0.279449020	1.496339108	1.180740083
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H	0.098197007	3.474866250	-0.115794008
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13B

H	-0.032730002	-1.368020097	1.158468081
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O	3.006409217	-1.008816073	-1.648432116
O	0.026202002	-1.886346138	-1.521468111
C	2.049299149	0.741457052	0.965543069
O	-2.039120149	-2.257430165	0.338085024
H	-0.827779059	1.894065135	-0.068377005
H	-3.195745228	2.644655188	-0.379908028
C	-2.379003171	-1.065242079	0.263599019
N	-1.369744098	-0.079536006	0.258816019
O	3.633551262	2.113134150	-0.119822009
O	1.500720108	2.318934166	-0.804474056
C	0.017980001	-0.501291036	0.499024036
O	2.588493189	-1.468071105	1.795536131
C	0.721792053	-0.878500063	-0.807130060
C	2.172109155	-1.303918094	-0.532238037
C	-3.959348284	0.612083046	-0.031513002
C	2.766187199	-0.591953043	0.689271052
O	0.659050046	0.570922042	1.166505082
N	-5.256593379	0.945050066	-0.109641008
N	-3.662879265	-0.668027046	0.173465012
C	-1.668820119	1.219704086	-0.008272001
C	-2.951429214	1.614014116	-0.173908013
H	2.438635177	1.150200084	1.901298136
H	3.823494276	-0.394746029	0.501156036
H	2.175134154	-2.376663171	-0.318234023
H	0.746562056	0.014786001	-1.437117104

H	2.994264213	-1.077489076	2.579421186
H	-0.606772044	-2.320784165	-0.918768065
H	2.625973189	-1.429207105	-2.430003174
H	3.788976271	2.795049199	-0.794574059

13C

1	0.029033002	0.395824029	-1.641147118
1	-6.118870445	-0.701125051	-0.584517045
1	-5.846616423	-0.682224051	1.124680082
6	2.719111194	-2.140345153	-0.045928003
8	2.380183173	2.812657201	0.531041038
8	-0.301177022	2.630121187	-0.449905032
6	2.011161143	-0.820495061	-0.446734032
8	-1.321129098	-0.022773002	1.941500139
1	-1.832909131	-0.014407001	-2.398184175
1	-4.271656308	-0.410731030	-2.199919160
6	-2.060488147	-0.103122007	0.964540071
7	-1.513128108	0.022539002	-0.345622025
8	3.982149288	-2.087970152	-0.158215011
8	2.041835146	-3.110023223	0.323808023
6	-0.090246007	0.262401019	-0.559215038
8	4.016039291	0.543119037	-0.111206008
6	0.427456031	1.540639113	0.107633008
6	1.915911138	1.661610122	-0.172857013
6	-4.169069298	-0.411810029	0.000531000
6	2.651558189	0.398798029	0.243595017
8	0.621351046	-0.878232061	-0.134211010
7	-5.483756408	-0.613727047	0.188840013
7	-3.398494247	-0.308428022	1.072703076
6	-2.318322168	-0.101679008	-1.436702102
6	-3.645884261	-0.317328023	-1.326139094
1	2.143920153	-0.704804050	-1.533054108
1	2.543150181	0.273438020	1.330737094
1	2.064064147	1.803563131	-1.252147091
1	0.268132019	1.477143108	1.183983087
1	4.339270312	-0.391351028	-0.161035011
1	0.123774009	3.443696250	-0.150275011
1	3.325222237	2.901073210	0.354590026

13D

H	0.020975002	-1.347317095	1.229104089
H	-5.562021406	1.729118126	-0.279180020
H	-5.924818449	0.057806004	-0.014125001
C	2.128393156	1.995044145	-0.323014023
O	3.038222221	-1.420081100	-1.532236111
O	0.168817012	-1.964078143	-1.402123099

C	2.029703144	0.948263066	0.835158060
O	-1.938301141	-2.312945166	0.386319028
H	-0.824493058	1.854297132	-0.071043005
H	-3.229838234	2.547874183	-0.380615027
C	-2.307550167	-1.128332082	0.294133021
N	-1.328847095	-0.117207008	0.280867020
O	3.295986237	2.382391171	-0.552272042
O	1.071091075	2.369158173	-0.877683061
C	0.077171006	-0.487799035	0.556543042
O	3.144221229	-0.995877070	1.823694134
C	0.814514056	-0.896974064	-0.718524050
C	2.240823159	-1.296077095	-0.355676026
C	-3.935144283	0.499253036	-0.020470001
C	2.902091210	-0.289656021	0.597951045
O	0.692312048	0.587323044	1.218935086
N	-5.243678380	0.792360056	-0.105937007
N	-3.603522257	-0.771177054	0.194741014
C	-1.661066117	1.170833086	0.008283001
C	-2.956552211	1.526318110	-0.164674012
H	2.420337175	1.466679104	1.713258123
H	3.841322278	0.045801003	0.156954011
H	2.191065157	-2.258881164	0.165000012
H	0.841682058	-0.037308003	-1.391297101
H	3.592923260	-0.399460029	2.435142173
H	-0.485441035	-2.370474173	-0.800931055
H	2.577564186	-2.028341147	-2.125289155

14A

O	-2.040008146	1.591529115	0.028056002
H	0.493572036	-1.987067142	-0.052870004
C	-0.564774039	-0.229681017	0.524126038
N	-1.738622123	-1.081202080	0.662930048
C	-0.890059062	1.206209087	0.054555004
H	-2.415051175	-0.585529043	1.231574087
H	-0.146847010	-0.091142006	1.527658109
H	0.296964021	-0.865199061	-1.393739101
C	0.511794037	-0.929129065	-0.329315024
C	1.936807141	-0.478392034	-0.131346010
O	2.730930199	-0.304148022	-1.024600075
O	2.258008164	-0.328558024	1.166892086
H	3.192633232	-0.070673005	1.226080090
C	0.257177019	2.117583154	-0.294912021
H	1.024747075	2.085996152	0.480926035
H	0.724639053	1.787335127	-1.225898090
H	-0.103506007	3.136178227	-0.418388030
C	-2.384468170	-1.473099104	-0.593908041

H	-3.328241241	-1.964652141	-0.358467026
H	-2.594066187	-0.633544047	-1.267606089
H	-1.764798130	-2.194824157	-1.127767080

14B

O	-2.056958148	1.551731112	-0.028941002
H	0.556904041	-1.957747140	-0.051746004
C	-0.529561040	-0.217216016	0.515557037
N	-1.689396124	-1.090246079	0.692319049
C	-0.896985066	1.184239087	0.001913000
H	-2.385658173	-0.577437039	1.221584089
H	-0.103218007	-0.026068002	1.508746108
H	0.423418030	-0.805144057	-1.364948096
C	0.588208040	-0.890615063	-0.290648021
C	2.032376145	-0.429129031	0.031873002
O	2.860238205	-0.530347038	-0.906711063
O	2.268534161	-0.033705002	1.200314085
C	0.226104016	2.105045152	-0.396500028
H	1.002378070	2.103386149	0.370005027
H	0.694193051	1.736416126	-1.312708094
H	-0.154888011	3.110660226	-0.562420042
C	-2.310510167	-1.549386111	-0.552875039
H	-3.237568233	-2.070848151	-0.311330022
H	-2.546816183	-0.741335055	-1.257290091
H	-1.655273118	-2.259220165	-1.059338074

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P	-5.890054414	-0.281841020	-0.522836038
O	-6.685769459	-1.157097084	-1.552206112
O	-6.827325484	0.060908004	0.693621048
O	-5.245903380	0.860475063	-1.191462087
O	-4.877284350	-1.320238095	0.142293010
P	-3.655995262	-1.238896091	1.191022087
O	-4.236103307	-0.542708041	2.476603179
O	-3.031861219	-2.546962183	1.343280097
O	-2.766201201	-0.046043003	0.654236047
P	-1.929265138	0.190339014	-0.729280053
O	-2.699830193	1.379883097	-1.384713099
O	-1.744787128	-1.042196076	-1.494748110
O	-0.581129040	0.806515060	-0.225829016
C	-0.495496036	2.012240146	0.576023041
C	0.948167068	2.425497177	0.686393047
O	1.695805122	1.433094103	1.407337099
C	1.698172121	2.592927186	-0.632733046
O	1.346656095	3.820807272	-1.225674089
C	3.156586228	2.439302178	-0.176173013

O	3.576569260	3.656089265	0.411582030
C	3.010063218	1.335991094	0.895052066
N	3.222141229	-0.008820001	0.363519026
C	2.282904165	-0.921878066	-0.078397006
N	2.823231205	-2.029600145	-0.513685037
C	4.183599304	-1.845743135	-0.360361026
C	5.283445378	-2.703602195	-0.659326049
O	5.287811381	-3.833854275	-1.135467080
N	6.508026494	-2.076556148	-0.328085024
C	6.657780480	-0.823509059	0.207475015
N	7.920506566	-0.381671028	0.412299029
N	5.638066399	-0.039891003	0.483494035
C	4.446584320	-0.593437042	0.183114013
H	-0.911395065	1.805424131	1.562106114
H	-1.064055076	2.808921204	0.096137007
H	0.973243069	3.375665244	1.230909086
H	1.458444106	1.752755124	-1.290578092
H	1.668660123	3.835688276	-2.134248153
H	3.824398275	2.127471154	-0.981518073
H	4.516405326	3.592309256	0.618623042
H	3.738219267	1.482497106	1.693642120
H	1.230901090	-0.700293052	-0.036108003
H	8.688448642	-1.030372076	0.455318033
H	8.018481564	0.464672034	0.948519066
H	7.330378522	-2.628243190	-0.533327036
H	-3.694271266	1.252767091	-1.388370100
H	-4.559301328	-1.159585084	3.149146229
H	-7.358512548	0.863790063	0.588558043
H	-7.230143514	-1.867863135	-1.182415087

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C	-1.244075805	-0.865169252	0.576840937
C	-1.515582104	0.644146806	0.596315935
C	-0.493973160	1.364467047	-0.285400126
C	0.915556012	0.987731275	0.129011904
C	1.086386303	-0.532415803	0.103702901
O	0.100537340	-1.138891026	0.945009965
N	-2.858021270	1.045970591	0.191257908
O	-0.634821428	2.776208123	-0.165597118
O	1.891436976	1.553493495	-0.751839160
C	2.441250482	-0.990712585	0.633797941
O	3.506910499	-0.670196366	-0.252592124
O	-1.553477741	-1.343096341	-0.703583159
C	-1.532863477	-2.764313441	-0.820223164
H	-1.844979754	-1.380389398	1.334544990
H	-1.359254154	0.980098862	1.623882012

H	-0.640522117	1.061788996	-1.330186199
H	1.086178955	1.343533335	1.152996976
H	0.974952359	-0.884888846	-0.927539173
H	-3.536875283	0.832094452	0.911894957
H	-3.132791201	0.540901504	-0.644823153
H	-1.589223527	2.945764959	-0.184446119
H	1.796336792	2.513721549	-0.728111159
H	2.605075413	-0.557671523	1.628824014
H	2.423834682	-2.076307668	0.737464949
H	3.400758321	0.261107680	-0.498881142
H	-1.838098460	-3.001454515	-1.837205236
H	-0.531058337	-3.160447285	-0.639074150
H	-2.233059446	-3.222193602	-0.113612114

17A

O	-3.127685223	-1.035061073	-0.495367036
O	-0.974596069	-0.215128016	0.352550025
H	2.993842215	0.337241024	-0.901915066
O	-3.003910215	0.259201019	1.771435129
C	1.341157096	1.422874103	-0.075454005
O	2.937744209	-1.932637140	0.350215025
H	3.974699287	-0.016182001	1.366897098
H	0.815011059	1.491533110	0.881258066
C	0.853211063	-1.341367095	-0.735161054
H	-0.069899005	-3.015612218	-1.182081087
H	3.946136284	1.539440113	0.905187064
C	1.823168132	2.794175199	-0.497994036
H	-2.624848190	2.239908159	-0.085356006
O	-2.755240200	1.395971102	-0.539276041
H	2.544928185	-2.806778201	0.469456034
C	-0.193886014	-0.232556017	-0.871067065
H	-4.081895294	-0.970351067	-0.638531045
P	-2.514758181	0.127804009	0.394760028
O	0.282412020	-2.594766188	-0.389627028
O	0.397519028	1.001213071	-1.090400080
H	2.367284171	2.734854196	-1.442658103
C	2.468684179	0.391662028	0.063077005
H	1.369996098	-1.403619099	-1.697987121
H	-0.857313060	-0.422072030	-1.714938123
H	2.478819177	3.220880232	0.260842019
C	1.873315137	-0.984341069	0.335088024
N	3.353697239	0.760969055	1.169469084
H	1.371750098	-0.970849071	1.310319097
H	0.973125067	3.464733247	-0.625357045

17B

O	2.753625579	1.261472359	-0.011832714
O	0.938226029	-0.486080683	0.294358499
H	-3.047119564	0.136992365	-0.839273651
O	2.974907110	-0.671508789	1.725899024
C	-1.750127706	-1.336139814	0.025711055
O	-2.244507196	2.370629254	0.237103757
H	-3.769466702	0.919687034	1.419174958
H	-1.236656517	-1.498479847	0.978175466
C	-0.506742702	1.098686541	-0.880067407
H	1.253930456	1.916151390	-0.446717097
H	-4.232942066	-0.596010547	1.072662382
C	-2.640681644	-2.521147150	-0.286339944
H	3.220514258	-1.992734244	-0.557173096
O	3.165743794	-1.061068775	-0.804794679
H	-1.582804109	3.073778302	0.190820215
C	0.188140842	-0.267751429	-0.901963846
P	2.535179004	-0.165752181	0.399714057
O	0.376008773	2.203078925	-0.805245125
O	-0.765244675	-1.285186945	-1.030147594
H	-3.173461839	-2.362661120	-1.226381298
C	-2.515612273	-0.007341781	0.113208501
H	-1.054554302	1.181292983	-1.824958524
H	0.844817386	-0.353717007	-1.769918666
H	-3.369667877	-2.675615306	0.509389517
C	-1.522991665	1.137231912	0.256061355
N	-3.421363414	-0.020495457	1.265713354
H	-0.992147989	1.036395494	1.210508832
H	-2.040566724	-3.427240981	-0.374400986

17C

O	2.638712189	1.260040093	0.365236026
O	0.936349069	-0.618294042	0.244225018
H	-3.023393219	0.241226017	-0.817306059
O	2.994771218	-0.937652067	1.628974115
C	-1.799719129	-1.301185095	0.033825002
O	-2.056760146	2.435796178	0.225877016
H	-3.658474261	1.087562076	1.441775102
H	-1.277255091	-1.484326107	0.978353069
C	-0.424804031	1.044981078	-0.911128063
H	1.338719098	1.799804131	-0.342837024
H	-4.218452304	-0.400176029	1.120413083
C	-2.771319197	-2.432308175	-0.240304017
O	3.198168230	-0.868177064	-0.936241069
H	-1.346226096	3.076483223	0.081381006
C	0.198194015	-0.360129026	-0.916561068

P	2.597115185	-0.279431020	0.326696024
O	0.519828037	2.095203153	-0.865328063
O	-0.844205059	-1.316844095	-1.040899073
H	-3.317024239	-2.251835163	-1.169316083
C	-2.483379177	0.072564005	0.126760009
H	-0.983669072	1.150742083	-1.848306131
H	0.826504059	-0.491565035	-1.801986130
H	-3.489336253	-2.534698183	0.574022042
C	-1.419522103	1.153215082	0.239542017
N	-3.370064241	0.126275009	1.294900094
H	-0.878579064	1.025863073	1.184951085
H	-2.230707158	-3.374941245	-0.333445024

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H	-1.973146140	-0.707394050	2.028350143
C	4.997705359	-1.010737071	-0.088174006
C	1.487897106	-1.228740089	0.001634000
C	-2.248115164	-0.256679019	1.066736078
C	0.644939048	1.159658084	0.104750008
N	1.672871119	0.134684010	0.027819002
N	2.605959187	-1.907339139	-0.042566003
O	-1.510070109	3.133012223	-0.420608030
N	3.706430267	1.491394105	0.014046001
C	3.033437220	0.335592024	0.002353000
C	-1.550080111	1.095354079	0.957552069
C	3.592907258	-0.939962069	-0.046585003
O	-5.919767452	-0.520572037	0.068123005
O	-3.643277264	-0.082049006	0.986628073
O	-4.154898301	-2.388633171	-0.003828000
C	5.022311360	1.297535095	-0.026655002
H	-1.883153135	-0.924616066	0.279802020
H	5.163801371	-3.047124221	-0.203548015
H	0.021937002	1.788085130	-1.898013136
N	5.692956421	0.140479010	-0.077976005
H	-2.502944183	1.366812096	-0.974887069
C	-0.329280024	1.169564087	-1.074940077
O	-0.144334010	0.939641070	1.266808090
H	-1.980963141	1.782314129	1.690387119
O	-3.929777282	-0.366038026	-1.545711112
H	1.180606084	2.106165150	0.190638014
H	-0.488630035	0.156923011	-1.444681105
C	-1.607937118	1.700170125	-0.447446032
H	5.636643389	2.191876158	-0.019033001
H	0.500177036	-1.659141118	0.032498002
N	5.663660427	-2.178967154	-0.125314009
H	6.664523469	-2.180313159	-0.221800016

P	-4.484095325	-0.918083066	-0.234331017
H	-2.316282168	3.482465251	-0.023462002

19

H	-0.241074017	1.489484109	-1.861655135
C	0.846295061	2.047256149	1.260015089
H	1.722597122	1.398974103	1.321463093
H	1.090729081	3.012637215	1.694942124
H	0.029644002	1.591505117	1.814303132
C	0.479531034	2.261544163	-0.187010014
H	0.019412001	-1.952731138	0.377711027
H	-0.698028052	-0.602028044	-1.454386105
H	-3.545898257	-0.892910062	0.748295054
H	0.539556039	-0.570957042	1.328264095
O	0.671325048	3.344765240	-0.737552052
C	-1.881804135	0.048314003	0.224819016
C	-0.528845038	-0.078133005	-0.514386037
N	-0.013960001	1.220742089	-0.915623064
S	2.071723151	-1.051264073	-0.477121034
C	0.430488031	-0.946455069	0.312794022
O	-2.178091154	1.079729078	0.820404058
N	-2.708195194	-1.016207075	0.197366014
C	2.801608202	-2.321929167	0.595703042
H	2.828180203	-1.982468142	1.631007119
H	2.245486163	-3.256603236	0.526525038
H	3.820754275	-2.484386180	0.247926018
C	-2.535792183	-2.311428168	-0.444926032
H	-2.073123148	-3.039487219	0.224912016
H	-3.514876252	-2.685747193	-0.738042054
H	-1.930594140	-2.227784158	-1.344398095

20

N	0.386143028	-0.446458032	-0.470767034
H	4.303481308	-2.207909160	-0.939670069
H	-4.196115303	2.655911190	0.065282005
O	2.760134200	2.351898168	-0.002417000
H	4.306654308	1.624453116	1.317837097
C	2.057321148	1.183784085	0.395175028
C	-4.943936357	0.369130026	0.331010024
H	-5.134675370	1.010057073	1.192977084
C	3.600192261	-0.476551034	-0.409307030
N	-3.505051251	0.171436012	0.138655010
H	1.364781098	-2.345909167	-0.289721021
O	-3.744966272	-2.075456147	0.632789043
N	-0.729444051	-2.302134165	0.102728007
O	4.123487298	0.744152056	1.677974119

H	1.290813094	1.406182101	1.137325079
C	-2.712495193	1.244986090	-0.204591015
H	2.158634154	3.104695223	-0.009286001
H	2.617900188	-0.592485041	1.487333109
C	-1.597473114	-1.225943086	0.058313004
C	-0.918948065	-0.070328005	-0.294201021
C	1.484441108	0.453752032	-0.829307058
C	-2.996778218	-1.158580082	0.309825023
N	-3.313890240	2.450531176	-0.369326027
H	1.101845078	1.158110082	-1.566982112
C	0.436467031	-1.804091128	-0.213783015
O	3.819805275	-1.837881132	-0.190716014
H	4.500700324	0.009232001	-0.792017059
O	2.555442185	-0.274845020	-1.380079099
H	-5.387056410	0.807333057	-0.562792043
H	-2.686728193	3.230286230	-0.481893034
C	3.104254223	0.180183013	0.889967064
N	-1.414961103	1.169565082	-0.425716031
H	-5.389312398	-0.601526045	0.513584037

21A

C	-0.631428147	-0.814928159	-0.746693102
P	0.715561911	0.096291959	0.022080956
O	-2.440156339	0.674901879	0.008597955
O	1.963421000	0.065015006	-0.978258118
H	-0.345956088	-1.865900221	-0.821901106
H	-1.723730308	1.251969944	0.318912978
O	0.332153830	1.459066043	0.462515988
H	-0.752008174	-0.425182136	-1.759747170
O	1.182578984	-0.899248092	1.174863040
H	-1.822014229	-1.017571220	1.057890029
H	-2.710754279	-1.279283274	-0.443324077
C	-1.947734249	-0.660330200	0.028822957
H	1.775380013	-0.501241042	1.828163089
H	2.016648976	0.846500064	-1.545738159

21B

C	-0.585721045	-1.039948073	-0.487160035
P	0.813942058	0.077345006	-0.110543008
O	-2.330248166	0.659351047	-0.159309011
O	2.019597144	-0.317249023	-0.900385067
H	-0.304384022	-2.059095146	-0.211171015
H	-1.521073112	1.215156088	-0.162430011
O	0.288077021	1.495382107	-0.164945012
H	-0.735982052	-1.020707072	-1.570198112
O	1.146247082	-0.268314019	1.464755106

H	-1.750921128	-0.705691052	1.305180092
H	-2.685069196	-1.339699097	-0.049337004
C	-1.886209134	-0.643499046	0.216005016
H	0.630501045	0.297173022	2.052105148

21C

C	-0.578679040	-1.012802074	-0.529059038
P	0.845807059	0.051441004	0.029808002
O	-2.258498161	0.714230051	-0.079927006
O	1.990500143	-0.215054015	-0.945751067
H	-0.340205024	-2.062766149	-0.331999024
H	-1.380773099	1.193628083	-0.070938005
O	0.270931020	1.488484107	-0.087156006
H	-0.688341049	-0.900660064	-1.613217116
O	1.142673082	-0.349358025	1.475369105
H	-1.829642134	-0.855161060	1.222917086
H	-2.722769196	-1.267041092	-0.243140018
C	-1.903025138	-0.651538047	0.143890010

22A

H	3.937109282	-1.435699105	-0.736037054
H	3.875576276	-0.235909017	0.433881031
C	2.045377146	-0.584361043	-0.306098022
N	3.412641245	-1.100758080	0.070048005
C	1.050565078	-0.960137068	0.804261056
C	2.217982160	0.959195069	-0.458396033
O	3.224417231	1.429985102	0.138925010
H	1.371187101	-0.484495035	1.734083126
H	1.754611129	-1.031056075	-1.252971089
H	1.111380080	-2.041672149	0.958261071
O	1.354012098	1.552938113	-1.117836079
C	-0.376857027	-0.586040043	0.498494036
C	-0.999415069	0.478820034	1.144331085
C	-1.115728081	-1.306088092	-0.442841032
C	-2.316793168	0.824170059	0.863904063
H	-0.449398032	1.055787078	1.877893134
C	-2.429717175	-0.973505070	-0.737524053
H	-0.659068049	-2.145074156	-0.955317068
C	-3.035421217	0.097170007	-0.081757006
H	-2.784415202	1.655708118	1.378153100
H	-2.997542217	-1.536907111	-1.466581106
O	-4.333505312	0.381541027	-0.403068029
H	-4.647001334	1.132783082	0.115971008
H	3.399737247	-1.839223131	0.771920056

22B

H	-4.099734277	-0.994634736	0.700871210
H	-3.817498227	-0.589337728	-0.835915900
C	-2.135070108	-0.616990864	0.283722178
N	-3.459723245	-1.157404800	-0.071156847
C	-1.131791071	-1.036467976	-0.806570899
C	-2.138394987	0.926608249	0.456119191
O	-2.655541973	1.584425334	-0.483991877
H	-1.458026056	-0.589903916	-1.749462970
H	-1.830983122	-1.065039922	1.232076245
H	-1.202693160	-2.121554048	-0.919285907
O	-1.631275914	1.392717238	1.506936269
C	0.293668065	-0.641917060	-0.519386879
C	0.862550195	0.500902978	-1.079944919
C	1.085301061	-1.400381175	0.347334183
C	2.170031319	0.880421902	-0.792154899
H	0.271876203	1.113321070	-1.750413970
C	2.391839186	-1.038571254	0.646194203
H	0.672195963	-2.296227208	0.797091213
C	2.938864313	0.108269785	0.074400163
H	2.591787423	1.772326930	-1.241630932
H	2.997633183	-1.636302347	1.315347254
O	4.233118435	0.421678705	0.396287186
H	4.501112517	1.227367742	-0.062704846

22C

H	4.074770293	-0.941399066	-0.738519054
H	3.777108270	-0.659276047	0.859159063
C	2.026954147	-0.620823044	-0.315532023
N	3.412219247	-1.117124082	0.019962001
C	1.055061073	-1.025646073	0.811389058
C	2.042538148	0.887251062	-0.522423038
O	2.890959209	1.486326106	0.321257023
H	1.391020098	-0.569304040	1.744205128
H	1.742500124	-1.085090078	-1.255653092
H	1.129349082	-2.108757150	0.930848065
O	1.335797097	1.447672105	-1.313185094
C	-0.371449027	-0.635853048	0.518224037
C	-0.937920069	0.498397036	1.095451077
C	-1.152106085	-1.395531101	-0.355756026
C	-2.245485163	0.873072064	0.811508060
H	-0.354913026	1.102847081	1.779867129
C	-2.457704179	-1.034475073	-0.649604047
H	-0.737111051	-2.286901162	-0.811686059
C	-3.008960217	0.105701008	-0.065489005
H	-2.671486195	1.756854126	1.271283093
H	-3.061586222	-1.627666116	-1.323594095

O	-4.298316311	0.414432030	-0.385926028
H	-4.576351329	1.214477085	0.077736006
H	2.863781206	2.449484178	0.192576014
H	3.404296247	-2.125397155	0.190267014

22D

H	-4.107582124	-0.921103086	0.680539114
H	-3.788514104	-0.652702062	-0.896664003
C	-2.108841982	-0.674408040	0.276900082
N	-3.454440077	-1.131201091	-0.066470942
C	-1.116583908	-1.084726051	-0.828260996
C	-2.030159004	0.827071067	0.537223103
O	-2.436995045	1.545958116	-0.526481975
H	-1.447933937	-0.645004026	-1.771403066
H	-1.813415956	-1.149060072	1.213006152
H	-1.193685896	-2.168809131	-0.929868002
O	-1.660468983	1.336151111	1.569030176
C	0.305953189	-0.677969001	-0.536258974
C	0.861394213	0.471701089	-1.096139018
C	1.097121256	-1.425193042	0.340466087
C	2.160097297	0.869757139	-0.796611995
H	0.271469159	1.072362121	-1.777983068
C	2.394515346	-1.043709994	0.649578107
H	0.692494244	-2.325535113	0.788421120
C	2.930468366	0.110349095	0.080073068
H	2.573503312	1.765875206	-1.244624027
H	3.002512398	-1.630820028	1.325696157
O	4.213713453	0.442222139	0.415237092
H	4.477208458	1.251625201	-0.040215940
H	-2.378759051	2.489694182	-0.305706959

23A

C	1.070337076	-0.354757026	-0.360952026
N	1.985996141	-1.441040101	-0.033685002
C	-0.353984025	-0.756638057	0.051612004
C	-1.426264102	0.262774019	-0.313303023
C	-2.821132202	-0.217590015	-0.005266000
O	-3.742245269	0.712369051	-0.326139024
H	1.099776080	-0.204336014	-1.444200104
H	-0.366612026	-0.930455066	1.130514081
H	-0.576540042	-1.709746122	-0.428421031
O	-3.113894224	-1.289837095	0.467335033
C	1.455354102	0.968541069	0.331333024
O	1.755358126	0.966203069	1.508496109
H	-1.396736101	0.509582037	-1.378516100
H	-1.293502092	1.209453087	0.216754015

H	-4.621928334	0.360232026	-0.112675008
C	3.354441241	-1.233588088	-0.506457037
H	3.354957242	-1.169432083	-1.596509117
H	3.835552278	-0.326876024	-0.113200008
H	3.965648287	-2.089679151	-0.219684016
H	1.993568143	-1.559228114	0.974583072
C	1.465525106	2.220075162	-0.498958036
H	1.581877112	3.102316222	0.126999009
H	2.302467165	2.156067157	-1.201556085
H	0.560094038	2.296603167	-1.103877082

23B

C	1.018757075	-0.371204027	-0.341917024
N	1.927807138	-1.450576103	0.031515002
C	-0.413790030	-0.730629053	0.087422006
C	-1.481807107	0.284474021	-0.302055022
C	-2.940583213	-0.151457011	-0.022317002
O	-3.802466275	0.761102053	-0.109707008
H	1.047431073	-0.269558020	-1.431311103
H	-0.417266030	-0.870487060	1.172925082
H	-0.655424050	-1.696842124	-0.354716026
O	-3.157415226	-1.358732100	0.245670018
C	1.416984100	0.976201069	0.284700021
O	1.747389124	1.028049073	1.453869104
H	-1.419867100	0.501218036	-1.374604099
H	-1.328671096	1.240043088	0.205025015
C	3.300317235	-1.267664092	-0.438010032
H	3.309352238	-1.246611088	-1.529969111
H	3.782599273	-0.347277025	-0.078624006
H	3.907552283	-2.113553152	-0.113725008
H	1.927611136	-1.529153109	1.043559073
C	1.402410099	2.193303159	-0.596739044
H	1.513435110	3.102215223	-0.008622001
H	2.235208160	2.111277150	-1.302599094
H	0.489592035	2.231257159	-1.193108087

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H	-1.207908265	-0.488342780	-1.801771130
C	-3.362982447	-0.610170293	-0.587484041
H	-3.736248659	-1.425511268	0.032487002
H	-4.077432308	0.211220928	-0.520653038
H	-3.303333519	-0.945187334	-1.621819115
C	-2.043415243	-0.139076563	-0.011532001
H	0.672970149	0.706823877	-1.665326121
H	2.005176503	-2.523931665	0.359738026
O	-1.968365156	0.225385446	1.159529082

C	1.336248813	-0.954930398	-0.629863047
C	0.395501027	0.271011908	-0.703924049
N	-1.001528169	-0.148404802	-0.876545065
C	0.664653298	1.366248925	0.348508025
O	2.086582819	-1.169786585	-1.585002116
N	1.330755626	-1.775457453	0.436741031
H	0.338307195	1.021957973	1.326191096
C	-0.117611469	2.635331196	0.003238000
H	0.182664641	3.020858153	-0.975150070
H	-1.191476586	2.455320426	-0.012376001
H	0.081420723	3.411650207	0.744347053
C	2.167439473	1.660541602	0.410475030
H	2.547904574	1.979098537	-0.563580041
H	2.358167669	2.463445615	1.124007080
H	2.743589315	0.790326407	0.729785053
C	0.627379597	-1.674597285	1.705997123
H	0.291312346	-2.667735280	2.003683144
H	1.283221734	-1.281098405	2.486766181
H	-0.241947318	-1.032805043	1.623593118

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H	-2.229241311	-3.235495197	-0.135227962
H	2.691340099	-0.533349103	1.587068161
H	2.471534052	-2.063274207	0.723748098
H	2.012469111	2.519339131	-0.462091985
H	-0.547035060	3.213819234	-0.909756018
H	-3.041625296	0.353577077	-0.715443005
H	-3.564215331	0.609058105	0.832949110
H	1.001449968	-0.863642094	-0.928783020
H	1.100481018	1.332953066	1.190504133
H	-0.616283110	1.060217080	-1.306852049
H	-1.396401164	0.974053091	1.642592163
H	-1.773627240	-1.425313075	1.370978145
C	-1.523295254	-2.774381176	-0.831283011
O	-1.523073222	-1.350179076	-0.675506003
O	3.529635154	-0.680574130	-0.321307976
C	2.494384074	-0.979689130	0.604579091
O	1.893531084	1.595589069	-0.713013002
O	-0.762884084	2.742480202	-0.096936959
N	-2.858929275	0.877873110	0.145331058
O	0.154046902	-1.145253097	0.954663116
C	1.128149987	-0.522229070	0.103573055
C	0.940531003	0.995761042	0.160470059
C	-0.481584093	1.357644101	-0.262534971
C	-1.186142189	-0.905973051	0.607093090
H	3.441288165	0.254861939	-0.556169993

H	-1.833273279	-2.972627187	-1.853868085
H	-0.524744188	-3.180693226	-0.663192001
C	-1.463425177	0.601450066	0.622580092
H	-2.961368259	1.879403184	-0.043830956

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N	-0.890212063	-0.120847009	-0.372814027
N	-1.844886132	-2.000658145	0.396515028
N	-4.890062351	0.058975004	-0.064941005
N	-2.890598210	1.240855089	-0.684372051
N	-4.898635350	-2.113662152	0.747588052
C	0.131618009	0.827408058	-0.825860061
C	0.362579026	1.958134143	0.181701013
C	1.539182113	1.408756103	1.007026072
C	2.343354167	0.651164046	-0.051404004
C	-0.720151053	-1.410619104	0.074642005
C	-2.815284201	-1.050709077	0.146559010
C	-2.241916159	0.123416009	-0.336646024
C	-4.217028304	-1.053084078	0.280845020
C	-4.205481302	1.115943080	-0.517501037
O	0.754578055	3.111634224	-0.540270037
O	2.341754168	2.426288175	1.578480112
O	1.355387096	0.141105010	-0.969702068
H	-0.193921014	1.230957088	-1.785448129
H	1.374034101	3.599785260	0.022518002
H	-0.527903038	2.151731153	0.783649058
H	1.987075144	2.662762189	2.443748177
H	1.168301084	0.721038054	1.771198126
H	2.978815217	1.368093097	-0.581066042
H	-4.422812318	-2.973506214	0.957038068
H	-5.903556424	-2.090565153	0.774086057
H	0.258635018	-1.855633135	0.122335009
H	-4.804520346	1.981261142	-0.781037055
C	3.183156228	-0.474344034	0.509831037
H	3.866900278	-0.048069003	1.246906088
H	2.547824181	-1.207205089	1.010653074
S	4.166230299	-1.303830092	-0.785435057
C	5.167937372	-2.385312171	0.274627020
H	5.779541408	-1.797716129	0.959233069
H	4.533167328	-3.068006222	0.839308058
H	5.817933429	-2.963011211	-0.380974028

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H	-0.630840030	1.023541075	-1.907079096
C	-1.322221076	2.429771183	1.064358120
H	-0.377810006	2.619059192	1.578843154

H	-1.943510113	3.316026248	1.174174125
H	-1.819702116	1.583674124	1.523950153
C	-1.043005056	2.243328168	-0.407580987
H	-0.179072012	-1.578984111	1.249236135
H	-0.594771039	-0.992590069	-1.127465036
H	-3.647494262	-2.185744142	0.342968067
H	-0.233434008	0.108722009	1.683209163
O	-0.970338044	3.222468234	-1.151200038
C	-2.390067167	-0.692912040	-0.007091958
C	-0.928148060	-0.324172019	-0.334014981
N	-0.814715043	1.002949074	-0.915331022
C	0.012099007	-0.574113039	0.873265103
O	-3.244654223	0.169670028	0.174430055
N	-2.690925193	-2.006302132	0.073830048
C	1.465968112	-0.444098039	0.493857078
C	2.109158155	-1.479858115	-0.188156971
C	2.189413172	0.712471040	0.782343101
C	3.438556251	-1.361217116	-0.576254000
H	1.565908109	-2.390453181	-0.413585987
C	3.521161264	0.836289044	0.396925071
H	1.712246140	1.523451102	1.317936137
C	4.149396308	-0.199561034	-0.286041978
H	3.921025278	-2.176306176	-1.101043036
H	4.066378309	1.742057108	0.631198088
H	5.185279379	-0.105503032	-0.586313998
C	-1.845120140	-3.170168218	-0.147559968
H	-1.109614083	-2.981606209	-0.926605027
H	-1.324111101	-3.480087245	0.760912094
H	-2.474203190	-3.993450276	-0.479953992

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H	-1.226546184	-0.429604217	-1.903117082
C	-2.282675317	0.084957707	1.235621145
H	-2.125603418	1.155095799	1.374563151
H	-3.252046353	-0.187847417	1.644465170
H	-1.497027202	-0.450628247	1.763041182
C	-2.281415277	-0.249457317	-0.236260963
H	0.812269895	0.208134048	-1.407321049
H	2.413407281	-2.304799964	0.640386102
O	-3.321358318	-0.565669450	-0.816397006
C	0.790492050	-1.274292064	0.155848066
C	0.253298874	0.023357974	-0.489944981
N	-1.122707203	-0.150072185	-0.938822015
O	0.024807084	-2.085399203	0.670967102
N	2.123436167	-1.472441934	0.148135065
C	0.485430764	1.210510087	0.438441086

C	1.506231722	2.264041272	0.090706061
C	0.041232585	2.578441134	0.002025054
H	0.381688780	0.992880058	1.492955162
H	2.052844774	2.154456320	-0.836484003
H	2.081403719	2.691520364	0.900968119
H	-0.399095516	3.226881133	0.747450106
H	-0.397915455	2.660445096	-0.983640015
C	3.177188157	-0.621926759	-0.386450974
H	2.905746094	-0.224000759	-1.362899042
H	3.408889082	0.209265326	0.280109075
H	4.070590285	-1.229441704	-0.512135983

Ado-H

N	-0.220422015	-0.292878997	-0.430681046
N	-1.654634073	-1.892738154	0.217838001
N	-3.993743323	0.977957985	0.091850992
N	-1.753043182	1.603625096	-0.513634052
N	-4.606809306	-1.175437192	0.697718033
C	1.023549055	0.372399087	-0.823467074
C	1.679056080	1.127635161	0.339830009
C	2.696975186	0.094401116	0.853457046
C	3.130463234	-0.601832920	-0.435681046
C	3.642890314	-2.012903010	-0.272420034
C	-0.415223990	-1.614585098	-0.104125022
C	-2.318455155	-0.687542087	0.100790992
C	-1.443735122	0.319043011	-0.302677037
C	-3.659531261	-0.308083100	0.301026007
C	-3.044911281	1.838838075	-0.294663037
O	2.343179094	2.261455262	-0.190728029
O	3.822966247	0.688795195	1.478639092
O	1.941671148	-0.605757955	-1.258693104
H	0.778266018	1.063088131	-1.631483135
H	3.140291146	2.394522294	0.344092010
H	0.944839019	1.419774161	1.094549063
H	3.633037229	0.823786194	2.414572159
H	2.203784170	-0.615200948	1.522969096
H	3.887681269	0.023189147	-0.920551080
H	2.895460280	-2.645488076	0.209421000
H	4.541528376	-2.002548980	0.346513010
H	-4.390203262	-2.149306251	0.816500043
H	-5.560597390	-0.869950194	0.786771039
H	0.396121089	-2.320796124	-0.143420025
H	-3.376868334	2.860371135	-0.447631047
H	3.898229344	-2.445303032	-1.240114103

Cartesian Coordinates of all the transition states between substrates and CH₃ radical.

1A-TS-CH₃

H	-7.414761550	0.446216032	-0.151757011
H	-4.533381327	-1.418143104	-0.647372046
H	-4.259147304	0.058845004	-1.530106109
H	-2.880766208	0.949477067	0.387781028
H	-3.149628224	-0.540359039	1.266141094
H	-2.001396146	-1.823908133	-0.560540039
H	-1.731164126	-0.329511024	-1.436660101
H	-0.369171026	0.541333038	0.472953034
H	-0.628807048	-0.954633069	1.345421096
H	0.511578037	-2.236418161	-0.459380033
H	0.781730054	-0.761213053	-1.368216099
H	1.247794090	1.697715123	-0.853287064
H	2.690547196	0.967610072	-1.663642120
H	2.947633214	2.492221178	-0.532030038
H	3.132405225	-2.650944190	-0.251416018
H	1.837865130	-1.303929096	1.439393106
H	2.137048156	1.001021069	1.365659099
H	4.637859331	0.959311070	0.585134044
O	-5.571554375	0.879569065	1.161965086
O	-6.661457468	0.035075003	-0.606447044
C	-5.549281411	0.259725019	0.124580009
C	-4.332376312	-0.350354025	-0.517951037
C	-3.042939217	-0.124210009	0.260817019
C	-1.832638134	-0.749287055	-0.429786031
C	-0.531159039	-0.532822037	0.339344024
C	0.677214050	-1.159413086	-0.355699026
C	2.274929162	1.360706100	-0.737912051
O	5.424700386	-1.421149101	-0.097304007
C	4.290258307	-0.997495071	0.096924007
N	3.115175224	-1.644704120	-0.197335014
C	1.975408140	-0.954019070	0.407898029
C	2.529470182	0.503911036	0.478339035
N	3.959505286	0.216432016	0.651370049
C	3.646703264	3.636069262	-0.267635019
H	4.631607335	3.466745248	-0.693121049
H	3.641882263	3.715893268	0.815762057
H	3.080469224	4.415759317	-0.768172057

1B-TS-CH₃

H	-4.596781328	-1.431678104	-0.634192045
H	-4.315604309	0.031298002	-1.540366110
H	-2.943116210	0.944568070	0.357816026
H	-3.203493229	-0.531745039	1.253667089

H	-2.058510146	-1.837816134	-0.561231039
H	-1.789596127	-0.352745025	-1.452110103
H	-0.429239031	0.538702037	0.449738032
H	-0.688455050	-0.948021068	1.337004098
H	0.458432033	-2.246545164	-0.453043033
H	0.731756053	-0.778885055	-1.373005100
H	1.194757088	1.684445120	-0.876804060
H	2.643866190	0.948945070	-1.670772122
H	2.892132210	2.483302176	-0.550881041
H	3.081116223	-2.655136189	-0.229238016
H	1.774009126	-1.297813093	1.444229103
H	2.067951149	1.007265070	1.353980098
H	4.574704329	0.963255070	0.592675042
O	-5.542928373	1.111059081	1.015313073
O	-6.770217469	-0.090280007	-0.426881031
C	-5.679157383	0.276451020	0.085620006
C	-4.407943316	-0.359759026	-0.520102038
C	-3.107143224	-0.129826009	0.239839017
C	-1.892663138	-0.760975056	-0.439863031
C	-0.590026044	-0.537113040	0.326153024
C	0.622475045	-1.168408083	-0.357502026
C	2.221436158	1.349737097	-0.751430053
O	5.370522373	-1.420648103	-0.066441005
C	4.233786305	-0.997628070	0.116490008
N	3.062044220	-1.648613121	-0.181751013
C	1.916626136	-0.955574068	0.410801030
C	2.467936176	0.503531036	0.473831034
N	3.897188283	0.219712016	0.660069046
C	3.589718256	3.629487260	-0.292069021
H	4.580125332	3.453217249	-0.701717052
H	3.570224255	3.723638270	0.790012059
H	3.031815218	4.403466317	-0.810517059

2A-TS-CH₃

O	3.552166256	-2.348103168	-0.559899042
P	2.215105161	-1.621900116	-0.140336010
O	2.614324188	-0.072801005	-0.155911011
O	1.354342098	-1.863301135	-1.441200103
O	1.608754115	-2.044310145	1.135470080
C	1.779309128	0.913332065	0.430101031
C	0.745516053	1.427623103	-0.528844038
C	-0.149038011	2.520554180	0.052618004
O	-0.154378011	0.330815024	-0.904104066
C	-1.508773106	0.678939051	-0.612984045
C	-1.408688099	1.746632125	0.479060034
N	-2.270106161	-0.490953035	-0.284208020

O	-0.456483033	3.447265249	-0.977511068
O	-2.580572183	2.539161185	0.465860033
C	-2.156992154	-1.336893097	0.813823057
C	-3.182309227	-2.235569160	0.680527049
N	-3.917272284	-1.970570142	-0.459929033
C	-3.342884243	-0.939067066	-1.016637074
N	-1.198339084	-1.142762085	1.808393132
H	4.090711292	-2.628734187	0.192635014
H	0.626048045	-1.204097088	-1.485097108
H	1.399270098	0.601186043	1.401861098
H	2.600579190	1.926540140	0.675396051
H	1.227139090	1.779350128	-1.441649105
H	0.323559023	3.024697218	0.900210062
H	-1.976716144	1.120216080	-1.496189107
H	-1.251559091	1.267543091	1.444791105
H	-1.306221095	3.851865278	-0.747895054
H	-2.741688198	2.882903206	1.351912095
H	-3.422976246	-3.050070219	1.344521097
H	-3.632571262	-0.460964033	-1.939074142
H	-0.249226018	-1.371825098	1.514944107
H	-1.419224102	-1.692528123	2.628104191
C	3.502557254	2.930611212	0.878469064
H	4.452256322	2.409264172	0.944196069
H	3.178418229	3.392879242	1.805606131
H	3.398248243	3.563499259	0.002524000

2B-TS-CH₃

O	3.992970285	-0.831977059	0.882306065
P	2.882354205	-1.344508096	-0.199005014
O	2.274218165	0.069462005	-0.771088057
O	3.608009257	-1.956577140	-1.340616097
O	1.798637131	-2.063891148	0.543055039
C	1.495611108	0.889205065	0.047035003
C	0.321557023	1.449927104	-0.704811051
C	-0.534108038	2.399259172	0.133108010
O	-0.559710041	0.364829026	-1.120403081
C	-1.858416136	0.567507039	-0.592832044
C	-1.668295117	1.484328107	0.618187042
N	-2.491430180	-0.696100053	-0.316860023
O	-1.046955073	3.424379248	-0.709365050
O	-2.876892207	2.174634156	0.886418063
C	-2.103896149	-1.687218120	0.572918040
C	-3.094942222	-2.634589189	0.509076037
N	-4.073336291	-2.253873162	-0.390858028
C	-3.678455264	-1.105188082	-0.872383065
N	-0.968501069	-1.573297112	1.369090099

H	3.619571261	-0.798819056	1.771189125
H	1.216562086	0.416026030	0.989917073
H	2.223477158	1.914574140	0.389039028
H	0.670660047	1.957229139	-1.606346115
H	0.028392002	2.831649203	0.965135068
H	-2.498922182	1.077872079	-1.319542095
H	-1.339731096	0.895448065	1.474428106
H	-1.881272138	3.719096267	-0.315427023
H	-2.904571209	2.412387175	1.820133131
H	-3.147936228	-3.559110258	1.061297078
H	-4.182608303	-0.513591037	-1.620028114
H	-0.079488006	-1.581017115	0.863171063
H	-0.941777068	-2.313368169	2.057790147
C	3.050457217	3.015600216	0.713702049
H	4.051479292	2.632121191	0.543544041
H	2.821131202	3.226789231	1.753632124
H	2.743294198	3.793381275	0.021086002

2C-TS-CH₃

O	3.865436277	-0.876108065	0.999088070
P	2.927778209	-1.356631097	-0.095760007
O	2.270897165	0.068429005	-0.779969058
O	3.591346259	-1.991898144	-1.301046096
O	1.702501124	-2.107208153	0.428770031
C	1.509903106	0.891754064	0.017697001
C	0.341357025	1.481161108	-0.731372055
C	-0.513137037	2.415098172	0.120658009
O	-0.556616042	0.421791030	-1.184319083
C	-1.832300133	0.575717044	-0.594797043
C	-1.622734115	1.481133104	0.621635045
N	-2.423696175	-0.709110050	-0.311185022
O	-1.060336076	3.437480248	-0.707113051
O	-2.835506202	2.151867157	0.928903069
C	-2.010385142	-1.688049119	0.583336043
C	-2.975413215	-2.663411193	0.513310037
N	-3.959593282	-2.313670165	-0.392613028
C	-3.594684256	-1.153951082	-0.872384065
N	-0.884631063	-1.545180110	1.386104100
H	1.211449085	0.430271031	0.962838068
H	2.207964157	1.905590139	0.373503027
H	0.700055049	2.003106145	-1.621015115
H	0.057425004	2.853887205	0.943566068
H	-2.519478183	1.076160079	-1.285343095
H	-1.266189090	0.886881066	1.462236105
H	-1.892402137	3.713502266	-0.295561021
H	-2.838764203	2.381830174	1.864919132

H	-3.005346217	-3.587721257	1.067998076
H	-4.111908296	-0.578360041	-1.623746119
H	0.024282002	-1.597149115	0.892409064
H	-0.879347064	-2.259364165	2.102858152
C	3.021297217	3.068103220	0.733875053
H	2.738078198	3.290758236	1.758080129
H	2.732939199	3.828112273	0.013864001
H	4.034813288	2.697523192	0.617376047

3-TS-CH₃

H	3.617572000	-2.076604000	0.040087000
H	-5.810838000	0.428558000	0.117043000
H	-2.466748000	0.437347000	1.544535000
H	-2.349739000	1.521573000	0.185980000
H	-1.369086000	-0.327909000	-1.207456000
H	-1.481995000	-1.412989000	0.158353000
H	0.054477000	0.078042000	1.470948000
H	0.164598000	1.165326000	0.101430000
H	1.155412000	-0.687960000	-1.278400000
H	1.048383000	-1.762178000	0.100355000
H	2.586410000	-0.081574000	1.367187000
H	2.679982000	0.971509000	-0.191205000
O	-4.019469000	-0.929555000	-0.784670000
C	5.073631000	-0.506168000	0.298740000
C	3.735216000	-1.018577000	-0.231249000
C	-3.855667000	0.023639000	-0.021456000
C	-2.481917000	0.467073000	0.449915000
C	-1.337907000	-0.364541000	-0.115363000
C	0.026520000	0.114487000	0.376043000
C	1.186739000	-0.708880000	-0.182391000
C	2.545695000	-0.241408000	0.286044000
H	3.734258000	-0.990524000	-1.326767000
H	5.907461000	-1.092258000	-0.092637000
H	5.233975000	0.536325000	0.015671000
H	5.107146000	-0.562433000	1.389736000
C	2.793209000	2.231878000	-0.798291000
H	2.714084000	2.937912000	0.022979000
H	3.767201000	2.220365000	-1.278030000
H	1.959550000	2.269168000	-1.493200000
N	-4.907494000	0.735028000	0.444330000
C	-4.855689000	1.882478000	1.336803000
H	-4.390579000	1.630140000	2.291498000
H	-4.308049000	2.716420000	0.893085000
H	-5.874156000	2.209625000	1.531553000

4-TS-CH₃

C	-0.540137208	2.885428148	0.626624065
C	-3.002030138	-1.320075220	-0.134131344
C	-1.750520060	-0.517334266	0.130437733
O	-1.372777877	-0.259498831	1.266969346
N	-1.050900126	-0.115293653	-0.970536491
C	0.083851501	0.747411285	-0.909480978
C	1.388401639	0.227998795	-0.368223046
O	2.343121853	0.999926297	-0.249506509
N	1.455678155	-1.071694453	-0.035586200
C	2.657435443	-1.666030551	0.520556121
H	-2.888056461	-2.301706177	0.327301160
H	-0.193100238	1.746427419	-0.145804498
H	0.250388690	1.232599686	-1.866955639
H	-1.462355017	-0.282501960	-1.874916825
H	3.494380053	-1.578386575	-0.174352250
H	0.643392697	-1.648558706	-0.171183602
H	-0.137499447	3.714073587	0.053980493
H	-1.622555327	2.830016702	0.660947623
H	2.467439464	-2.718460926	0.716286588
H	2.936903537	-1.174447345	1.454099825
H	-3.224578487	-1.448209532	-1.192190330
H	-3.840891893	-0.821045813	0.351717423
H	-0.041672655	2.691307486	1.569530894

5-TS-CH₃

C	3.069091056	-1.696971042	-1.351360385
N	2.098819794	-1.446437683	-0.583263635
C	1.725792750	-0.048711955	-0.382127879
C	1.969867072	0.426952680	1.088748799
O	2.294136571	-0.424405767	1.945938793
C	0.268059573	0.113225277	-0.792473385
C	-0.778640940	-0.362002722	0.188680783
C	-2.200101033	-0.204697969	-0.353535815
C	-3.228197758	-0.695320781	0.648370233
N	-4.628120306	-0.536415738	0.107294688
O	1.810675119	1.658582667	1.265632644
H	3.651660427	-0.919163540	-1.861662236
H	2.337401526	0.607391906	-1.018881421
H	0.102861135	-0.278979764	-1.798688445
H	-0.595435786	-1.415047941	0.433699106
H	-0.679812596	0.195214620	1.125024010
H	-2.301119748	-0.766709337	-1.286505596
H	-2.388803270	0.846376411	-0.587192210
H	-3.104468127	-1.752549179	0.874469553
H	-3.191870211	-0.130516360	1.577719076
H	-5.328241640	-0.868010632	0.772454054

H	-4.837911361	0.442337883	-0.097423428
H	-4.753168229	-1.063786555	-0.758827729
H	0.051594726	1.397565566	-0.984807338
H	3.363382368	-2.729949215	-1.530632207
C	-0.250201552	2.719068654	-1.260756890
H	-0.958967226	2.686479035	-2.083181373
H	0.710576940	3.152803775	-1.519050692
H	-0.665083894	3.093849201	-0.330574784

6A-TS-CH₃

C	2.479880807	-2.213672932	-0.765626307
N	1.806464620	-1.506293377	0.035754422
C	1.306047567	-0.227868577	-0.458875498
C	1.710948735	0.933050136	0.439220557
O	1.942897554	0.592802510	1.715094299
C	-0.217409281	-0.288958665	-0.587096757
C	-1.036854788	-0.345581177	0.676198024
O	1.787345737	2.070904159	0.039288711
H	2.727018865	-1.903620256	-1.787491039
H	1.720987042	0.014409837	-1.445768252
H	-0.502117408	-1.057828263	-1.302415088
H	-0.732540071	-1.214850091	1.273029415
H	-0.860797290	0.532989082	1.299780479
H	-0.577983600	0.809573679	-1.209482239
H	2.840362228	-3.187722657	-0.442187329
C	-2.558778341	-0.484458009	0.428689369
O	-2.918507473	-1.211043719	-0.530929551
O	-3.311783035	0.121184530	1.232416289
H	2.158660994	1.403632059	2.205805188
C	-1.029458780	1.962257207	-1.836700586
H	-0.258138627	2.190746793	-2.565374853
H	-1.982727709	1.672718320	-2.267754307
H	-1.103854486	2.684617358	-1.030233670

6B-TS-CH₃

C	2.465001031	-2.277495635	-0.755530775
N	1.666084342	-1.619414226	-0.030483646
C	1.334771822	-0.256143220	-0.441614657
C	1.853915976	0.752196640	0.644467784
O	1.361461453	0.670233001	1.793125258
C	-0.160570471	-0.138474069	-0.692455805
C	-1.090298177	-0.522645760	0.429919178
O	2.725520214	1.562006972	0.248708411
H	2.912872630	-1.880708252	-1.674775311
H	1.850642755	-0.002066888	-1.375271979
H	-0.445025747	-0.592445289	-1.641739791

H	-0.923549467	-1.561410558	0.738024141
H	-0.887363967	0.072542342	1.320996787
H	-0.374483373	1.140222992	-0.915105650
H	2.735432323	-3.293058654	-0.471339004
C	-2.545494505	-0.398981338	0.076079555
O	-3.002830455	-0.155950000	-1.016886301
O	-3.334727568	-0.610365909	1.152589954
H	-4.260552291	-0.539106271	0.868456353
C	-0.587967137	2.504113410	-1.060373500
H	0.372955492	2.936484847	-0.801012406
H	-0.870876254	2.625816081	-2.101481418
H	-1.384182885	2.726816544	-0.356615396

6C-TS-CH₃

C	2.381217413	-2.242914161	-0.813298166
N	1.691456354	-1.550779519	-0.013251581
C	1.277442759	-0.214244321	-0.448574537
C	1.784495879	0.829211970	0.547381544
O	3.083928260	0.644791519	0.828243459
C	-0.225288147	-0.178659105	-0.643037545
C	-1.079817297	-0.408229245	0.577764801
O	1.135495105	1.739679684	0.999573886
H	2.708024889	-1.886160328	-1.795970067
H	1.754257353	0.055519039	-1.403678330
H	-0.513152181	-0.811431419	-1.479744750
H	-0.817307541	-1.353117931	1.067830396
H	-0.921292368	0.368312194	1.327495063
H	-0.519031229	1.024828839	-1.105816247
H	2.674079613	-3.250295560	-0.526405057
C	-2.551944673	-0.470039488	0.268638258
O	-3.049018384	-0.480725538	-0.832560032
O	-3.287537758	-0.528432873	1.397144378
H	-4.224868223	-0.584512711	1.149124864
H	3.370562959	1.347206519	1.435153904
C	-0.859283827	2.259300912	-1.596957235
H	0.093854284	2.735683714	-1.803199771
H	-1.454419020	2.044786283	-2.478898787
H	-1.414773447	2.715576312	-0.783846372

6D-TS-CH₃

C	2.679900340	-2.031729623	-0.780080503
N	1.875194484	-1.453018827	0.002675563
C	1.334605348	-0.158887611	-0.407282934
C	1.728602004	0.989418721	0.576595700
O	2.072881615	0.693496146	1.743198966
C	-0.179149948	-0.294538321	-0.539653265

C	-1.003768605	-0.355547571	0.723103089
O	1.646638322	2.141761596	0.084226941
H	3.002938915	-1.604746073	-1.738587102
H	1.736775575	0.126122776	-1.390131705
H	-0.442291994	-1.094802888	-1.231556127
H	-0.677416428	-1.214232187	1.324086092
H	-0.840081355	0.535396706	1.331041693
H	-0.609381512	0.753699335	-1.193585749
H	3.088518434	-3.005185886	-0.512486556
C	-2.516478124	-0.529546292	0.461750068
O	-2.854108057	-1.435140907	-0.343901740
O	-3.296360011	0.234526942	1.087978835
C	-1.206417440	1.807947920	-1.888091576
H	-0.470888335	2.093066854	-2.633998654
H	-2.116554810	1.381631165	-2.299269696
H	-1.374156262	2.560328439	-1.124308573

7A-TS-CH₃

C	0.916557067	-0.846993061	-0.375399027
C	0.527581038	0.484858035	-0.301208022
C	1.498593107	1.481683105	-0.066553005
N	-0.017101001	-1.808078129	-0.572868044
C	-1.416138099	-1.492449105	-0.796702056
C	-1.755510127	-0.180123013	-0.092493006
N	-0.827075057	0.845395062	-0.452141033
C	-3.192882231	0.198535014	-0.230785017
O	-3.395412244	1.521971110	-0.092844007
O	-4.094402293	-0.597217045	-0.373484027
O	1.290198095	2.699487196	0.047890003
N	4.409675318	-0.702822048	0.163121012
H	-1.647113121	-0.438263032	1.090392079
H	3.524960254	1.669411120	0.226467016
H	0.293132021	-2.764134198	-0.614397043
H	-2.034465146	-2.290289167	-0.390502028
H	-1.637779116	-1.402677100	-1.865258133
H	-1.027913074	1.758263124	-0.065609005
H	4.643243334	-1.649012121	-0.090424006
H	5.141326372	-0.023057002	0.035473003
N	2.206279156	-1.259837090	-0.246620018
C	3.114005224	-0.340377024	-0.034751003
N	2.807119202	0.982016071	0.045064003
H	-4.350283311	1.694033124	-0.130350009
C	-1.294109096	-0.847111062	2.601768187
H	-1.428716103	-1.920835138	2.559578182
H	-2.045955146	-0.282386020	3.139622223
H	-0.274376020	-0.489852035	2.673360191

7B-TS-CH₃

C	0.876134064	-0.848707061	-0.375123027
C	0.501389036	0.490450035	-0.308218022
C	1.485106109	1.474069107	-0.078052005
N	-0.065148005	-1.797226127	-0.590154042
C	-1.476238104	-1.475950104	-0.777308054
C	-1.798584128	-0.150078011	-0.104380008
N	-0.845372059	0.843045060	-0.477912035
C	-3.250777233	0.325613024	-0.223429016
O	-3.437288247	1.564742115	-0.129753009
O	-4.123724295	-0.568141041	-0.345613025
O	1.301501093	2.699822197	0.019096001
N	4.372294317	-0.746592055	0.197230014
H	-1.675893118	-0.389551028	1.091453080
H	3.512544253	1.635335117	0.231818017
H	0.238935017	-2.755895199	-0.616342045
H	-2.083258152	-2.261660164	-0.332830024
H	-1.724905124	-1.423587100	-1.843156130
H	-1.087099078	1.773060126	-0.164422012
H	4.590360329	-1.694127122	-0.066860005
H	5.107724368	-0.079006006	0.028546002
N	2.162195157	-1.277552092	-0.233907017
C	3.078339222	-0.369251026	-0.020538001
N	2.787620201	0.956356070	0.047933003
C	-1.367743099	-0.749670052	2.599132186
H	-1.578859114	-1.812445133	2.632589190
H	-2.067761148	-0.112412008	3.127945224
H	-0.322580023	-0.476172034	2.686588194

8A-TS-CH₃

O	2.653760223	-1.552044168	-2.045627183
O	4.411538424	1.692383022	0.292006985
C	1.176286178	1.104285056	0.502143000
C	0.502054131	1.185946081	-0.889983098
C	-0.976412967	1.464582133	-0.768667092
C	-4.140214241	-0.389302924	0.138106973
C	-2.315804146	-1.964063082	0.224847980
O	-1.419559977	2.583751226	-0.966356107
H	5.482010441	-0.100241132	0.794211023
O	-5.940404359	1.145129232	0.055707968
O	5.186636417	-0.930131183	0.390756992
H	2.879110280	0.329567961	1.703473085
C	-1.889722061	0.343859076	-0.369474063
O	-6.407539439	-0.976050910	0.613494008
C	-3.251127151	0.616849129	-0.224930053

C	-3.666333237	-1.685577030	0.363417990
H	3.437497251	-2.566043262	-0.414379066
H	3.234555325	1.167324011	-1.335685134
H	4.878719405	-0.564008151	-1.631165152
H	4.914210471	2.201786050	-0.354815062
H	1.923957151	-2.181894198	-2.094699186
C	-5.596100315	-0.133539870	0.298000985
C	-1.428789061	-0.957090028	-0.140174047
H	1.391999219	2.108842125	0.869637027
H	0.940871180	1.991391129	-1.476112144
H	0.501040118	0.643600039	1.226063050
H	0.667589120	0.248921008	-1.423423140
H	-3.602488155	1.622342207	-0.401472065
H	-4.365599304	-2.460370069	0.645947009
H	-1.949203145	-2.966394162	0.401126992
H	-0.378365989	-1.195023069	-0.235648054
O	2.202762202	-1.059657121	0.190525977
C	3.602977342	0.746309972	-0.395846065
C	4.333641364	-0.579289139	-0.684608085
C	3.168259259	-1.559058180	-0.737206091
C	2.450901251	0.299530969	0.490627999
H	-6.899463403	1.227743257	0.180664977
C	3.268402307	0.261163947	3.082748184
H	3.635528358	1.258601011	3.299261199
H	4.029534343	-0.511483127	3.069619186
H	2.352837235	-0.009339051	3.599299222

8B-TS-CH₃

O	2.673068265	-1.618827041	-1.999927139
O	4.360500263	1.720973257	0.255835025
C	1.135665056	1.068272095	0.477117040
C	0.463540005	1.109106073	-0.915892061
C	-1.012684115	1.418397041	-0.803188054
C	-4.226457279	-0.341337204	0.141380016
C	-2.419912092	-1.954043254	0.243747024
O	-1.420827181	2.549332109	-1.023446067
H	5.469420415	-0.031805825	0.797773063
O	-6.043339441	1.192817839	0.051987010
O	5.194893418	-0.878328895	0.414580036
H	2.853777205	0.365026107	1.697928128
C	-1.947321142	0.329366928	-0.387401022
O	-6.473596423	-0.927216327	0.654039055
C	-3.306185250	0.627540901	-0.240371011
C	-3.766870199	-1.638409282	0.382369034
H	3.480241358	-2.572562080	-0.343759018
H	3.196071201	1.133259172	-1.359228092

H	4.874163384	-0.570502886	-1.614827112
H	4.853004280	2.224803313	-0.402987023
H	1.942915233	-2.249780114	-2.025237142
C	-5.713487387	0.006134766	0.295914027
C	-1.508820060	-0.977903152	-0.139781004
H	1.328059034	2.084074175	0.827230064
H	0.915127008	1.887183143	-1.529282106
H	0.467159024	0.604852035	1.205537090
H	0.616955049	0.151858009	-1.414985096
H	-3.653752312	1.632850958	-0.428426025
H	-4.483457221	-2.391810362	0.680296058
H	-2.076588026	-2.963042316	0.435139038
H	-0.464322976	-1.240674132	-0.235445011
O	2.212822211	-1.079693020	0.223394022
C	3.571973244	0.742053159	-0.409697024
C	4.331406346	-0.574014908	-0.666769044
C	3.187956300	-1.580255020	-0.691562045
C	2.428440175	0.292824086	0.486791041
C	3.237835235	0.346330120	3.082120225
H	3.517941215	1.373478206	3.289932243
H	4.061041318	-0.359893901	3.085307227
H	2.343603182	0.005849062	3.594675266

9-TS-CH₃

H	-1.850423131	-0.234819017	1.805995129
C	-2.045642148	-2.111338154	-0.970391068
H	-1.385976102	-2.970095212	-0.827586057
H	-2.970245212	-2.467155179	-1.419246100
H	-1.552256114	-1.418119101	-1.646660118
C	-2.367669168	-1.537588109	0.388614028
H	0.721988054	-1.394830100	-0.550963037
H	-0.277872020	1.131624084	1.083824079
H	-2.085803150	2.014041143	-2.077604152
H	0.826341062	-1.171180083	1.189970088
O	-3.270398236	-2.007694143	1.076658078
C	-0.826770061	0.860587064	-1.077701075
C	-0.503251036	0.176394013	0.238260017
N	-1.619227115	-0.501740036	0.858565062
C	0.785167055	-0.639516045	0.237174017
O	-0.089610006	0.711957050	-2.055699146
N	-1.928238137	1.637952120	-1.154453081
C	2.059158150	0.181872013	0.054142004
H	2.038451148	0.714205053	-0.893952065
H	2.170748159	0.907782065	0.860023061
S	3.515022252	-0.921202069	0.075226005
C	4.822114346	0.318457023	-0.150037011

H	5.773532441	-0.211585015	-0.160530012
H	4.695611339	0.844874061	-1.096111078
H	4.821081345	1.034532076	0.671891051
C	-0.014157001	2.044679146	2.148908156
H	0.732726050	1.523852107	2.737721199
H	-0.969087069	2.176535156	2.645895188
H	0.346927025	2.914447207	1.611068117
C	-2.915552209	1.965218144	-0.135937010
H	-3.657498263	1.174595086	-0.014248001
H	-2.443615174	2.152563157	0.824149062
H	-3.423063248	2.877795206	-0.441896032

10A-TS-CH₃

C	1.990641142	0.131866009	0.844552062
C	2.444669178	-0.865628065	-0.202640015
O	2.130805151	-0.519393037	-1.462409104
C	0.800859055	-0.508445036	1.634084115
C	-0.408043029	-0.823061057	0.811221060
C	-0.690440052	-2.025852146	0.216271016
C	-1.484475107	0.062733005	0.457162033
N	-1.868038134	-1.940740140	-0.489943035
C	-2.382894169	-0.674693050	-0.359218026
C	-1.786839129	1.398472099	0.758034053
C	-3.550364254	-0.113936008	-0.877205066
C	-2.946419213	1.957988143	0.247742018
C	-3.818983273	1.209270087	-0.564431043
O	3.010745216	-1.903070139	0.060558005
H	0.542340041	0.184894013	2.437205176
H	1.172451082	-1.420303100	2.105354154
H	-0.132763009	-2.947885214	0.243132017
H	-1.121063082	1.984937140	1.378207098
H	-3.188969230	2.988813216	0.473884034
H	-4.220942305	-0.692892048	-1.499709110
H	-4.716766337	1.675339123	-0.950520071
H	2.821582204	0.194575014	1.552293114
H	-2.295503166	-2.696806193	-0.996201074
C	1.686737119	1.509488110	0.312234023
H	0.933529068	1.546030111	-0.468702034
H	1.496862110	2.236037159	1.099334079
H	2.791117200	1.961793140	-0.275767020
H	2.426675173	-1.230690086	-2.054308150
C	3.956321284	2.376479171	-0.857249061
H	4.148360301	3.356002240	-0.429282031
H	4.685385338	1.622858117	-0.573369042
H	3.736967271	2.394100170	-1.920484140

10B-TS-CH₃

C	2.016845147	0.115308008	0.738166051
C	2.503412182	-0.929580066	-0.303457022
O	2.331016167	-0.683866051	-1.522277112
C	0.833692059	-0.483223035	1.556836112
C	-0.394093029	-0.809065060	0.764013057
C	-0.686158050	-2.010364144	0.173078012
C	-1.486911106	0.068781005	0.440584032
N	-1.886134133	-1.932927140	-0.501777036
C	-2.404775172	-0.671311046	-0.353278026
C	-1.787729126	1.402936101	0.749820053
C	-3.588858258	-0.114831008	-0.837327062
C	-2.963428213	1.958920141	0.272311020
C	-3.855388275	1.207213085	-0.515782037
O	3.029476218	-1.968455142	0.176966013
H	0.576096041	0.221849016	2.352856169
H	1.204807085	-1.389946101	2.038235148
H	-0.117489009	-2.925684212	0.174640012
H	-1.106234080	1.991319145	1.350790096
H	-3.203499230	2.988935213	0.505494037
H	-4.274146309	-0.695818049	-1.441974104
H	-4.765732341	1.669465118	-0.876564063
H	2.836138203	0.231563017	1.456574105
H	-2.321566167	-2.689824192	-0.999498071
C	1.695247120	1.465246108	0.153377011
H	1.031060075	1.440937102	-0.705875052
H	1.390331099	2.210509161	0.888809066
H	2.819842201	1.966167144	-0.327175024
C	4.025470288	2.470922180	-0.767265053
H	4.076665293	3.481850252	-0.372630027
H	4.765626342	1.797382129	-0.344697025
H	3.963147284	2.424629173	-1.850507132

11A-TS-CH₃

C	-2.247968163	0.298541022	0.908292065
C	-3.095821222	-0.235718017	-0.229751017
O	-4.360954313	-0.477516034	0.176004013
C	-0.882290062	0.821882061	0.474099034
C	0.181328013	-0.098567007	0.051015004
C	0.094163007	-1.327058095	-0.567019042
C	1.593281115	0.178594013	0.175473012
N	1.352569095	-1.822561134	-0.814657061
C	2.294321164	-0.924651066	-0.375055027
C	2.325592169	1.252363091	0.697877051
C	3.686772263	-0.980308072	-0.410640030
C	3.710567269	1.202924087	0.664115050

C	4.384355314	0.096722007	0.115310008
O	-2.740861200	-0.429145031	-1.367876097
H	-0.511278037	1.499111108	1.244305092
H	-1.109814080	1.642033119	-0.460785033
H	-0.776478055	-1.885843134	-0.860079064
H	1.818913129	2.111477153	1.120216080
H	4.286604306	2.027670145	1.064726078
H	4.202860302	-1.832789130	-0.834060059
H	5.466952385	0.086326006	0.102645007
H	-2.812765201	1.154237082	1.291653094
H	1.547336110	-2.707031194	-1.251213088
C	-2.156183153	-0.733698054	2.050121146
H	-1.645952116	-1.637784117	1.718454125
H	-1.585818112	-0.307572022	2.875961204
H	-3.146821225	-1.002741070	2.414314174
H	-4.862218351	-0.819823059	-0.581837042
C	-1.412017100	2.654022192	-1.489825105
H	-2.475300180	2.833092206	-1.371238098
H	-1.134189080	2.132994156	-2.399370172
H	-0.772096055	3.487578252	-1.220173085

11B-TS-CH₃

C	-2.406798175	0.329089024	0.861398060
C	-3.064183223	-0.280286020	-0.413544030
O	-3.299278238	-1.516378108	-0.426057030
C	-0.976178071	0.814453058	0.622056043
C	0.059981004	-0.130032009	0.178663013
C	-0.077402005	-1.374934099	-0.394941028
C	1.478994106	0.133126010	0.213210015
N	1.161833082	-1.891954136	-0.704830048
C	2.136257153	-0.994049069	-0.345020025
C	2.249855162	1.214561087	0.657749048
C	3.523927252	-1.064235075	-0.459669033
C	3.630609264	1.150340083	0.545237038
C	4.260995308	0.020808001	-0.007689001
O	-3.315687236	0.527900038	-1.342150098
H	-0.625494044	1.390935102	1.482696109
H	-1.022845075	1.741317127	-0.237566017
H	-0.978009072	-1.931626142	-0.591534041
H	1.773433127	2.090373151	1.081031077
H	4.236569306	1.980814141	0.885661064
H	4.007709290	-1.933725139	-0.886998062
H	5.340966395	-0.001854000	-0.083095006
H	-2.993715218	1.226757088	1.081915078
H	1.322929094	-2.794828204	-1.116214082
C	-2.477747180	-0.594664045	2.081391151

H	-1.902043138	-1.504593109	1.914879137
H	-2.078971149	-0.092252006	2.967143212
H	-3.508910255	-0.886246064	2.288277166
C	-0.980155071	2.885692208	-1.163965085
H	-1.641975116	3.614722262	-0.707934049
H	-1.360354097	2.428295175	-2.068971149
H	0.068674005	3.164199226	-1.179081086

12A-TS-CH₃

O	0.517515037	-1.608026115	1.519830112
H	-0.716486050	1.912788135	-0.202394014
N	2.147073155	-1.657550120	-0.033954002
C	0.219304016	-0.135805010	-0.365703026
C	-2.436447177	-0.362306026	1.262744093
H	1.602222115	2.697122192	1.528504110
C	-2.269331165	-0.827569060	-0.162251011
N	-1.079363078	-0.649141049	-0.800284057
H	-2.550962181	0.723058051	1.280868091
C	0.980252069	-1.202455088	0.455844033
H	-1.097692079	-0.990550070	-1.750121123
H	0.748134051	0.056951004	-1.296880095
H	2.607425187	-2.333452165	0.558275039
H	-3.343899242	-0.810544057	1.658954118
H	-0.195187014	1.077096078	1.418583099
O	-3.205426229	-1.339631097	-0.775430056
H	-1.582597116	-0.636825046	1.876314133
C	0.165600012	1.178930085	0.401917029
C	-1.655312119	2.717499194	-0.883639062
H	-1.181964086	2.863421206	-1.849599133
H	-1.706907123	3.609264259	-0.266872019
H	-2.569243186	2.133994153	-0.914954068
C	2.823822201	-1.280908092	-1.269859093
H	2.190783159	-1.450112104	-2.141112153
H	3.144885225	-0.238610017	-1.253250093
H	3.706991269	-1.906717139	-1.370437098
S	1.750405128	2.031056144	0.373392027

12B-TS-CH₃

O	0.767739058	-1.845965135	1.000292070
H	-0.829245060	1.957892140	0.143240010
N	2.565593186	-0.928455067	0.000342000
C	0.341764024	0.099255007	-0.360427026
C	-2.220062160	-0.703737049	1.201935087
H	1.316348092	2.576537186	1.428591101
C	-2.017422146	-0.934932070	-0.275517020
N	-0.889735062	-0.475675034	-0.882422065

H	-2.469517178	0.343680024	1.380034098
C	1.247714089	-0.985267071	0.264837019
H	-0.867480063	-0.691492051	-1.868127137
H	0.835566061	0.534868037	-1.227395090
H	3.106117223	-1.652012117	0.451468032
H	-3.055434219	-1.317874097	1.527731109
H	-0.164110012	0.954456070	1.616435117
O	-2.879744208	-1.495278108	-0.952377070
H	-1.329814097	-0.957811069	1.770944126
O	1.303801093	2.039604145	0.628082043
C	0.147380010	1.252562088	0.616655043
C	-1.812296132	2.821110204	-0.424570031
H	-1.421237103	3.017255218	-1.418048101
H	-1.809657131	3.680604263	0.238577017
H	-2.730811198	2.243459161	-0.411144030
C	3.270520233	-0.044309003	-0.922953069
H	2.978923216	-0.229677016	-1.958801140
H	3.094626224	1.000462073	-0.677505050
H	4.334756314	-0.246413018	-0.829175060

13A-TS-CH₃

H	-0.230879017	0.465195034	-1.787714129
H	-6.292357449	-0.698669049	-0.390329028
H	-5.923185408	-0.687289050	1.300679096
C	2.534127180	-2.055470149	-0.369564026
O	2.251558160	2.826999201	0.280367020
O	-0.505495036	2.664140193	-0.471597034
C	1.808415130	-0.779602058	-0.768919054
O	-1.359904100	-0.014043001	1.857379134
H	-2.125669152	0.019047001	-2.446838175
H	-4.543596327	-0.403864029	-2.107314152
C	-2.156867157	-0.091088006	0.927360067
N	-1.687249119	0.050317004	-0.413162030
O	3.744291269	-2.135206154	-0.393041028
O	1.734156126	-3.057321217	-0.025992002
C	-0.289480021	0.311563023	-0.704860053
O	3.824833274	0.626404043	-0.635299047
C	0.276375020	1.563013113	-0.031504002
C	1.732630127	1.718802122	-0.445834032
C	-4.313838313	-0.409827029	0.084035006
C	2.518169184	0.451560033	-0.189183013
O	0.461736033	-0.838553060	-0.345893025
N	-5.613207398	-0.620034046	0.345780025
N	-3.483333250	-0.306452022	1.110619081
C	-2.553329186	-0.078065006	-1.459262103
C	-3.868494276	-0.307467022	-1.271402089

H	1.871224136	-0.734666051	-1.869554137
H	2.520793183	0.259595019	1.098611080
H	1.767732126	1.934277140	-1.525163112
H	0.220605016	1.447054105	1.050106075
H	4.277692310	-0.231261016	-0.568634044
H	-0.081308006	3.469404252	-0.148833011
H	3.155602228	2.987838213	-0.016817001
H	2.281972162	-3.831049276	0.192567014
C	2.579430187	-0.025826002	2.490069179
H	2.201527161	0.880300065	2.951492213
H	1.939232138	-0.893519066	2.613125188
H	3.634912263	-0.214129015	2.658929189

13B-TS-CH₃

H	0.297482021	-1.356119096	-1.126019080
H	5.893210427	1.821030129	0.188164014
H	6.275112462	0.154861011	-0.083100006
C	-2.005294145	1.852873131	0.141747010
O	-2.668729192	-0.886976064	1.754369125
O	0.300090022	-1.865872132	1.550596112
C	-1.756437129	0.770219058	-0.913485066
O	2.311216164	-2.273378165	-0.368370027
H	1.170918082	1.893817136	0.082039006
H	3.555536258	2.608352190	0.344552025
C	2.670110191	-1.086910077	-0.295929021
N	1.676140123	-0.085865006	-0.265605019
O	-3.277969233	2.259916160	0.110497008
O	-1.165393085	2.308104168	0.875906063
C	0.277021020	-0.484688035	-0.470909034
O	-2.341309167	-1.446275104	-1.682113121
C	-0.398499029	-0.846625061	0.856612064
C	-1.872100136	-1.242018088	0.626969046
C	4.281403309	0.565716038	-0.027016002
C	-2.442440178	-0.555179040	-0.603709044
O	-0.359396026	0.596243041	-1.130841081
N	5.584890383	0.878854061	0.025603002
N	3.961467284	-0.708810049	-0.231009016
C	2.000435144	1.207544085	0.000659000
C	3.291889236	1.582231116	0.140069010
H	-2.155714154	1.165957082	-1.850393132
H	-3.715019269	-0.345306025	-0.399055029
H	-1.908518135	-2.320867166	0.450093033
H	-0.389645028	0.048163003	1.484006108
H	-2.655806191	-1.021928074	-2.491119177
H	0.901538064	-2.317376168	0.928952065
H	-2.272107166	-1.285694093	2.539238185

H	-3.408099248	2.947117214	0.785120054
C	-5.117262369	-0.301757022	-0.354111026
H	-5.322948386	0.248333018	0.556538041
H	-5.397217407	-1.350136097	-0.329597023
H	-5.387245379	0.218018016	-1.268085090

13C-TS-CH₃

H	-0.211059015	0.383640027	-1.781765129
H	-6.289386436	-0.731377051	-0.417715030
H	-5.941416411	-0.665690046	1.276588090
C	2.565876185	-2.138052154	-0.326941024
O	2.271888166	2.808065202	0.211251015
O	-0.491099035	2.626425191	-0.547232041
C	1.818624129	-0.837865061	-0.727440051
O	-1.387791101	0.038429003	1.869693136
H	-2.095659151	-0.071260005	-2.441047177
H	-4.519828325	-0.477921034	-2.121232154
C	-2.169540158	-0.071739005	0.929598069
N	-1.682925122	0.023060002	-0.406612029
O	3.819930278	-2.074622148	-0.517986037
O	1.924075137	-3.102700225	0.107841008
C	-0.273063020	0.259673019	-0.693852049
O	3.836733274	0.524931038	-0.571501041
C	0.288134021	1.537241112	-0.063561004
C	1.746805124	1.671201121	-0.472840034
C	-4.317359310	-0.418438030	0.071315005
C	2.512130181	0.404805029	-0.167361012
O	0.461401033	-0.878299066	-0.298381022
N	-5.620733410	-0.622550045	0.323979023
N	-3.499746254	-0.281782020	1.104012080
C	-2.536163184	-0.135835010	-1.456417103
C	-3.855497275	-0.357006026	-1.279873090
H	1.855196135	-0.785902056	-1.828996130
H	2.479881178	0.256720019	1.110823078
H	1.789861128	1.847161134	-1.559719112
H	0.223713016	1.462969106	1.021044073
H	4.150362300	-0.420771030	-0.613242045
H	-0.054423004	3.440563245	-0.266780019
H	3.201013230	2.896514211	-0.035062003
C	2.537250183	0.016261001	2.538909185
H	1.901104135	0.782780059	2.968843215
H	2.156269155	-0.994786070	2.639062192
H	3.593925257	0.126965009	2.760847198

13D-TS-CH₃

H	-0.314755022	-1.336963097	1.230800086
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H	-5.862947415	1.786466128	-0.280940020
H	-6.243409453	0.123691009	0.014089001
C	1.874810137	1.987031142	-0.301790022
O	2.714539193	-1.388226100	-1.576257112
O	-0.172638013	-2.011952147	-1.382504102
C	1.748729128	0.914188068	0.831730060
O	-2.284340167	-2.290959163	0.410199030
H	-1.123779078	1.853306136	-0.121683009
H	-3.521633253	2.573966183	-0.416347030
C	-2.639002189	-1.103179081	0.302894022
N	-1.646736119	-0.106777007	0.261925019
O	3.004132215	2.516663182	-0.374973027
O	0.859179061	2.245247161	-0.986755070
C	-0.242898017	-0.491690035	0.541589038
O	2.720348194	-1.079871078	1.830651132
C	0.487819035	-0.934736068	-0.728036053
C	1.927322137	-1.329691096	-0.385365028
C	-4.249349307	0.540548040	-0.018511001
C	2.548235183	-0.365345026	0.621843043
O	0.379305027	0.593278045	1.182353084
N	-5.554813377	0.848965061	-0.094097007
N	-3.931125282	-0.730202055	0.212568015
C	-1.966977140	1.181325083	-0.024970002
C	-3.259482236	1.552015111	-0.188702013
H	2.129797153	1.407616102	1.727978125
H	3.749583269	-0.074804005	0.221200016
H	1.902982137	-2.317597168	0.086502006
H	0.517108037	-0.086699006	-1.415144104
H	3.014446218	-0.467955034	2.517482179
H	-0.840464062	-2.384873171	-0.773204056
H	2.260662163	-1.985908144	-2.184845155
C	5.151338373	0.042384003	0.012596001
H	5.225372377	0.549769039	-0.941960068
H	5.500037393	-0.985514070	0.011734001
H	5.488260395	0.631061047	0.860179063

14A-TS-CH₃

O	-2.673595892	-1.063219468	-0.077514890
H	1.064191895	1.454192463	0.089799121
C	-0.621131035	0.114274382	-0.487934920
N	-1.411014357	1.335574943	-0.569057925
C	-1.463862844	-1.134164203	-0.100671892
H	-2.215421530	1.144022415	-1.154225969
H	-0.267788145	-0.113686847	-1.499652991
H	0.386974207	0.393360795	1.457571218
C	0.602992162	0.294458658	0.398248144

C	1.789482735	-0.563386119	0.205388129
O	2.565616602	-0.870190604	1.087065195
O	1.987000530	-0.921320260	-1.083348963
H	2.807433280	-1.437680794	-1.131232969
C	1.596037700	2.733151235	-0.258094904
H	1.679635661	2.656627183	-1.336133982
H	2.535363777	2.744611675	0.284047136
H	0.838148059	3.418702743	0.100683122
C	-0.739460566	-2.424103731	0.176948127
H	0.012474369	-2.617675197	-0.589486929
H	-0.214391487	-2.350248040	1.132924198
H	-1.450290114	-3.246094363	0.223348131
C	-1.882487070	1.869988269	0.710885164
H	-2.594282637	2.670233754	0.509306152
H	-2.374540551	1.126815508	1.349831211
H	-1.052002746	2.304325800	1.268410206

14B-TS-CH₃

O	2.729651199	-0.872148063	0.018994001
H	-1.195746084	1.351150096	-0.089599006
C	0.599817041	0.143081010	0.490156035
N	1.309290095	1.417674100	0.587169043
C	1.525400110	-1.027559076	0.084938006
H	2.153050154	1.259154091	1.126022081
H	0.256131018	-0.130416009	1.495711107
H	-0.451826033	0.300578022	-1.437550103
C	-0.648413049	0.216213016	-0.370633027
C	-1.791363129	-0.745777054	-0.071030005
O	-2.531291181	-1.047185074	-1.043575075
O	-1.933248139	-1.121462081	1.122170083
C	-1.869539135	2.563173185	0.227627017
H	-1.841030134	2.584281187	1.311759094
H	-2.856241208	2.409491174	-0.197515014
H	-1.281243093	3.336194241	-0.254368018
C	0.892122064	-2.368971172	-0.171526012
H	0.149085011	-2.592103188	0.594698044
H	0.356346026	-2.335909167	-1.123914082
H	1.656997120	-3.141890224	-0.213736015
C	1.691520119	2.016025145	-0.693423051
H	2.348001169	2.865245206	-0.500006036
H	2.214749157	1.327167095	-1.369006097
H	0.808532057	2.392588173	-1.210036087

15-TS-CH₃

P	5.485431836	-0.757175801	0.234027586
O	6.173288334	-1.773719217	1.210872626

O	6.280547853	-0.726965173	-1.123729468
O	5.266414533	0.537555824	0.898638887
O	4.149792291	-1.502815375	-0.221430779
P	2.814766824	-1.092870216	-1.023414268
O	3.304467461	-0.516523194	-2.402460726
O	1.865929030	-2.199193865	-1.042149514
O	2.355305281	0.258655602	-0.341957251
P	1.927090013	0.619938916	1.195647773
O	3.020930989	1.662432013	1.596940714
O	1.751682678	-0.577065859	2.017567210
O	0.612900260	1.442779925	1.008279524
C	0.530550760	2.662046032	0.231915503
C	-0.873881018	2.831474802	-0.290667998
O	-1.190460211	1.787728660	-1.225446199
C	-2.004497998	2.812331186	0.719099212
O	-2.086546062	4.009479213	1.414304744
C	-3.206073588	2.361917123	-0.095740038
O	-3.758521777	3.479568757	-0.776075235
C	-2.537106543	1.390319023	-1.093250092
N	-2.578921896	-0.005045744	-0.644455666
C	-1.517618177	-0.848922632	-0.381545461
N	-1.899956328	-2.049037841	-0.033275973
C	-3.279591765	-2.007201786	-0.074255608
C	-4.253571750	-3.014841964	0.192475421
O	-4.098801809	-4.179164560	0.545765162
N	-5.559849874	-2.508773102	-0.004319965
C	-5.884960289	-1.237875800	-0.401659358
N	-7.200548906	-0.934021038	-0.497411653
N	-4.980907410	-0.314817016	-0.647821212
C	-3.716453461	-0.745682162	-0.463380181
H	1.230656574	2.618596611	-0.602704824
H	0.785395750	3.503383824	0.876056174
H	-0.892691787	3.798868526	-0.811660590
H	-1.845078276	1.851963989	1.597674233
H	-2.898862339	4.028696195	1.935623933
H	-3.960585384	1.858165878	0.508758083
H	-4.631143300	3.235807078	-1.108155914
H	-3.035728986	1.446806779	-2.062202771
H	-0.502807898	-0.510206273	-0.472101740
H	-7.889455186	-1.664470552	-0.565465351
H	-7.427886998	-0.060881184	-0.943966411
H	-6.299724072	-3.173476412	0.177570806
H	3.943429489	1.321807990	1.417118559
H	3.268212263	-1.150829831	-3.132833430
H	7.125084844	-0.253292655	-1.099307499
H	6.435600756	-2.624940187	0.830934072

C	-1.894512332	0.950647343	2.688745845
H	-1.380935017	0.069210427	2.324234374
H	-2.955520326	0.817663460	2.876667714
H	-1.360377756	1.491862448	3.463083473

16-TS-CH₃

C	0.795370043	1.317853141	0.566790025
C	1.911763198	0.268375149	0.626861025
C	1.550042259	-0.918975963	-0.265845037
C	0.181951199	-1.465405099	0.098218989
C	-0.864785958	-0.343891096	0.070128987
O	-0.453642006	0.735549010	0.910504047
N	3.241596262	0.743972279	0.261747001
O	2.503066401	-1.966276969	-0.120651026
O	-0.245519760	-2.458111201	-0.842510078
C	-2.223711022	-0.765776223	0.582194025
O	-2.819019991	-1.823582345	-0.110902026
O	0.788585001	1.872493182	-0.719443072
C	-0.081160143	2.993549199	-0.869313080
H	0.949232995	2.097540212	1.321031078
H	1.952841228	-0.090415874	1.657860102
H	1.517274233	-0.585323939	-1.310824112
H	0.226415233	-1.894085127	1.106287061
H	-0.963395990	-0.003281079	-0.968102085
H	3.635560246	1.325448348	0.991467055
H	3.188387214	1.306994318	-0.580754060
H	3.368712432	-1.529453877	-0.106631025
H	0.357158338	-3.210001215	-0.790001074
H	-2.232956013	-0.912767237	1.666967105
H	-2.978665153	0.273855796	0.391940011
H	-2.118665904	-2.328829331	-0.559268056
H	0.041484840	3.352918237	-1.888826153
H	-1.122561198	2.708765107	-0.705694068
H	0.187987819	3.789830279	-0.167473030
C	-3.784123293	1.386052817	0.056935986
H	-3.551797287	1.568274849	-0.988082088
H	-3.449174324	2.168169896	0.730926033
H	-4.798847343	1.043289721	0.235139999

17A-TS-CH₃

O	-3.185223232	-0.947025066	-0.708991048
O	-1.026457075	-0.184032013	0.176630013
H	2.889974209	0.722056054	-1.120513081
O	-3.008830219	-0.011095001	1.723926125
C	1.258446089	1.543280109	-0.003020000
O	2.914866210	-1.786791128	-0.313102023

H	3.977764287	-0.087788006	1.008831075
H	0.779481056	1.387368098	0.967154069
C	0.777037057	-1.049701074	-1.171257084
H	-0.115701008	-2.653818189	-1.865704135
H	3.957227283	1.522485110	0.803595060
C	1.683293123	2.988798214	-0.143664010
H	-2.770253202	2.244408161	0.180442013
O	-2.892709209	1.474503106	-0.391816028
H	2.515721183	-2.659971192	-0.430357031
C	-0.289082021	0.044298003	-1.047466073
H	-4.147394298	-0.904730067	-0.796230056
P	-2.572366184	0.088551006	0.326852023
O	0.249717018	-2.360777169	-1.023235073
O	0.279361020	1.308829092	-1.044857076
H	2.175645154	3.152410226	-1.104368079
C	2.419154172	0.548094039	-0.137932010
H	1.219693090	-0.929546067	-2.168823155
H	-0.977185069	0.008162001	-1.892181137
H	2.370294168	3.263755236	0.656473048
C	1.873592135	-0.862790060	-0.147564011
N	3.363799243	0.718024051	0.968156072
H	1.358774100	-1.086875077	1.031390075
H	0.812209061	3.641306264	-0.081334006
C	0.917626064	-1.443980104	2.332059170
H	0.422641030	-0.550389039	2.695882192
H	1.833319132	-1.701290123	2.854711203
H	0.250491018	-2.278865161	2.145774157

17B-TS-CH₃

O	-2.673836191	-1.245110087	-0.136159010
O	-0.968043071	0.609640041	0.210193015
H	3.045131217	0.198120014	-1.030635072
O	-2.985569217	0.597538044	1.677194122
C	1.734154126	1.411732101	0.152356011
O	2.186384156	-2.238213162	-0.506908036
H	3.708431266	-1.131132081	1.010500073
H	1.208064086	1.338522095	1.107897077
C	0.457855033	-0.733934051	-1.283442094
H	-1.243439088	-1.686684122	-0.892324062
H	4.243401307	0.400216029	0.967964070
C	2.626894190	2.634942187	0.146764011
H	-3.357610240	1.992031142	-0.543351039
O	-3.244030234	1.077681078	-0.832178062
H	1.508970108	-2.878304205	-0.769817057
C	-0.214608015	0.616670045	-0.998125073
P	-2.534351181	0.177160013	0.324889023

O	-0.431081031	-1.821498133	-1.446711103
O	0.764589056	1.614496117	-0.899907066
H	3.168353230	2.710199193	-0.798736060
C	2.501911181	0.100376007	-0.074743006
H	0.973962072	-0.605978045	-2.244809161
H	-0.861013062	0.900120065	-1.831369130
H	3.348555239	2.587117185	0.962464067
C	1.516702108	-1.033231073	-0.239794017
N	3.405800248	-0.164162012	1.049156074
H	0.911715064	-1.203852084	0.902989063
H	2.027530146	3.536334252	0.277764020
C	0.322097023	-1.577626115	2.139623154
H	0.255452018	-0.647951045	2.694125196
H	1.017193075	-2.302636163	2.551811183
H	-0.637368046	-1.984229144	1.838073134

17C-TS-CH₃

O	-2.612590190	-1.244432089	0.057604004
O	-0.974657073	0.688090050	0.220786016
H	3.021898219	0.149206011	-1.053171075
O	-3.050042220	0.737802051	1.618757115
C	1.770247126	1.382779099	0.170634013
O	2.080755149	-2.271710161	-0.548412038
H	3.681849264	-1.241512089	0.943817067
H	1.246447090	1.304039096	1.127868079
C	0.393169028	-0.696037049	-1.270076093
H	-1.330929095	-1.593994112	-0.785821055
H	4.265088308	0.272366020	0.922693068
C	2.708328197	2.572928186	0.193620014
O	-3.236186234	1.026684076	-0.932088065
H	1.366363100	-2.863438204	-0.828447060
C	-0.231051017	0.676607047	-0.959846068
P	-2.619828187	0.285485021	0.240352017
O	-0.539713041	-1.748188124	-1.405285103
O	0.812416059	1.636696118	-0.871550061
H	3.247206234	2.654524190	-0.753255053
C	2.492834177	0.051160004	-0.088742007
H	0.895948063	-0.587960041	-2.242963163
H	-0.853953060	0.996118073	-1.800296128
H	3.433274247	2.479094180	1.002822071
C	1.464587108	-1.040980074	-0.253923018
N	3.411481246	-0.266492019	1.011035072
H	0.872062061	-1.208219088	0.897246066
H	2.142894152	3.492184253	0.350901025
C	0.260323019	-1.594613112	2.114478154
H	0.373449027	-0.729506054	2.759743196

H	0.822188058	-2.468479175	2.432035177
H	-0.757205054	-1.781835129	1.788931131

18-TS-CH₃

H	1.935646137	-0.382300027	-2.211271161
C	-4.518549325	-1.148984082	0.093083007
C	-1.459317106	-0.555460038	-1.544316111
C	2.106448154	-0.055657004	-1.177497083
C	-0.625094044	1.689834124	-0.634183044
N	-1.592861112	0.584834043	-0.793380056
N	-2.458662175	-1.394920103	-1.399836101
O	1.844557132	3.283813234	0.531796036
N	-3.318974236	1.311025093	0.769653055
C	-2.771561201	0.457895033	-0.105560008
C	1.668217122	1.400130101	-1.054770074
C	-3.295494240	-0.774826054	-0.494311035
O	5.451432410	-1.096745080	0.334692024
O	3.473938248	-0.151330011	-0.853619059
O	3.408518245	-2.595970188	-0.093948007
C	-4.468557320	0.848617059	1.253707090
H	1.493069110	-0.687218051	-0.528353038
H	-4.680275338	-2.994875217	-0.770256058
H	-0.320369023	2.296421167	1.475158106
N	-5.085698365	-0.306462022	0.973909070
H	2.210502160	1.283853090	1.037772075
C	0.097334007	1.661730118	0.701056052
O	0.353056026	1.589179113	-1.637992116
H	2.358193170	2.029603145	-1.619144119
O	3.271851235	-0.720053054	1.636738119
H	-1.199077085	2.610440185	-0.771667056
H	-0.030185002	0.440083032	1.229444091
C	1.556820115	1.877980137	0.394134028
H	-4.975412360	1.485223105	1.971448142
H	-0.605229042	-0.700454049	-2.182641158
N	-5.143219371	-2.304382168	-0.205280015
H	-5.954530428	-2.577411185	0.322886023
P	3.938613283	-1.242560088	0.366472026
H	2.798562200	3.400307245	0.443878032
C	-0.116188008	-0.777307053	1.825106132
H	-0.648888049	-0.580383043	2.750966199
H	-0.670580046	-1.394861099	1.124543083
H	0.934125069	-1.035556076	1.934673139

19-TS-CH₃

H	-1.383997281	1.477196978	-1.765012028
C	0.362024813	2.153441110	1.016786170

H	1.346723904	1.743789126	0.783918155
H	0.488125775	3.130125185	1.476206205
H	-0.144302191	1.485591036	1.709135224
C	-0.423910252	2.330705085	-0.258227919
H	0.230186000	-1.885905185	-0.015153902
H	-1.241305165	-0.678039175	-1.472800007
H	-3.243441259	-1.733230347	1.344504196
H	0.670856964	-0.447396063	0.888851162
O	-0.632463324	3.449479157	-0.724869954
C	-2.036610235	-0.399464191	0.511424136
C	-0.942898167	-0.166867121	-0.558222942
N	-0.856144229	1.232489982	-0.940236966
S	1.722556042	-0.494439015	-1.277291991
C	0.370977958	-0.808994102	-0.091751907
O	-2.379372304	0.507224857	1.264019188
N	-2.581851215	-1.629560306	0.588088139
C	2.992178180	-1.450323024	-0.488435936
H	3.282729172	-0.929143971	0.665985147
H	2.705310209	-2.478617111	-0.271434920
H	3.912066244	-1.391914974	-1.065720979
C	-2.304110139	-2.820912377	-0.201503916
H	-1.532113051	-3.442235387	0.257620117
H	-3.218020172	-3.406974466	-0.278088921
H	-1.992205125	-2.561297346	-1.210217986
C	3.603914166	-0.355555913	1.918835240
H	2.748357117	-0.581827972	2.547734285
H	4.521488259	-0.853394905	2.216444260
H	3.719899124	0.697982167	1.683132221

20-TS-CH₃

N	-0.775513058	0.582968042	-0.495766036
H	-4.816494346	2.086518148	-0.322064023
H	3.988853286	-2.246372160	-0.693349051
O	-2.907602210	-2.432881173	-0.282079020
H	-4.355388315	-2.046441147	1.270446094
C	-2.244083161	-1.289833095	0.236811017
C	4.617583334	0.068224005	-0.265444019
H	4.948254354	-0.683180047	0.756782057
C	-3.961223286	0.350844025	-0.146683010
N	3.190377227	0.178666013	-0.317582023
H	-1.850783135	2.354944170	0.052707004
O	3.329594242	2.327269168	0.531820040
N	0.268570019	2.410764173	0.270064019
O	-4.196283301	-1.220290086	1.750434126
H	-1.394847103	-1.564338115	0.862475062
C	2.429575175	-0.902940067	-0.724945055

H	-2.262948161	-3.124271225	-0.469028034
H	-2.804689199	0.243854017	1.649248118
C	1.194723083	1.421602103	-0.008658001
C	0.560484042	0.283708020	-0.481724035
C	-1.844226132	-0.335045024	-0.898412066
C	2.610274188	1.424259102	0.121786009
N	3.087354222	-2.036148147	-1.086303079
H	-1.492861106	-0.883603062	-1.771376126
C	-0.887352066	1.879350134	-0.028651002
O	-4.239400304	1.640462119	0.310174022
H	-4.864331350	-0.135665010	-0.522133038
O	-3.008597217	0.383431028	-1.226857086
H	5.039426365	-0.413010030	-1.143074082
H	2.492183178	-2.833092206	-1.246994090
C	-3.298238235	-0.461348033	0.978811072
N	1.117733080	-0.887411064	-0.828106058
H	5.064382364	1.028677074	-0.048354003
C	5.227668376	-1.478563108	1.870932136
H	4.245122308	-1.753987128	2.241637161
H	5.808244405	-2.305444168	1.473713108
H	5.783408423	-0.811938058	2.522342180

21A-TS-CH₃

C	-0.441441174	-0.690109851	-0.145071059
P	1.239715585	-0.048433839	-0.049454606
O	-1.512128810	1.528305012	-0.155235839
O	2.209209608	-1.057399100	-0.823192013
H	-0.486955830	-1.659544283	0.353447945
H	-0.608525726	1.788726895	-0.411648620
O	1.336717077	1.356244850	-0.516862831
H	-0.652112665	-0.845148058	-1.207067603
O	1.624619579	-0.309707074	1.472077247
H	-1.412704289	0.325184397	1.543398354
H	-2.614341841	-0.266696555	0.218627379
C	-1.456653577	0.266943831	0.451662843
H	2.437636963	0.129195601	1.760541714
H	2.357433663	-0.812170103	-1.747190148
C	-3.866716727	-0.804119258	-0.135866203
H	-3.903527069	-1.754895334	0.387007001
H	-3.814060601	-0.888018020	-1.216972457
H	-4.577047150	-0.065964809	0.223029530

21B-TS-CH₃

C	-0.412878983	-0.764777078	-0.041692625
P	1.317893703	-0.162328623	-0.133311123
O	-1.365070368	1.492073061	-0.236580312

O	2.220839299	-1.239901977	-0.636314115
H	-0.453813077	-1.652563593	0.592203879
H	-0.450113987	1.586400064	-0.597544150
O	1.263490085	1.183904510	-0.824219024
H	-0.679311582	-1.070762466	-1.058655621
O	1.717289771	0.090883322	1.440582172
H	-1.368074517	0.416309523	1.541151727
H	-2.567900071	-0.210996902	0.254358764
C	-1.397628538	0.273115294	0.454237598
H	1.433319305	0.966453650	1.730531199
C	-3.867265976	-0.731291858	-0.077529838
H	-3.955077480	-1.632004417	0.522574531
H	-3.802453299	-0.909813285	-1.146585358
H	-4.550730170	0.063957305	0.203791278

21C-TS-CH₃

C	-0.386371240	-0.777721426	0.040876134
P	1.370148173	-0.132717604	-0.015403713
O	-1.297768494	1.483707435	-0.162569005
O	2.187852681	-1.182654429	-0.760673145
H	-0.438464850	-1.659228544	0.685450143
H	-0.347618946	1.520319643	-0.514397603
O	1.195230538	1.186692829	-0.817192196
H	-0.635113978	-1.098585405	-0.977021341
O	1.804013111	0.103859348	1.429186213
H	-1.413886567	0.380749872	1.592043724
H	-2.546585896	-0.199540368	0.248031824
C	-1.391782251	0.254454997	0.500405941
C	-3.879331487	-0.697899128	-0.148698516
H	-3.788899175	-0.807850259	-1.225287144
H	-4.564073793	0.083636092	0.166592344
H	-3.987292171	-1.634585098	0.390127490

22A-TS-CH₃

H	-3.790056274	0.789423059	-1.156298084
H	-3.813509273	-0.051695004	0.294831021
C	-1.954516143	0.001425000	-0.456347033
N	-3.299358239	0.661204046	-0.273818020
C	-0.948457068	0.614324043	0.500235036
C	-2.193229159	-1.516733107	-0.137298010
O	-3.255427235	-1.750553128	0.498714036
H	-1.251081090	0.454994033	1.536370113
H	-1.653963119	0.122223009	-1.492551109
H	-1.065941074	1.873271136	0.359280026
O	-1.315064097	-2.303601166	-0.513552037
C	0.479395034	0.298181022	0.278302020

C	1.292640094	-0.104353007	1.341788098
C	1.082168077	0.457820033	-0.977417071
C	2.646933190	-0.357604026	1.165305083
H	0.858380061	-0.230589016	2.326145169
C	2.430770174	0.209533015	-1.168106082
H	0.491324035	0.789149056	-1.822156133
C	3.220758230	-0.203550015	-0.094836007
H	3.256078234	-0.676309051	2.003225146
H	2.887293207	0.335060024	-2.141323152
O	4.543566328	-0.436884031	-0.340037024
H	4.988798359	-0.713216053	0.470800034
C	-1.185148087	3.324796239	0.173333012
H	-1.485022107	3.428661245	-0.864384064
H	-0.165440012	3.625390258	0.387650028
H	-1.919566139	3.649359262	0.903596066
H	-3.254261235	1.561122114	0.200767015

22B-TS-CH₃

H	-4.106642295	0.204403015	-0.710700053
H	-3.701887264	0.194432014	0.851161062
C	-2.103672154	0.024286002	-0.369726027
N	-3.429904245	0.577179039	-0.051576004
C	-1.056459075	0.712974049	0.494321036
C	-2.019298143	-1.520464108	-0.148149011
O	-2.495484181	-1.948322139	0.934172066
H	-1.337968094	0.655971050	1.547501113
H	-1.901394134	0.220269016	-1.423840105
H	-1.175075087	1.943085142	0.228357017
O	-1.479268104	-2.198950157	-1.055182075
C	0.370045027	0.371438027	0.290910021
C	1.206853085	0.096019007	1.377423100
C	0.953067069	0.370444026	-0.984909072
C	2.558991187	-0.181464013	1.209154086
H	0.791464058	0.091622007	2.378347172
C	2.299187166	0.098301007	-1.169366084
H	0.342328025	0.590201043	-1.851109135
C	3.109817225	-0.181763013	-0.069628005
H	3.183231228	-0.399296029	2.068480147
H	2.736992200	0.100626007	-2.159544153
O	4.431697320	-0.446333032	-0.308389022
H	4.889436350	-0.616783045	0.524076037
C	-1.250034092	3.363856241	-0.137691010
H	-1.470159106	3.321129237	-1.199206088
H	-0.256789019	3.723924269	0.110066008
H	-2.050761149	3.757244269	0.478601034

22C-TS-CH₃

H	-4.021163415	0.318960256	-0.866427112
H	-3.682388390	0.376348246	0.745775006
C	-1.968418280	0.043341151	-0.436900079
N	-3.333097353	0.634919251	-0.180234060
C	-0.956902181	0.685067157	0.504812989
C	-1.997272347	-1.468128955	-0.241397064
O	-2.882610428	-1.825870947	0.696929003
H	-1.256606209	0.557776157	1.544982065
H	-1.731770257	0.243452156	-1.478412154
H	-1.092490140	1.941168250	0.303717975
O	-1.263354325	-2.214964040	-0.827650109
C	0.467190907	0.351484072	0.284696973
C	1.281268954	0.009491013	1.369228050
C	1.060775955	0.426032053	-0.983250117
C	2.631699035	-0.262244062	1.202332038
H	0.851087919	-0.050713973	2.361342124
C	2.405730036	0.155851977	-1.163411131
H	0.470294922	0.706937100	-1.846133181
C	3.199044082	-0.191931081	-0.068976052
H	3.243093071	-0.530860107	2.055738098
H	2.857670071	0.214082963	-2.144772202
O	4.515842165	-0.447860154	-0.305806069
H	4.967742189	-0.671371187	0.517748990
C	-1.202545085	3.364594358	0.031262955
H	-1.355445099	3.412536367	-1.042197124
H	-0.222871004	3.684981342	0.368119979
H	-2.031431135	3.712592419	0.638941999
H	-2.850717465	-2.787502014	0.835131013
H	-3.295769311	1.655392321	-0.230091064

22D-TS-CH₃

H	3.965095181	-0.032863971	-1.417068065
H	3.590855156	-0.869265031	-0.067638967
C	1.959787034	-0.028379977	-0.978542033
N	3.279116135	-0.658506020	-1.009406036
C	0.920785966	-1.041065055	-0.491890997
C	1.930006028	1.283355118	-0.197684976
O	2.449261066	1.160617112	1.038026112
H	1.358068998	-1.495366083	0.647606085
H	1.698855019	0.254717043	-2.002028105
H	0.991324971	-1.921437114	-1.129826045
O	1.506552996	2.329722191	-0.628332005
C	-0.483534138	-0.606751025	-0.292124983
C	-0.853425168	0.263967035	0.740405090
C	-1.503675209	-1.099002063	-1.116985041

C	-2.173642261	0.648863061	0.927653105
H	-0.103064114	0.634593067	1.426476143
C	-2.827428306	-0.723317041	-0.942147031
H	-1.253668190	-1.786291113	-1.916426102
C	-3.167210334	0.158485020	0.081620044
H	-2.435203282	1.321830104	1.735956165
H	-3.605043361	-1.106648071	-1.590147079
O	-4.483844431	0.498497041	0.213841053
H	-4.598111437	1.104214083	0.956968106
H	2.417981061	2.027255175	1.475306143
C	1.800982032	-2.030868122	1.878458174
H	2.128200054	-1.156807057	2.430419213
H	0.905497967	-2.505444159	2.266978200
H	2.593768091	-2.721357171	1.608417156

23A-TS-CH₃

C	-1.182084087	-0.322810023	0.252067018
N	-2.135848152	-1.422038103	0.336793024
C	0.187143013	-0.878952065	-0.169291012
C	1.308989094	0.133145010	-0.176490013
C	2.663085194	-0.419978030	-0.383773028
O	3.560242258	0.542408040	-0.698468052
H	-1.097444081	0.124582009	1.245695087
H	0.084485006	-1.317353095	-1.168360081
H	0.437839032	-1.694312122	0.509497037
O	2.981987216	-1.582940113	-0.244947018
C	-1.629371120	0.765413054	-0.745830056
O	-2.029646146	0.442282032	-1.846132133
H	1.379565099	0.622480046	1.012014071
H	1.143797081	1.025294075	-0.775649056
H	4.435322317	0.128045009	-0.769096053
C	-3.445099247	-1.038379073	0.863991060
H	-3.328874238	-0.664828048	1.883441135
H	-3.959883287	-0.265309019	0.276167020
H	-4.088281294	-1.917964140	0.898976063
H	-2.249546159	-1.819632132	-0.590451043
C	1.423740101	1.113616081	2.353799168
H	0.739627051	1.954553143	2.347086168
H	2.471759180	1.371261101	2.459335178
H	1.096311080	0.254167018	2.928387212
C	-1.576362112	2.197458158	-0.297126021
H	-1.786572128	2.873099207	-1.123470081
H	-2.320517168	2.337795171	0.493023035
H	-0.607567042	2.431308173	0.148148011

23B-TS-CH₃

C	-1.136667079	-0.341604025	0.239620017
N	-2.088298152	-1.447385106	0.273333020
C	0.237208017	-0.861158062	-0.219688016
C	1.355294098	0.154127011	-0.214904015
C	2.771512199	-0.358599026	-0.435732032
O	3.610204258	0.487679035	-0.847465061
H	-1.045423073	0.053424004	1.254923092
H	0.117471009	-1.271723093	-1.230740088
H	0.510971037	-1.696541123	0.424832031
O	3.003795214	-1.563924113	-0.157187011
C	-1.591080113	0.796026058	-0.691925050
O	-2.035695145	0.536274040	-1.793393127
H	1.411356099	0.619812045	0.986607070
H	1.163247086	1.049857076	-0.804269058
C	-3.398747246	-1.091686076	0.815543057
H	-3.285744239	-0.771457057	1.853587134
H	-3.911712282	-0.287989021	0.268062019
H	-4.043815292	-1.970897142	0.803566056
H	-2.200569159	-1.799612129	-0.672101049
C	1.462213107	1.069944078	2.342943171
H	0.760531055	1.895802138	2.396713173
H	2.503224181	1.354783098	2.455690178
H	1.169032084	0.193283014	2.911621210
C	-1.488749108	2.205948161	-0.182687013
H	-1.673251122	2.923064208	-0.980063068
H	-2.234376161	2.337222167	0.607927042
H	-0.515194037	2.384444172	0.275657020

24-TS-CH₃

H	-1.243501129	-1.785244094	0.336795995
C	-3.489754282	-0.753893992	-0.237630046
H	-4.114934317	-0.271704949	0.515371008
H	-3.966709314	-0.610528975	-1.206999117
H	-3.430767291	-1.819024071	-0.018963030
C	-2.145697172	-0.063063959	-0.255848048
H	0.796036023	-1.147289074	1.021880046
H	0.905442080	2.836972213	1.135365054
O	-2.033733151	1.117376124	-0.579675073
C	0.355188018	0.959887085	0.972858039
C	0.275237996	-0.338695008	0.173644983
N	-1.084354109	-0.815139025	0.117416979
C	1.102073053	-0.569535037	-1.097341108
O	0.022260994	0.921928084	2.159599124
N	0.861257071	2.101122160	0.445396003
H	0.789216039	0.158961021	-1.848835160
C	0.838787014	-1.958633131	-1.690266149

H	1.083140023	-2.747265192	-0.974920100
H	-0.201279060	-2.081502130	-1.991668175
H	1.463094061	-2.105582150	-2.572971213
C	2.599908161	-0.393254041	-0.821138091
H	2.960923178	-1.190572101	-0.167897041
H	3.163412202	-0.444703052	-1.753702156
H	2.827273193	0.557040024	-0.339136054
C	1.255158046	-2.090425148	2.006372116
H	0.366211980	-2.239327149	2.608846161
H	2.046643108	-1.529368113	2.489883152
H	1.582034056	-2.955898212	1.441155076
C	0.875880075	2.543880192	-0.945230097
H	0.880255090	3.631955268	-0.944643097
H	1.764668137	2.205600159	-1.478324136
H	-0.018386994	2.203563181	-1.462850136

25-TS-CH₃

H	3.049059221	2.725572195	0.540624041
H	-2.525151180	0.983940069	1.266536093
H	-1.914666138	2.565296185	0.757781053
H	-2.029626149	-1.758991129	-1.452550103
H	0.351483025	-2.873145209	-1.722135124
H	3.131571226	-0.820396057	-0.641148049
H	3.346726239	-1.398424103	0.893237062
H	-0.523284037	1.440824102	-0.989545072
H	-1.348372095	-1.126083079	0.759559057
H	0.755413054	-0.767831055	-1.624365119
H	1.039343075	-1.382944102	1.353174098
H	1.993094143	0.862772063	1.604484115
C	2.357909171	2.583394185	-0.294634021
O	2.014294143	1.198999084	-0.430029031
O	-3.105017222	1.670160118	-0.619260045
C	-2.138839152	1.554917114	0.415452030
O	-1.926379138	-0.804777057	-1.335582098
O	0.288009021	-2.614407189	-0.795855055
N	2.711748196	-1.398270102	0.092944007
O	0.126836009	1.128906081	0.965246068
C	-0.839008062	0.920277067	-0.076373005
C	-0.955687068	-0.567718043	-0.358437026
C	0.384944028	-1.196781086	-0.686527051
C	1.416290100	0.637272048	0.702037051
H	-3.234755233	0.789396055	-0.997574072
H	2.840218202	2.873998205	-1.224129087
H	1.464006103	3.189010230	-0.137749010
C	1.352725096	-0.872453065	0.445454032
C	-1.821179129	-1.754789128	1.934906141

H	-1.433500103	-1.141026082	2.741644197
H	-2.899431210	-1.715586122	1.817369132
H	-1.399129099	-2.753232200	1.882907137
H	2.629903187	-2.361021168	-0.246159018

26-TS-CH₃

N	-1.296616078	-0.116039957	-0.372946106
N	-2.171415208	-2.031338063	0.403650950
N	-5.283131364	-0.042471812	0.102661929
N	-3.340708181	1.199665207	-0.577130122
N	-5.205148434	-2.227811971	0.876215986
C	-0.322491975	0.865427078	-0.855880138
C	-0.056164916	1.978594152	0.163974933
C	1.196121154	1.453408069	0.888329985
C	1.942095183	0.745769989	-0.244363096
C	-1.076028108	-1.408182057	0.045378924
C	-3.174664251	-1.102416960	0.210533936
C	-2.651115167	0.093418106	-0.275770098
C	-4.569270350	-1.142732916	0.401186950
C	-4.644110280	1.038872245	-0.358716104
O	0.242290147	3.162995226	-0.552697119
O	2.005529248	2.486129115	1.421050023
O	0.904893090	0.208185989	-1.087472159
H	-0.711760990	1.286637123	-1.783759207
H	0.880652211	3.661514236	-0.020975080
H	-0.906946970	2.124950191	0.832980982
H	1.715824236	2.687206140	2.318784086
H	0.906996110	0.737611028	1.661970042
H	2.504479252	1.496637024	-0.808779135
H	-4.700917426	-3.079990049	1.047103999
H	-6.208706485	-2.231351934	0.939573986
H	-0.085665052	-1.829399125	0.044738924
H	-5.274619294	1.893036330	-0.582174123
C	2.866492212	-0.352842120	0.227972938
H	3.590694281	0.084478886	0.917406989
H	2.303716145	-1.124124155	0.756668977
S	3.783237249	-1.117198209	-1.154015160
C	4.873361295	-2.159403318	-0.219870095
H	5.680287388	-1.434390296	0.493639957
H	4.360829231	-2.799022346	0.497922957
H	5.512471312	-2.727204384	-0.892304144
C	6.552615445	-0.635364268	1.272220012
H	7.515130493	-1.131865341	1.197728006
H	6.118406462	-0.646851256	2.267151082
H	6.503726505	0.327504802	0.772360977

27-TS-CH₃

H	0.726927167	1.105312078	1.709637217
C	1.847522308	2.347441114	-1.199278993
H	0.981389260	2.669637175	-1.782172035
H	2.610722401	3.118117132	-1.280046999
H	2.226955292	1.418394024	-1.612452021
C	1.444361276	2.240067124	0.251011113
H	0.022151001	-1.330481067	-1.528615015
H	0.363592045	-0.918820051	1.092890172
H	3.316140180	-2.485357305	-0.508449942
H	0.213640096	0.372125048	-1.822815038
O	1.503805328	3.219497190	0.992646167
C	2.276359184	-0.860043138	-0.075267911
C	0.897231117	-0.240823029	0.117972103
N	0.953922183	1.062449060	0.726220144
C	-0.079463960	-0.353878990	-1.062231981
O	3.292274291	-0.173949139	0.042954098
N	2.365760130	-2.177963236	-0.361139931
C	-1.520445053	-0.126054904	-0.671891956
C	-2.370098166	-1.209519943	-0.443824938
C	-2.027425025	1.164172215	-0.506510942
C	-3.688552252	-1.012669864	-0.046885909
H	-1.998710185	-2.218415032	-0.578753945
C	-3.344644111	1.366288290	-0.108484913
H	-1.389168941	2.018671243	-0.690689956
C	-4.179224225	0.277604252	0.126420103
H	-4.331639338	-1.866769897	0.124766103
H	-3.719906094	2.374537381	0.014861096
H	-5.205095289	0.433848312	0.435134126
C	-0.213562021	-1.427503059	2.288951259
H	-0.739864017	-0.570231974	2.695177291
H	-0.862693105	-2.227362086	1.952918234
H	0.657066028	-1.744704126	2.853312302
C	1.339088008	-3.206045261	-0.434129937
H	0.465790956	-2.928785201	0.145672105
H	1.031876977	-3.402224264	-1.463936013
H	1.737529991	-4.127485348	-0.011883906

28-TS-CH₃

H	1.241897087	-0.081104006	1.782671128
C	2.376674172	-0.144437010	-1.366181100
H	2.185450158	0.862982062	-1.737418123
H	3.357106241	-0.468319034	-1.705076122
H	1.612179114	-0.804997057	-1.771026128
C	2.368039169	-0.145713011	0.142892010
H	-0.841115061	0.231883017	1.278527090

H	-2.063316149	-2.555414181	-0.837093060
O	3.406637247	-0.252765018	0.793254059
C	-0.585968043	-1.410824102	-0.182769013
C	-0.151651011	-0.004004000	0.219938016
N	1.176011085	0.013818001	0.779005056
O	0.213051016	-2.347551167	-0.152712011
N	-1.869543136	-1.606422115	-0.553893039
C	-0.459438033	1.079277076	-0.790724057
C	-1.355954099	2.254517161	-0.464623033
C	0.118441009	2.458471179	-0.627060043
H	-0.540314038	0.722114052	-1.810892130
H	-1.766090126	2.311690164	0.534094036
H	-2.020370145	2.601444188	-1.244385088
H	0.480408035	2.959576210	-1.514797107
H	0.703014050	2.639957190	0.264886019
C	-2.977853215	-0.665148047	-0.619343046
H	-2.924846212	0.058996004	0.187530013
H	-3.003106214	-0.125979009	-1.567711112
H	-3.904442281	-1.225434086	-0.510537036
C	-1.372561099	0.464393033	2.600077186
H	-1.109756082	-0.452310032	3.117427223
H	-0.833570062	1.348189095	2.923835209
H	-2.434281175	0.608298043	2.436607174

Cartesian Coordinates of all the transition states between substrates and 5'-dAdo[•] radical.

1A-TS-Ado

N	11.673095000	1.401737000	3.232226000
N	10.237344000	2.824514000	2.256898000
N	13.010919000	3.016220000	-0.192329000
N	13.504378000	1.522033000	1.624870000
N	11.030779000	4.211337000	-0.371620000
C	12.243777000	0.452352000	4.190705000
C	13.290816000	1.100396000	5.104694000
C	12.450292000	1.464343000	6.341553000
C	11.451006000	0.301137000	6.402463000
C	10.153764000	0.587991000	7.083415000
C	10.446674000	2.023398000	3.272581000
C	11.389336000	2.729790000	1.501444000
C	12.293111000	1.848163000	2.090546000
C	11.797962000	3.331640000	0.295935000
C	13.775749000	2.150366000	0.483041000
O	14.256976000	0.116881000	5.429707000
O	13.210393000	1.503061000	7.536307000
O	11.208889000	-0.032753000	5.016041000

H	12.693040000	-0.359289000	3.616710000
H	14.553137000	0.302116000	6.333567000
H	13.755847000	1.969235000	4.632643000
H	13.577467000	2.387575000	7.651563000
H	11.925316000	2.407880000	6.174124000
H	11.957435000	-0.544224000	6.882093000
H	9.563502000	1.376119000	6.620928000
H	10.245239000	0.708627000	8.160279000
H	10.095788000	4.409360000	-0.061294000
H	11.336698000	4.566997000	-1.261063000
H	9.752004000	1.827232000	4.071010000
H	14.741830000	1.936230000	0.038142000
H	-0.891979000	-2.173157000	4.988482000
H	1.894096000	-4.167297000	5.507217000
H	2.476140000	-2.852477000	4.523010000
H	3.395585000	-1.717194000	6.580103000
H	2.816401000	-3.042689000	7.565506000
H	4.290262000	-4.629841000	6.297084000
H	4.870646000	-3.300169000	5.312629000
H	5.775641000	-2.181391000	7.357644000
H	5.203372000	-3.510236000	8.344365000
H	6.663150000	-5.098120000	7.100600000
H	7.252059000	-3.796546000	6.083543000
H	7.750296000	-1.291169000	6.333479000
H	9.283113000	-2.205515000	6.033197000
H	9.392021000	-0.520308000	6.930485000
H	9.120957000	-5.548098000	8.023740000
H	7.540669000	-3.916119000	9.116208000
H	7.999839000	-1.657929000	8.781203000
H	10.605439000	-1.897610000	8.716885000
O	0.599882000	-1.581661000	6.642162000
O	-0.079506000	-2.672437000	4.804582000
C	0.833524000	-2.361537000	5.748808000
C	2.127763000	-3.098610000	5.530699000
C	3.196777000	-2.792184000	6.571622000
C	4.494619000	-3.553537000	6.309981000
C	5.576731000	-3.257622000	7.346144000
C	6.872687000	-4.023902000	7.083018000
C	8.684833000	-1.653026000	6.754124000
O	11.377883000	-4.374530000	8.591026000
C	10.262452000	-3.894536000	8.420460000
N	9.158353000	-4.545657000	7.926493000
C	7.952118000	-3.737594000	8.114160000
C	8.567994000	-2.302180000	8.110259000
N	9.884175000	-2.600719000	8.689505000

1B-TS- Ado

N	12.046517000	1.142380000	3.327314000
N	10.770866000	2.638231000	2.244813000
N	13.676837000	2.570951000	-0.052903000
N	13.964216000	1.091779000	1.820076000
N	11.799197000	3.896229000	-0.366895000
C	12.497221000	0.182734000	4.337699000
C	13.523459000	0.787450000	5.303647000
C	12.631783000	1.229516000	6.477487000
C	11.562424000	0.128961000	6.497417000
C	10.246066000	0.505925000	7.092194000
C	10.867892000	1.850481000	3.287467000
C	11.951336000	2.442933000	1.555523000
C	12.756694000	1.514681000	2.211848000
C	12.465552000	2.983787000	0.361510000
C	14.340176000	1.670200000	0.681489000
O	14.405416000	-0.244506000	5.708180000
O	13.316921000	1.250002000	7.717161000
O	11.385261000	-0.220366000	5.105316000
H	12.930690000	-0.667017000	3.808485000
H	14.655859000	-0.056534000	6.625219000
H	14.069264000	1.615706000	4.845253000
H	13.729010000	2.113442000	7.839249000
H	12.175984000	2.198288000	6.259117000
H	11.988500000	-0.733830000	7.022267000
H	9.726838000	1.307050000	6.570582000
H	10.283364000	0.659608000	8.168094000
H	10.872667000	4.181936000	-0.103398000
H	12.183515000	4.219920000	-1.237844000
H	10.119026000	1.723770000	4.050077000
H	15.310448000	1.376926000	0.294583000
H	1.856835000	-3.930758000	5.344948000
H	2.503075000	-2.620775000	4.393797000
H	3.413664000	-1.555629000	6.482725000
H	2.759987000	-2.866524000	7.432961000
H	4.211759000	-4.494677000	6.192953000
H	4.861062000	-3.181992000	5.230272000
H	5.756641000	-2.104083000	7.298976000
H	5.113738000	-3.412799000	8.267887000
H	6.551386000	-5.049386000	7.066349000
H	7.205851000	-3.772565000	6.058140000
H	7.781612000	-1.284174000	6.306882000
H	9.287177000	-2.254842000	6.049042000
H	9.437516000	-0.567984000	6.933485000
H	8.974579000	-5.571576000	8.050908000
H	7.419342000	-3.885734000	9.097178000

H	7.954679000	-1.643818000	8.760348000
H	10.551134000	-1.965697000	8.774685000
O	0.588863000	-1.467148000	6.627932000
O	-0.028092000	-2.180454000	4.592717000
C	0.778327000	-2.097373000	5.557395000
C	2.108474000	-2.864514000	5.385267000
C	3.171473000	-2.622586000	6.449825000
C	4.451091000	-3.425047000	6.217495000
C	5.520087000	-3.172835000	7.279161000
C	6.796045000	-3.982466000	7.049492000
C	8.692759000	-1.675382000	6.751841000
O	11.250369000	-4.465584000	8.675795000
C	10.155206000	-3.952332000	8.472505000
N	9.045455000	-4.571251000	7.950667000
C	7.859760000	-3.725587000	8.104329000
C	8.519976000	-2.310188000	8.109019000
N	9.809852000	-2.646378000	8.725929000

2A-TS- Ado

O	2.300260000	-1.960844000	2.811326000
P	1.451326000	-1.322621000	1.644022000
O	2.292644000	-0.020348000	1.247498000
O	1.720328000	-2.378833000	0.502456000
O	0.038978000	-1.022479000	1.941275000
C	1.747289000	0.987106000	0.414316000
C	1.933144000	0.695762000	-1.045034000
C	1.403744000	1.797559000	-1.961012000
O	1.185639000	-0.517335000	-1.399244000
C	0.295461000	-0.250197000	-2.482435000
C	0.034030000	1.256010000	-2.405201000
N	-0.861621000	-1.093283000	-2.399749000
O	2.282408000	1.921459000	-3.069037000
O	-0.368220000	1.729995000	-3.675706000
C	-1.857887000	-1.123109000	-1.430912000
C	-2.768005000	-2.043116000	-1.880887000
N	-2.362679000	-2.577200000	-3.090024000
C	-1.222521000	-2.003476000	-3.363710000
N	-1.843162000	-0.277050000	-0.322507000
H	2.015573000	-1.681317000	3.692161000
H	1.524160000	-1.978974000	-0.374412000
H	0.740790000	1.271308000	0.717532000
H	2.522909000	2.053586000	0.665215000
H	2.986105000	0.507025000	-1.247568000
H	1.308490000	2.751978000	-1.436396000
H	0.783869000	-0.477120000	-3.433454000
H	-0.715240000	1.454809000	-1.639592000

H	1.767924000	2.293497000	-3.800488000
H	-0.948678000	2.491070000	-3.561696000
H	-3.684010000	-2.341857000	-1.397353000
H	-0.599036000	-2.187480000	-4.224247000
H	-1.121715000	-0.505138000	0.360194000
H	-2.739550000	-0.286483000	0.145781000
N	6.484889000	2.170618000	-1.845771000
N	5.947019000	3.156659000	-3.788230000
N	9.563167000	2.616678000	-4.388047000
N	8.866277000	1.800332000	-2.237364000
N	8.132731000	3.649141000	-5.894902000
C	6.349537000	1.556082000	-0.521006000
C	7.090540000	2.344967000	0.563698000
C	5.973795000	3.247318000	1.115979000
C	4.747151000	2.330141000	1.023161000
C	3.431422000	3.024676000	0.910896000
C	5.502362000	2.730983000	-2.630577000
C	7.294619000	2.856631000	-3.773258000
C	7.646973000	2.235364000	-2.577156000
C	8.329669000	3.046855000	-4.708210000
C	9.755927000	2.031071000	-3.200325000
O	7.524924000	1.426066000	1.550579000
O	6.185032000	3.630023000	2.462879000
O	4.985320000	1.540640000	-0.166668000
H	6.736966000	0.537945000	-0.583739000
H	7.493995000	1.890646000	2.400224000
H	7.930533000	2.908911000	0.153294000
H	6.708453000	4.439919000	2.484948000
H	5.844353000	4.118102000	0.468631000
H	4.754600000	1.663549000	1.891254000
H	3.337540000	3.685655000	0.051899000
H	3.085400000	3.471216000	1.838833000
H	7.206039000	3.907153000	-6.185546000
H	8.883895000	3.694224000	-6.561977000
H	4.476538000	2.766621000	-2.306582000
H	10.770873000	1.703399000	-3.001166000

2B-TS- Ado

O	4.199299000	-0.627278000	0.446042000
P	3.024833000	-1.139426000	-0.565330000
O	2.226187000	0.256582000	-0.902646000
O	3.670184000	-1.547008000	-1.838462000
O	2.100580000	-2.038768000	0.195185000
C	1.506104000	0.909804000	0.094285000
C	0.229276000	1.489342000	-0.440790000
C	-0.563082000	2.259864000	0.613883000

O	-0.642798000	0.414423000	-0.904088000
C	-1.879312000	0.464142000	-0.217175000
C	-1.596340000	1.224345000	1.081234000
N	-2.410700000	-0.864002000	-0.048652000
O	-1.204740000	3.366265000	-0.008896000
O	-2.795310000	1.801122000	1.569344000
C	-1.860575000	-1.938123000	0.634760000
C	-2.802150000	-2.933732000	0.556980000
N	-3.907791000	-2.501547000	-0.151966000
C	-3.637741000	-1.273504000	-0.507883000
N	-0.639603000	-1.856143000	1.297470000
H	3.918710000	-0.696011000	1.366545000
H	1.371892000	0.310078000	0.996005000
H	2.226699000	1.941551000	0.481727000
H	0.451871000	2.133709000	-1.291167000
H	0.071936000	2.600422000	1.435977000
H	-2.625035000	1.021759000	-0.793458000
H	-1.147375000	0.547622000	1.808240000
H	-1.989126000	3.572555000	0.520282000
H	-2.733420000	1.896378000	2.526513000
H	-2.735790000	-3.926339000	0.972642000
H	-4.264502000	-0.621486000	-1.095340000
H	0.176936000	-1.723846000	0.697948000
H	-0.483033000	-2.682024000	1.859572000
N	1.806784000	5.796122000	-2.133669000
N	0.040714000	6.887646000	-1.281751000
N	1.009452000	9.309264000	-3.912823000
N	2.443709000	7.380680000	-3.879789000
N	-0.754827000	9.623074000	-2.438866000
C	2.798009000	4.737966000	-2.369670000
C	4.223520000	5.206433000	-2.061631000
C	4.387164000	4.761266000	-0.599532000
C	3.603209000	3.442178000	-0.569923000
C	3.048172000	3.041230000	0.753763000
C	0.784813000	5.810036000	-1.212011000
C	0.594206000	7.623898000	-2.310108000
C	1.688020000	6.957607000	-2.859046000
C	0.263607000	8.865065000	-2.885696000
C	2.031296000	8.558890000	-4.341679000
O	5.110083000	4.492286000	-2.905836000
O	5.737338000	4.524229000	-0.239818000
O	2.519553000	3.657504000	-1.512452000
H	2.712992000	4.427439000	-3.412382000
H	5.925509000	4.352885000	-2.401518000
H	4.335621000	6.284046000	-2.196347000
H	6.136079000	5.350464000	0.058257000

H	3.920070000	5.491820000	0.065629000
H	4.251229000	2.653526000	-0.965275000
H	2.382733000	3.770666000	1.210522000
H	3.786210000	2.637370000	1.440686000
H	-1.378750000	9.268387000	-1.735396000
H	-1.009279000	10.457857000	-2.938658000
H	0.623409000	4.984430000	-0.540588000
H	2.593290000	8.968543000	-5.174463000

2C-TS- Ado

O	3.914754000	-0.837083000	0.770826000
P	3.010028000	-1.221147000	-0.387746000
O	2.252240000	0.241703000	-0.858135000
O	3.711031000	-1.620595000	-1.669644000
O	1.839820000	-2.119922000	0.013199000
C	1.506079000	0.919397000	0.072666000
C	0.273144000	1.544563000	-0.524973000
C	-0.551838000	2.328486000	0.490949000
O	-0.617180000	0.509720000	-1.049551000
C	-1.857000000	0.541364000	-0.373530000
C	-1.603375000	1.301700000	0.930886000
N	-2.385244000	-0.791717000	-0.212700000
O	-1.171259000	3.433658000	-0.160845000
O	-2.814296000	1.886182000	1.385534000
C	-1.870937000	-1.855040000	0.517604000
C	-2.809427000	-2.851872000	0.402429000
N	-3.874764000	-2.433233000	-0.372873000
C	-3.584820000	-1.209988000	-0.731389000
N	-0.687102000	-1.766129000	1.241619000
H	1.298297000	0.342361000	0.977376000
H	2.193981000	1.930877000	0.505772000
H	0.559648000	2.186521000	-1.358033000
H	0.055468000	2.674629000	1.331061000
H	-2.603373000	1.091765000	-0.956504000
H	-1.179392000	0.623873000	1.671201000
H	-1.973400000	3.641860000	0.340024000
H	-2.772616000	1.991071000	2.342692000
H	-2.766340000	-3.837479000	0.837938000
H	-4.178844000	-0.567881000	-1.362467000
H	0.179034000	-1.724929000	0.676643000
H	-0.603424000	-2.559119000	1.864463000
N	1.966153000	5.884323000	-2.024831000
N	0.152668000	6.955543000	-1.250066000
N	1.263412000	9.435343000	-3.768562000
N	2.696017000	7.506437000	-3.698826000
N	-0.604204000	9.697438000	-2.417057000

C	2.971934000	4.830947000	-2.225009000
C	4.373947000	5.291854000	-1.813739000
C	4.439826000	4.812485000	-0.355454000
C	3.654239000	3.494210000	-0.401565000
C	3.009330000	3.066694000	0.870301000
C	0.895289000	5.878036000	-1.160867000
C	0.759929000	7.713131000	-2.231513000
C	1.884753000	7.060007000	-2.731843000
C	0.459387000	8.965975000	-2.798021000
C	2.308897000	8.694937000	-4.156002000
O	5.315984000	4.597748000	-2.614019000
O	5.764035000	4.562724000	0.086595000
O	2.640014000	3.728793000	-1.418772000
H	2.953802000	4.550992000	-3.279765000
H	6.090459000	4.435102000	-2.054973000
H	4.493249000	6.372331000	-1.916886000
H	6.144056000	5.380613000	0.428431000
H	3.932751000	5.529773000	0.294597000
H	4.328595000	2.712604000	-0.766343000
H	2.316545000	3.788870000	1.297160000
H	3.698100000	2.644564000	1.596280000
H	-1.166932000	9.405555000	-1.637356000
H	-0.733153000	10.621256000	-2.792773000
H	0.699542000	5.038182000	-0.516882000
H	2.917630000	9.124611000	-4.944709000

3-TS- Ado

N	0.903041000	-1.071330000	0.413652000
N	2.201064000	-0.745929000	2.216537000
N	4.758593000	-0.302367000	-0.426525000
N	2.583894000	-0.773400000	-1.334691000
N	5.202457000	-0.190431000	1.845921000
C	-0.279627000	-1.332025000	-0.390009000
C	-0.865297000	-2.747980000	-0.231308000
C	-2.105521000	-2.503673000	0.650800000
C	-2.539197000	-1.092406000	0.228343000
C	-3.338559000	-0.327382000	1.230866000
C	0.992236000	-1.004538000	1.786115000
C	2.960128000	-0.633436000	1.066631000
C	2.170748000	-0.826928000	-0.065029000
C	4.324090000	-0.367249000	0.843617000
C	3.883728000	-0.500102000	-1.419086000
O	-1.252325000	-3.209805000	-1.514602000
O	-3.149557000	-3.429445000	0.401913000
O	-1.289746000	-0.416481000	-0.008318000
H	0.021518000	-1.177673000	-1.426810000

H	-2.055543000	-3.737902000	-1.388392000
H	-0.145317000	-3.430980000	0.226968000
H	-3.040682000	-4.195388000	0.977796000
H	-1.823481000	-2.503706000	1.706266000
H	-3.091570000	-1.180929000	-0.715406000
H	-2.826277000	-0.164893000	2.177137000
H	-4.348877000	-0.706872000	1.356143000
H	4.888445000	-0.165094000	2.799895000
H	6.148741000	0.078257000	1.637230000
H	0.125342000	-1.137833000	2.412049000
H	4.292287000	-0.429840000	-2.421565000
H	-4.945204000	2.980933000	-1.325617000
H	4.602536000	2.872874000	0.941702000
H	1.125120000	3.627205000	1.746600000
H	1.210177000	1.889254000	1.681949000
H	0.305172000	1.917130000	-0.653390000
H	0.207487000	3.663269000	-0.600932000
H	-1.416521000	3.511574000	1.306719000
H	-1.253505000	1.762969000	1.291623000
H	-2.076608000	1.791848000	-1.126533000
H	-2.443234000	3.494673000	-0.921282000
H	-3.958998000	2.768097000	1.086149000
H	-3.530935000	0.962264000	0.734229000
O	2.863269000	2.982065000	-0.742140000
C	-6.172191000	1.680403000	-0.120604000
C	-4.837541000	2.037069000	-0.773346000
C	2.657782000	2.879175000	0.468184000
C	1.262245000	2.786713000	1.057726000
C	0.149814000	2.764551000	0.018718000
C	-1.233126000	2.649784000	0.654985000
C	-2.353420000	2.541903000	-0.379460000
C	-3.695421000	2.172250000	0.207695000
H	-4.578010000	1.282923000	-1.524970000
H	-6.970545000	1.610650000	-0.862024000
H	-6.113244000	0.721611000	0.398224000
H	-6.461112000	2.437240000	0.613019000
N	3.681602000	2.847728000	1.351216000
C	3.576493000	2.697068000	2.793528000
H	3.014810000	3.518050000	3.242735000
H	3.096128000	1.755322000	3.066235000
H	4.580209000	2.703056000	3.211036000

4-TS- Ado

C	2.347869000	-0.084665000	-1.449989000
C	0.924134000	0.121168000	-0.999008000
O	0.003747000	0.304076000	-1.791009000

N	0.713466000	0.104614000	0.343883000
C	-0.527739000	0.479392000	0.921953000
C	-1.791679000	-0.273994000	0.572346000
O	-2.867830000	0.326704000	0.622504000
H	2.967330000	-0.574433000	-0.699726000
H	-0.798292000	1.686761000	0.523398000
H	-0.435543000	0.595181000	1.998746000
N	-1.740777000	-1.582720000	0.244713000
H	-2.642364000	-1.966857000	0.003212000
H	1.518276000	0.056241000	0.947470000
H	2.779383000	0.893764000	-1.670733000
H	2.350361000	-0.669862000	-2.367439000
C	-0.625222000	-2.516556000	0.306739000
H	-0.005560000	-2.476917000	-0.590798000
H	0.001384000	-2.323013000	1.174392000
H	-1.034122000	-3.520808000	0.399909000
N	2.232105000	3.846887000	-2.392720000
N	1.655960000	3.093067000	-4.425861000
N	4.538182000	5.216581000	-5.381733000
N	4.135110000	5.243634000	-3.012100000
N	3.249677000	4.014313000	-6.890385000
C	2.236567000	4.042505000	-0.938496000
C	1.745340000	5.437046000	-0.541951000
C	0.243327000	5.187765000	-0.323790000
C	0.231682000	3.770349000	0.272521000
C	-1.017631000	2.993122000	0.037890000
C	1.383583000	3.064538000	-3.143635000
C	2.743496000	3.937614000	-4.530382000
C	3.119815000	4.412547000	-3.275782000
C	3.511206000	4.382150000	-5.623524000
C	4.785942000	5.589675000	-4.120713000
O	2.375754000	5.793305000	0.675326000
O	-0.342118000	6.095812000	0.592046000
O	1.360335000	3.110013000	-0.353262000
H	3.256289000	3.879543000	-0.586874000
H	1.740595000	6.328560000	1.174224000
H	1.946963000	6.175033000	-1.321925000
H	-0.646953000	6.876185000	0.114148000
H	-0.279055000	5.199291000	-1.283377000
H	0.434519000	3.857819000	1.345096000
H	-1.258886000	2.800365000	-1.003230000
H	-1.864360000	3.320107000	0.633061000
H	2.529345000	3.341876000	-7.086831000
H	3.862517000	4.306053000	-7.632289000
H	0.611394000	2.474820000	-2.678721000
H	5.627551000	6.261846000	-3.990231000

5-TS- Ado

N	-2.481089000	-0.094213000	-0.106614000
N	-3.176760000	-2.227964000	-0.074355000
N	-6.401097000	-0.569609000	-0.837099000
N	-4.600043000	1.006181000	-0.608800000
N	-6.142461000	-2.861269000	-0.587789000
C	-1.598596000	1.075242000	-0.016815000
C	-1.763620000	1.818807000	1.312659000
C	-0.665290000	1.167534000	2.170302000
C	0.450170000	0.927793000	1.145826000
C	1.396411000	-0.184401000	1.442460000
C	-2.154274000	-1.419032000	0.061506000
C	-4.241407000	-1.391823000	-0.346630000
C	-3.828013000	-0.061235000	-0.372738000
C	-5.607080000	-1.627876000	-0.594734000
C	-5.865045000	0.656672000	-0.831211000
O	-1.479329000	3.188968000	1.090529000
O	-0.191091000	2.019625000	3.200398000
O	-0.263098000	0.643741000	-0.091167000
H	-1.842041000	1.729724000	-0.855009000
H	-1.039778000	3.515964000	1.889907000
H	-2.766460000	1.688182000	1.727096000
H	-0.750863000	1.916249000	3.979080000
H	-1.023896000	0.218772000	2.577220000
H	1.016460000	1.853331000	1.017058000
H	0.938856000	-1.167881000	1.534133000
H	2.096576000	0.042679000	2.240498000
H	-5.559108000	-3.669732000	-0.462877000
H	-7.112089000	-2.987492000	-0.822128000
H	-1.140484000	-1.717102000	0.266346000
H	-6.556015000	1.468175000	-1.034177000
C	2.726011000	1.395457000	-3.643220000
N	3.474338000	0.951651000	-2.727948000
C	3.003496000	1.060723000	-1.348961000
C	3.891738000	2.017401000	-0.488437000
O	4.956684000	2.451900000	-0.979857000
C	2.953781000	-0.338962000	-0.754064000
C	4.263721000	-0.955859000	-0.326836000
C	4.094277000	-2.383807000	0.194217000
C	5.423280000	-2.963811000	0.640697000
N	5.259048000	-4.384793000	1.121366000
O	3.428577000	2.260670000	0.652597000
H	1.754114000	1.868145000	-3.452027000
H	1.987123000	1.476836000	-1.321931000
H	2.350546000	-1.008439000	-1.370726000

H	4.959929000	-0.956030000	-1.174194000
H	4.722197000	-0.334488000	0.448434000
H	3.663677000	-3.012504000	-0.590745000
H	3.392752000	-2.388848000	1.033132000
H	6.146652000	-2.996726000	-0.171674000
H	5.851689000	-2.405445000	1.470638000
H	6.146268000	-4.779745000	1.436999000
H	4.602241000	-4.440074000	1.901848000
H	4.901155000	-4.987914000	0.378434000
H	2.205093000	-0.260326000	0.342137000
H	3.040553000	1.318646000	-4.682926000

6A-TS- Ado

C	2.638874000	-1.268825000	0.742144000
N	1.376535000	-1.308515000	0.778322000
C	0.663201000	-0.066802000	0.495179000
C	-0.352006000	0.275760000	1.575817000
O	-0.828672000	-0.782026000	2.247165000
C	-0.028893000	-0.165229000	-0.862281000
C	-1.150998000	-1.148401000	-1.044033000
O	-0.721465000	1.407627000	1.785232000
H	3.210852000	-0.355543000	0.542132000
H	1.344211000	0.792581000	0.456722000
H	0.711955000	-0.208305000	-1.655382000
H	-0.794300000	-2.169628000	-0.862523000
H	-1.946978000	-0.982488000	-0.313980000
H	-0.560514000	1.028136000	-1.075095000
H	3.205359000	-2.181547000	0.913427000
C	-1.791751000	-1.141577000	-2.455005000
O	-1.185687000	-0.537651000	-3.376425000
O	-2.874204000	-1.769297000	-2.559710000
N	2.059162000	2.297065000	-3.916892000
N	1.998763000	0.449916000	-5.188043000
N	5.198848000	1.875243000	-6.393337000
N	4.171252000	3.244379000	-4.705780000
N	4.263020000	-0.093396000	-7.191319000
C	1.661358000	3.293770000	-2.940894000
C	0.457613000	4.157180000	-3.374192000
C	-0.150670000	4.523930000	-2.019326000
C	0.029013000	3.218567000	-1.231140000
C	-1.094110000	2.239344000	-1.398287000
C	1.382042000	1.145680000	-4.263374000
C	3.139105000	1.176117000	-5.471714000
C	3.197515000	2.327107000	-4.688441000
C	4.207588000	0.966929000	-6.362302000
C	5.125422000	2.936221000	-5.580676000

O	0.801737000	5.248891000	-4.190619000
O	0.653372000	5.586160000	-1.505974000
O	1.277501000	2.655088000	-1.743457000
H	2.534076000	3.933429000	-2.788813000
H	1.141940000	5.943421000	-3.607708000
H	-0.242760000	3.540018000	-3.937206000
H	0.192260000	6.010885000	-0.774657000
H	-1.197025000	4.823040000	-2.093268000
H	0.193018000	3.433934000	-0.175041000
H	-1.415101000	2.052059000	-2.419316000
H	-1.918381000	2.375551000	-0.704475000
H	3.590671000	-0.835425000	-7.104096000
H	5.096068000	-0.256169000	-7.730837000
H	0.458048000	0.846462000	-3.784851000
H	5.954365000	3.633127000	-5.647952000
H	-1.489778000	-0.460154000	2.882936000

6B-TS- Ado

C	2.460933000	-2.227979000	-0.885217000
N	1.692597000	-1.588956000	-0.111683000
C	1.380668000	-0.202406000	-0.455249000
C	1.910853000	0.755693000	0.669051000
O	1.483596000	0.575222000	1.832241000
C	-0.113785000	-0.052954000	-0.685440000
C	-1.042889000	-0.437426000	0.435156000
O	2.717104000	1.636305000	0.284381000
H	2.897543000	-1.796816000	-1.794379000
H	1.888579000	0.087663000	-1.382237000
H	-0.418893000	-0.464514000	-1.646673000
H	-0.916458000	-1.492448000	0.705201000
H	-0.805722000	0.116330000	1.344826000
H	-0.299937000	1.246843000	-0.878703000
H	2.715218000	-3.261422000	-0.655901000
C	-2.495898000	-0.238261000	0.104622000
O	-2.951546000	0.089588000	-0.966648000
O	-3.283348000	-0.484235000	1.174526000
H	-4.208076000	-0.357578000	0.906486000
N	-0.467792000	2.854454000	-5.190985000
N	-2.627306000	2.613797000	-5.754289000
N	-1.311129000	3.851886000	-8.988575000
N	0.407759000	3.669149000	-7.317913000
N	-3.539468000	3.334036000	-8.601680000
C	0.766362000	2.830226000	-4.393923000
C	1.213851000	4.237225000	-3.986942000
C	0.536611000	4.392755000	-2.614654000
C	0.617726000	2.971829000	-2.041545000

C	-0.445744000	2.596989000	-1.065264000
C	-1.735143000	2.489549000	-4.801920000
C	-1.910543000	3.085698000	-6.835940000
C	-0.565151000	3.238569000	-6.505983000
C	-2.273422000	3.419054000	-8.154651000
C	-0.056139000	3.949182000	-8.533713000
O	2.624175000	4.228344000	-3.851627000
O	1.224209000	5.290533000	-1.758247000
O	0.530291000	2.109556000	-3.212077000
H	1.533710000	2.341357000	-4.996052000
H	2.837573000	4.823015000	-3.116844000
H	0.893403000	4.989638000	-4.711686000
H	0.908213000	6.187429000	-1.919568000
H	-0.505637000	4.693603000	-2.746405000
H	1.601161000	2.831132000	-1.585545000
H	-1.466980000	2.698883000	-1.424673000
H	-0.295836000	3.009495000	-0.071507000
H	-4.256382000	2.934893000	-8.021489000
H	-3.737246000	3.504994000	-9.572755000
H	-1.925105000	2.127015000	-3.806464000
H	0.674361000	4.302711000	-9.253817000

6C-TS- Ado

C	2.385199000	-2.194917000	-1.092899000
N	1.581259000	-1.662186000	-0.276631000
C	1.421851000	-0.212147000	-0.348701000
C	1.686368000	0.455380000	0.996497000
O	1.290983000	-0.270028000	2.051171000
C	0.021842000	0.130740000	-0.842744000
C	-1.149634000	-0.333588000	-0.019211000
O	2.168994000	1.558029000	1.093648000
H	2.974604000	-1.627330000	-1.821382000
H	2.137392000	0.244952000	-1.041679000
H	-0.077204000	-0.101672000	-1.899320000
H	-1.126348000	-1.419594000	0.124746000
H	-1.140685000	0.090593000	0.987658000
H	-0.039482000	1.467001000	-0.866168000
H	2.508871000	-3.275424000	-1.086856000
C	-2.473820000	0.006180000	-0.654475000
O	-2.630111000	0.520542000	-1.737283000
O	-3.502833000	-0.344481000	0.138535000
H	-4.332052000	-0.117159000	-0.313500000
N	-0.347320000	2.759686000	-4.989813000
N	-2.496978000	2.222541000	-5.346145000
N	-1.704839000	3.690432000	-8.654307000
N	0.186276000	3.719046000	-7.170711000

N	-3.789561000	2.862535000	-8.061926000
C	0.961458000	2.868859000	-4.327017000
C	1.343588000	4.324244000	-4.054495000
C	0.729039000	4.547104000	-2.662149000
C	0.912312000	3.179439000	-1.986437000
C	-0.132663000	2.811693000	-0.982926000
C	-1.504401000	2.205817000	-4.488973000
C	-1.967982000	2.811577000	-6.477075000
C	-0.630034000	3.146178000	-6.277648000
C	-2.507455000	3.114648000	-7.741556000
C	-0.434309000	3.951986000	-8.324944000
O	2.756985000	4.399622000	-3.998225000
O	1.404488000	5.542175000	-1.911212000
O	0.900006000	2.222710000	-3.083401000
H	1.700713000	2.383392000	-4.965280000
H	2.975662000	5.067085000	-3.330841000
H	0.942113000	5.001426000	-4.811406000
H	1.032587000	6.406580000	-2.123837000
H	-0.333134000	4.782265000	-2.762668000
H	1.904787000	3.148905000	-1.529757000
H	-1.159421000	2.943730000	-1.314587000
H	0.051760000	3.187991000	0.018271000
H	-4.383086000	2.362215000	-7.423803000
H	-4.109451000	3.024134000	-9.001500000
H	-1.546827000	1.794118000	-3.494088000
H	0.163474000	4.413949000	-9.103687000
H	1.461555000	0.246459000	2.856908000

6D-TS- Ado

C	3.038151000	-1.141115000	0.073097000
N	1.821704000	-1.116427000	0.412922000
C	1.067227000	0.108073000	0.154046000
C	0.496121000	0.728586000	1.469618000
O	0.129698000	-0.038349000	2.386332000
C	-0.036120000	-0.195268000	-0.854510000
C	-1.166080000	-1.099931000	-0.442257000
O	0.436143000	1.986228000	1.470010000
H	3.553176000	-0.290192000	-0.391535000
H	1.723396000	0.870366000	-0.287691000
H	0.380704000	-0.469119000	-1.823644000
H	-0.762565000	-2.065600000	-0.111294000
H	-1.689798000	-0.691522000	0.422130000
H	-0.572427000	0.981084000	-1.141752000
H	3.626951000	-2.041998000	0.239768000
C	-2.215170000	-1.408962000	-1.533944000
O	-1.957304000	-1.089856000	-2.722682000

O	-3.260840000	-1.985216000	-1.133161000
N	-3.742454000	2.666143000	1.775520000
N	-2.693734000	2.767345000	3.755363000
N	-6.193948000	3.011703000	4.944145000
N	-6.056766000	2.825632000	2.551527000
N	-4.335051000	3.071503000	6.333841000
C	-3.941778000	2.611481000	0.341366000
C	-3.606417000	3.921110000	-0.396265000
C	-3.329399000	3.392988000	-1.802388000
C	-2.582385000	2.079039000	-1.511115000
C	-1.092505000	2.215803000	-1.460829000
C	-2.542940000	2.662590000	2.456493000
C	-4.059530000	2.849503000	3.944541000
C	-4.730581000	2.784273000	2.724734000
C	-4.858409000	2.971991000	5.095434000
C	-6.703969000	2.936028000	3.708748000
O	-4.605401000	4.907419000	-0.308435000
O	-4.612796000	3.176345000	-2.394448000
O	-3.089185000	1.636930000	-0.212678000
H	-4.997205000	2.366679000	0.189758000
H	-5.294437000	4.671815000	-0.946482000
H	-2.692136000	4.340350000	0.025688000
H	-4.503479000	3.007004000	-3.336518000
H	-2.734722000	4.080999000	-2.404635000
H	-2.867183000	1.320744000	-2.243104000
H	-0.706002000	2.832742000	-0.655000000
H	-0.643579000	2.426506000	-2.429392000
H	-3.351625000	2.918035000	6.474764000
H	-4.947294000	3.032995000	7.130976000
H	-1.591985000	2.538742000	1.951473000
H	-7.786866000	2.969915000	3.648707000

7A-TS- Ado

C	0.859288000	-0.710672000	-0.835972000
C	0.369291000	0.587044000	-0.782333000
C	1.270004000	1.671786000	-0.792266000
N	0.000577000	-1.751489000	-0.742889000
C	-1.438893000	-1.570319000	-0.749524000
C	-1.800130000	-0.226404000	-0.116106000
N	-1.007511000	0.827483000	-0.648601000
C	-3.271398000	0.033732000	-0.136803000
O	-3.567888000	1.345359000	-0.086998000
O	-4.112918000	-0.836545000	-0.112109000
O	0.977155000	2.873624000	-0.684397000
N	4.351229000	-0.246633000	-1.167349000
H	-1.612741000	-0.372681000	1.093958000

H	3.285482000	2.045632000	-0.953083000
H	0.383491000	-2.680576000	-0.788172000
H	-1.904244000	-2.371838000	-0.179522000
H	-1.838044000	-1.609352000	-1.768954000
H	-1.222016000	1.757589000	-0.316632000
H	4.646411000	-1.186921000	-0.957873000
H	5.014326000	0.469088000	-0.917347000
N	2.182002000	-1.007886000	-0.940142000
C	3.022027000	-0.005572000	-0.993165000
N	2.615636000	1.289620000	-0.925850000
H	-4.532473000	1.442228000	-0.031710000
N	3.001582000	0.148400000	2.455256000
N	3.652981000	2.294140000	2.391201000
N	6.906530000	0.669536000	1.677930000
N	5.144854000	-0.931285000	2.011348000
N	6.597622000	2.964604000	1.813165000
C	2.133500000	-1.013886000	2.525713000
C	1.946496000	-1.622048000	3.935510000
C	0.452942000	-1.346314000	4.229466000
C	-0.155886000	-1.294141000	2.815934000
C	-1.437964000	-0.568212000	2.665941000
C	2.645686000	1.474301000	2.559556000
C	4.736403000	1.467483000	2.163515000
C	4.351456000	0.128615000	2.201755000
C	6.092701000	1.721672000	1.882897000
C	6.399360000	-0.566514000	1.756057000
O	2.196149000	-3.014553000	3.863429000
O	-0.152019000	-2.374065000	4.994175000
O	0.861874000	-0.604151000	2.074605000
H	2.566554000	-1.771531000	1.868084000
H	1.551758000	-3.440584000	4.449913000
H	2.609285000	-1.147398000	4.663660000
H	-0.108546000	-2.145495000	5.929864000
H	0.338308000	-0.371836000	4.707848000
H	-0.248790000	-2.325015000	2.449540000
H	-1.433161000	0.477895000	2.959077000
H	-2.336502000	-1.119794000	2.916168000
H	5.999608000	3.765268000	1.917788000
H	7.562490000	3.100911000	1.565102000
H	1.622479000	1.759570000	2.734932000
H	7.105306000	-1.371903000	1.583645000

7B-TS- Ado

C	0.905394000	-0.612502000	-0.959979000
C	0.416480000	0.681016000	-0.809410000
C	1.317127000	1.762977000	-0.763573000

N	0.043796000	-1.652638000	-0.995185000
C	-1.396394000	-1.501523000	-0.806599000
C	-1.734287000	-0.176091000	-0.137554000
N	-0.960533000	0.883685000	-0.676851000
C	-3.230106000	0.152870000	-0.052263000
O	-3.524283000	1.370164000	0.048871000
O	-4.015657000	-0.825485000	-0.027761000
O	1.031437000	2.962840000	-0.601727000
N	4.407803000	-0.133345000	-1.220516000
H	-1.467525000	-0.328093000	1.070034000
H	3.335520000	2.139561000	-0.878713000
H	0.446514000	-2.573902000	-0.958734000
H	-1.763209000	-2.318364000	-0.187468000
H	-1.913035000	-1.565328000	-1.770175000
H	-1.244628000	1.804339000	-0.373624000
H	4.691390000	-1.087169000	-1.060365000
H	5.059569000	0.553357000	-0.874841000
N	2.231302000	-0.904572000	-1.070703000
C	3.070607000	0.097044000	-1.050680000
N	2.664186000	1.385907000	-0.916724000
N	2.977617000	-0.070703000	2.399935000
N	3.461039000	2.117568000	2.278012000
N	6.827766000	0.734188000	1.588106000
N	5.199199000	-0.990221000	1.978436000
N	6.341477000	3.001417000	1.672157000
C	2.197457000	-1.300129000	2.530532000
C	1.963800000	-1.729223000	3.986425000
C	0.556523000	-1.172066000	4.263183000
C	-0.138397000	-1.320848000	2.897769000
C	-1.258817000	-0.388522000	2.614484000
C	2.520698000	1.225469000	2.464691000
C	4.605629000	1.372120000	2.072871000
C	4.325365000	0.008230000	2.147554000
C	5.935748000	1.724394000	1.775637000
C	6.419337000	-0.535516000	1.702752000
O	1.956419000	-3.146354000	4.030833000
O	-0.147306000	-1.912415000	5.246478000
O	0.934721000	-1.084128000	1.952450000
H	2.751345000	-2.072282000	1.994959000
H	1.304170000	-3.399888000	4.701368000
H	2.725854000	-1.320543000	4.655691000
H	0.068494000	-1.566054000	6.120454000
H	0.619538000	-0.115388000	4.534970000
H	-0.469274000	-2.361011000	2.803051000
H	-1.053223000	0.665307000	2.788416000
H	-2.238232000	-0.712914000	2.948425000

H	5.678236000	3.753161000	1.741905000
H	7.285623000	3.205258000	1.392288000
H	1.477107000	1.440749000	2.618853000
H	7.184984000	-1.287352000	1.544001000

8A-TS- Ado

N	-1.128758000	-1.654946000	0.102937000
N	-0.955743000	-2.180728000	-2.070467000
N	-4.633178000	-2.437612000	-1.691391000
N	-3.547593000	-1.826096000	0.364211000
N	-3.496496000	-2.851226000	-3.671341000
C	-0.758971000	-1.191069000	1.444369000
C	-0.800951000	-2.310597000	2.487405000
C	0.651536000	-2.818462000	2.460312000
C	1.457266000	-1.534976000	2.201765000
C	2.756231000	-1.717865000	1.486320000
C	-0.306171000	-1.828058000	-0.986474000
C	-2.279733000	-2.234154000	-1.678949000
C	-2.407036000	-1.902758000	-0.331365000
C	-3.474294000	-2.511371000	-2.370194000
C	-4.604504000	-2.107032000	-0.394912000
O	-1.104570000	-1.727199000	3.742173000
O	1.057623000	-3.397424000	3.688971000
O	0.559431000	-0.714843000	1.403126000
H	-1.447927000	-0.388107000	1.711551000
H	-0.616139000	-2.231033000	4.410414000
H	-1.528115000	-3.083161000	2.225078000
H	0.819213000	-4.332043000	3.693467000
H	0.783200000	-3.518009000	1.631324000
H	1.611186000	-1.029847000	3.159603000
H	2.725209000	-2.384956000	0.628373000
H	3.612569000	-1.887064000	2.131083000
H	-2.651478000	-2.832258000	-4.214899000
H	-4.377936000	-2.958322000	-4.143524000
H	0.751530000	-1.634961000	-0.919450000
H	-5.570818000	-2.061322000	0.096142000
O	3.565826000	0.820397000	-3.145120000
O	5.452979000	0.264448000	0.760974000
C	2.487847000	1.645986000	0.615375000
C	2.324665000	2.878922000	-0.310557000
C	1.064021000	3.634134000	0.039978000
C	-2.646864000	2.919375000	0.151334000
C	-1.633109000	1.316828000	-1.336156000
O	1.110302000	4.726134000	0.580473000
H	5.395318000	-1.659318000	-0.197552000
O	-3.655881000	4.485945000	1.610717000

O	4.957480000	-1.716965000	-1.059861000
H	3.068437000	-0.513003000	0.808691000
C	-0.259221000	2.982520000	-0.242735000
O	-4.981233000	2.946051000	0.661655000
C	-1.400688000	3.498566000	0.372484000
C	-2.760408000	1.825447000	-0.712456000
H	3.147476000	-1.167918000	-2.728138000
H	4.902425000	1.613141000	-0.719883000
H	5.645033000	-0.129530000	-2.211133000
H	6.329062000	0.655741000	0.661193000
H	2.727928000	0.898258000	-3.617838000
C	-3.878410000	3.425148000	0.811834000
C	-0.385435000	1.878460000	-1.091366000
H	3.041938000	1.924492000	1.513476000
H	3.165693000	3.562612000	-0.213193000
H	1.512033000	1.294068000	0.943054000
H	2.279342000	2.546040000	-1.348849000
H	-1.300164000	4.348319000	1.031056000
H	-3.731909000	1.381330000	-0.879193000
H	-1.719320000	0.471749000	-2.004503000
H	0.485251000	1.439855000	-1.556767000
O	2.534078000	0.040082000	-1.203600000
C	4.665347000	0.602322000	-0.373343000
C	4.823611000	-0.391028000	-1.540327000
C	3.477342000	-0.249721000	-2.239834000
C	3.189402000	0.483497000	-0.036610000
H	-4.503755000	4.751795000	2.001307000

8B-TS- Ado

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N	-1.127947000	-1.654669000	0.079466000
N	-0.939916000	-2.164085000	-2.096685000
N	-4.608859000	-2.524636000	-1.720820000
N	-3.541714000	-1.891633000	0.337880000
N	-3.459751000	-2.901495000	-3.701416000
C	-0.772312000	-1.176379000	1.420071000
C	-0.824029000	-2.286816000	2.472191000
C	0.628257000	-2.795804000	2.461195000
C	1.437020000	-1.514914000	2.199232000
C	2.741251000	-1.703642000	1.494787000
C	-0.300830000	-1.799135000	-1.010428000
C	-2.262244000	-2.254389000	-1.706403000
C	-2.398973000	-1.932983000	-0.357184000
C	-3.448005000	-2.562656000	-2.398929000
C	-4.589990000	-2.198759000	-0.422828000

O	-1.137478000	-1.692741000	3.719686000
O	1.023761000	-3.365710000	3.697794000
O	0.545960000	-0.699613000	1.388816000
H	-1.463771000	-0.370518000	1.671769000
H	-0.654812000	-2.191369000	4.395923000
H	-1.549624000	-3.060995000	2.210676000
H	0.783464000	-4.299789000	3.707639000
H	0.766193000	-3.502056000	1.638924000
H	1.584507000	-1.003401000	3.154785000
H	2.714561000	-2.373779000	0.639041000
H	3.591724000	-1.873432000	2.147210000
H	-2.617967000	-2.838893000	-4.246914000
H	-4.338883000	-3.014705000	-4.176660000
H	0.751683000	-1.580118000	-0.940917000
H	-5.557408000	-2.182446000	0.067964000
O	3.586988000	0.788821000	-3.150416000
O	5.448431000	0.275346000	0.774694000
C	2.481680000	1.654907000	0.590117000
C	2.320809000	2.873074000	-0.353261000
C	1.076894000	3.658676000	0.002937000
C	-2.657645000	3.050715000	0.158848000
C	-1.672664000	1.365973000	-1.276777000
O	1.165638000	4.759100000	0.526522000
H	5.399527000	-1.654690000	-0.163420000
O	-3.698155000	4.721345000	1.497380000
O	4.972931000	-1.723312000	-1.030581000
H	3.062519000	-0.502405000	0.813267000
C	-0.258694000	3.034520000	-0.253568000
O	-4.977489000	3.066097000	0.682668000
C	-1.391726000	3.595485000	0.344601000
C	-2.785286000	1.927507000	-0.662279000
H	3.170906000	-1.196252000	-2.715511000
H	4.907176000	1.609436000	-0.722714000
H	5.662177000	-0.145016000	-2.193038000
H	6.324690000	0.666827000	0.677309000
H	2.742438000	0.875107000	-3.609874000
C	-3.886230000	3.667924000	0.840427000
C	-0.410056000	1.903839000	-1.065248000
H	3.030354000	1.945873000	1.487942000
H	3.174959000	3.544113000	-0.281783000
H	1.503857000	1.306509000	0.914738000
H	2.253467000	2.521639000	-1.383883000
H	-1.283613000	4.465784000	0.975430000
H	-3.768046000	1.499872000	-0.806603000
H	-1.785324000	0.498769000	-1.913764000
H	0.447065000	1.430832000	-1.522562000

O	2.544745000	0.025352000	-1.208185000
C	4.668420000	0.601731000	-0.368672000
C	4.837261000	-0.402545000	-1.524918000
C	3.494926000	-0.272226000	-2.233947000
C	3.190052000	0.485193000	-0.041511000

9-TS- Ado

H	-1.801168000	0.069922000	1.471428000
C	-2.626240000	-0.537269000	-1.722845000
H	-1.613197000	-0.665728000	-2.098834000
H	-3.254787000	-1.350597000	-2.075546000
H	-3.012850000	0.402304000	-2.122760000
C	-2.699301000	-0.501390000	-0.215629000
H	0.514063000	-0.772852000	-1.204000000
H	-0.089912000	1.418720000	1.009049000
H	-1.617835000	3.258507000	-1.891952000
H	0.526571000	-1.074181000	0.528851000
O	-3.642989000	-0.998438000	0.393518000
C	-0.639881000	1.709005000	-1.162381000
C	-0.481890000	0.713889000	-0.029806000
N	-1.703243000	0.131393000	0.466514000
C	0.645076000	-0.297197000	-0.227819000
O	0.141024000	1.681029000	-2.116328000
N	-1.643994000	2.611327000	-1.118288000
C	2.048166000	0.297193000	-0.132759000
H	2.143344000	1.164153000	-0.783243000
H	2.264316000	0.598879000	0.892029000
S	3.291956000	-0.944602000	-0.623856000
C	4.797765000	0.023624000	-0.321111000
H	5.647108000	-0.605179000	-0.584516000
H	4.810247000	0.920015000	-0.941224000
H	4.871993000	0.303231000	0.729922000
C	-2.557336000	2.930702000	-0.032031000
H	-3.396214000	2.236232000	0.019260000
H	-2.045859000	2.938962000	0.926261000
H	-2.950148000	3.928991000	-0.209203000
N	-0.430380000	5.855369000	0.488539000
N	-2.452439000	6.708580000	0.971389000
N	-2.694159000	6.705752000	-2.725827000
N	-0.591197000	5.837792000	-1.949432000
N	-4.368574000	7.459551000	-1.309713000
C	0.851392000	5.186505000	0.632614000
C	1.610733000	5.523639000	1.920121000
C	1.275940000	4.326089000	2.833807000
C	1.167974000	3.169217000	1.828573000
C	0.265914000	2.046925000	2.229299000

C	-1.33466000	6.23730800	1.45782800
C	-2.29576600	6.62263200	-0.39922100
C	-1.05189200	6.08711100	-0.71932300
C	-3.14201300	6.94118200	-1.47942400
C	-1.47443400	6.18117100	-2.88579800
O	2.99248600	5.53359800	1.60781800
O	2.29529100	4.05206100	3.77620700
O	0.64844400	3.78008900	0.63352400
H	1.44159700	5.46438600	-0.23940100
H	3.45984900	5.22061900	2.39723600
H	1.30455100	6.48119700	2.34856500
H	2.13108300	4.55831600	4.58062400
H	0.31529400	4.48574000	3.32860500
H	2.17977800	2.80228300	1.63174900
H	-0.70814500	2.34762600	2.60623200
H	0.72792900	1.25269000	2.80684300
H	-4.72831600	7.63448100	-0.38800000
H	-4.94554800	7.65740400	-2.10911500
H	-1.10999600	6.15245000	2.50820200
H	-1.17076400	6.00921400	-3.91288400

10A-TS- Ado

C	2.01445600	-0.19766700	0.50054900
C	2.36534000	-0.73899000	-0.87100000
O	2.08129500	0.10255700	-1.88013200
C	0.75865000	-0.97897400	1.01565300
C	-0.46956500	-0.81941800	0.17727500
C	-0.87134500	-1.65163500	-0.83583700
C	-1.44188000	0.23866900	0.23750700
N	-2.02560400	-1.17411100	-1.41223500
C	-2.40452600	-0.01849800	-0.77474300
C	-1.60304800	1.36886600	1.05166200
C	-3.49990400	0.81786100	-0.99020600
C	-2.69044200	2.20042100	0.84200600
C	-3.62910900	1.92835500	-0.17110500
O	2.82754600	-1.84156000	-1.05993900
H	0.56865100	-0.63822700	2.03555000
H	1.03029000	-2.03458200	1.07534900
H	-0.41439400	-2.55943300	-1.19499800
H	-0.88499400	1.58982100	1.83099700
H	-2.82383600	3.07618200	1.46475400
H	-4.22219200	0.60581100	-1.76836900
H	-4.46788000	2.59833900	-0.31211200
H	2.84360300	-0.50090600	1.14505600
H	-2.52333500	-1.61822800	-2.16446100
C	1.85213200	1.29863300	0.56467100

H	1.106189000	1.715502000	-0.103764000
H	1.756112000	1.676770000	1.579836000
H	2.996014000	1.857488000	0.132944000
H	2.301949000	-0.340700000	-2.716018000
N	2.917182000	6.255656000	-1.568980000
N	3.229492000	7.609413000	0.193635000
N	2.510519000	10.164970000	-2.391038000
N	2.443642000	7.931535000	-3.277455000
N	2.990254000	10.654018000	-0.174766000
C	2.816707000	5.036275000	-2.375716000
C	4.068268000	4.797796000	-3.228587000
C	4.887365000	3.857266000	-2.327584000
C	3.792374000	3.013079000	-1.662976000
C	4.134794000	2.417679000	-0.338323000
C	3.206769000	6.369194000	-0.229339000
C	2.940358000	8.360225000	-0.928638000
C	2.741255000	7.535959000	-2.034280000
C	2.811935000	9.744835000	-1.149364000
C	2.347040000	9.256666000	-3.360125000
O	3.671733000	4.133492000	-4.415380000
O	5.763029000	3.015146000	-3.057602000
O	2.681474000	3.932592000	-1.511425000
H	1.937197000	5.140347000	-3.012805000
H	4.393321000	3.532625000	-4.654712000
H	4.586003000	5.733168000	-3.455259000
H	6.605830000	3.466750000	-3.184409000
H	5.429286000	4.437148000	-1.576638000
H	3.498733000	2.226510000	-2.363718000
H	4.412068000	3.140171000	0.426864000
H	4.830337000	1.584720000	-0.404178000
H	3.148381000	10.359966000	0.772982000
H	2.826105000	11.627871000	-0.363998000
H	3.373273000	5.495740000	0.377241000
H	2.104681000	9.657670000	-4.338692000

10B-TS- Ado

C	0.489471000	2.340811000	-0.852706000
C	-0.158015000	3.562379000	-0.149746000
O	-0.336500000	3.514558000	1.090717000
C	-0.594594000	1.558227000	-1.652647000
C	-1.709514000	0.971918000	-0.844480000
C	-2.927744000	1.549861000	-0.601618000
C	-1.722951000	-0.288984000	-0.152228000
N	-3.692911000	0.734123000	0.204916000
C	-2.983648000	-0.404337000	0.494076000
C	-0.801677000	-1.338042000	-0.023239000

C	-3.331603000	-1.520662000	1.254855000
C	-1.144337000	-2.449692000	0.729340000
C	-2.397342000	-2.539110000	1.364838000
O	-0.464631000	4.523983000	-0.906483000
H	-0.093132000	0.762291000	-2.211933000
H	-1.010652000	2.249917000	-2.388471000
H	-3.311065000	2.498432000	-0.940759000
H	0.166472000	-1.276132000	-0.503464000
H	-0.439027000	-3.264775000	0.834725000
H	-4.297232000	-1.587961000	1.740467000
H	-2.636072000	-3.419328000	1.948611000
H	1.170200000	2.748700000	-1.604152000
H	-4.631229000	0.931303000	0.506261000
C	1.289266000	1.469597000	0.076905000
H	0.755207000	1.114685000	0.953378000
H	1.860794000	0.682416000	-0.415203000
H	2.228612000	2.270221000	0.585182000
N	3.660931000	5.568450000	-2.398034000
N	1.951452000	7.018711000	-2.488407000
N	4.320225000	8.770717000	-4.734024000
N	5.223781000	6.710119000	-3.888182000
N	2.217716000	9.576850000	-4.172869000
C	4.449556000	4.370026000	-2.079683000
C	5.693343000	4.704586000	-1.249564000
C	5.177827000	4.488978000	0.181709000
C	4.215808000	3.305597000	0.013220000
C	3.117490000	3.212617000	1.018246000
C	2.382804000	5.882962000	-1.992212000
C	2.993818000	7.476105000	-3.268710000
C	4.062865000	6.583310000	-3.233070000
C	3.161904000	8.623030000	-4.066718000
C	5.261566000	7.827293000	-4.610625000
O	6.700365000	3.758590000	-1.567918000
O	6.207004000	4.144466000	1.094821000
O	3.659577000	3.493226000	-1.315996000
H	4.735557000	3.901789000	-3.023278000
H	7.200923000	3.600183000	-0.753569000
H	6.041814000	5.723278000	-1.431083000
H	6.600279000	4.951466000	1.447442000
H	4.630028000	5.373235000	0.516433000
H	4.811640000	2.386537000	0.008384000
H	2.492466000	4.099533000	1.088920000
H	3.447098000	2.846818000	1.987486000
H	1.312469000	9.439866000	-3.758450000
H	2.344040000	10.330324000	-4.826844000
H	1.805251000	5.228067000	-1.359835000

H	6.171889000	8.000410000	-5.175094000
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11A-TS- Ado

C	-2.194579000	0.220274000	1.096612000
C	-2.769718000	-0.886821000	0.231250000
O	-3.257420000	-0.427694000	-0.937953000
C	-0.932306000	0.858000000	0.507928000
C	0.249844000	0.043162000	0.220975000
C	0.365575000	-1.318714000	0.041219000
C	1.556261000	0.590344000	-0.058401000
N	1.650203000	-1.636619000	-0.331633000
C	2.404925000	-0.490688000	-0.403317000
C	2.076115000	1.890072000	-0.065233000
C	3.742913000	-0.305597000	-0.747477000
C	3.405347000	2.081006000	-0.409210000
C	4.230107000	0.992939000	-0.747009000
O	-2.823928000	-2.057151000	0.530799000
H	-0.675600000	1.740269000	1.096045000
H	-1.267877000	1.448166000	-0.587284000
H	-0.370352000	-2.095262000	0.154598000
H	1.448763000	2.735764000	0.188079000
H	3.818362000	3.081795000	-0.420346000
H	4.375483000	-1.144300000	-1.009321000
H	5.264294000	1.172436000	-1.012438000
H	-2.958299000	1.004020000	1.101121000
H	1.987400000	-2.569826000	-0.493851000
C	-1.976773000	-0.267060000	2.531733000
H	-1.228210000	-1.057531000	2.565188000
H	-1.631010000	0.561723000	3.150145000
H	-2.902690000	-0.654243000	2.958463000
H	-3.619440000	-1.185406000	-1.426465000
N	-1.066455000	-0.376376000	-4.964736000
N	-3.110051000	-1.231649000	-5.323925000
N	-1.407913000	-2.472385000	-8.372454000
N	0.063161000	-1.190865000	-6.967956000
N	-3.632568000	-2.887549000	-7.863285000
C	0.033593000	0.345487000	-4.316001000
C	0.296020000	1.707381000	-4.966011000
C	-0.576234000	2.635096000	-4.103342000
C	-0.439005000	2.003283000	-2.708751000
C	-1.564485000	2.249735000	-1.764969000
C	-2.358057000	-0.523490000	-4.516988000
C	-2.269168000	-1.572722000	-6.365072000
C	-0.993245000	-1.051240000	-6.158409000
C	-2.456470000	-2.319313000	-7.543982000
C	-0.236487000	-1.914666000	-8.044218000

O	1.669177000	2.015174000	-4.800554000
O	-0.099744000	3.969525000	-4.069061000
O	-0.315998000	0.583586000	-2.976057000
H	0.920299000	-0.287084000	-4.377947000
H	1.728259000	2.974388000	-4.676620000
H	0.015400000	1.713335000	-6.022270000
H	-0.471965000	4.459504000	-4.811768000
H	-1.614907000	2.592276000	-4.440159000
H	0.503184000	2.353948000	-2.277353000
H	-2.533618000	1.872748000	-2.076832000
H	-1.590006000	3.256791000	-1.358795000
H	-4.443935000	-2.736684000	-7.290125000
H	-3.735643000	-3.363635000	-8.742960000
H	-2.668173000	-0.094939000	-3.579582000
H	0.570379000	-2.074937000	-8.751636000

11B-TS- Ado

C	-2.274973000	0.164510000	0.842203000
C	-2.810179000	-0.813083000	-0.246070000
O	-3.355677000	-0.278785000	-1.247679000
C	-0.961180000	0.840504000	0.447634000
C	0.254899000	0.055297000	0.215393000
C	0.399993000	-1.296568000	-0.001427000
C	1.568827000	0.626602000	0.042010000
N	1.714401000	-1.589076000	-0.293651000
C	2.456396000	-0.433226000	-0.276466000
C	2.067660000	1.933232000	0.098581000
C	3.810994000	-0.219020000	-0.524869000
C	3.414137000	2.153340000	-0.151390000
C	4.277316000	1.086458000	-0.459068000
O	-2.671420000	-2.047251000	-0.056565000
H	-0.758548000	1.689298000	1.106363000
H	-1.183026000	1.484060000	-0.638981000
H	-0.354523000	-2.064310000	0.018474000
H	1.409265000	2.762470000	0.327134000
H	3.810235000	3.160493000	-0.112433000
H	4.473177000	-1.040812000	-0.767517000
H	5.324041000	1.287276000	-0.650375000
H	-3.017130000	0.966712000	0.893668000
H	2.075181000	-2.511271000	-0.465815000
C	-2.174265000	-0.480571000	2.228633000
H	-1.457421000	-1.300371000	2.225234000
H	-1.854546000	0.254797000	2.972037000
H	-3.140511000	-0.882568000	2.540436000
N	-1.011872000	-0.406179000	-4.861963000
N	-3.029722000	-1.376366000	-4.995687000

N	-1.732597000	-2.263016000	-8.350935000
N	-0.144004000	-0.995021000	-7.067825000
N	-3.847665000	-2.828823000	-7.579799000
C	0.149353000	0.305537000	-4.304920000
C	0.402691000	1.632584000	-5.023121000
C	-0.436971000	2.601110000	-4.176102000
C	-0.278718000	2.032826000	-2.755463000
C	-1.419002000	2.287523000	-1.831943000
C	-2.209061000	-0.683990000	-4.238910000
C	-2.337875000	-1.572022000	-6.173953000
C	-1.076791000	-0.982211000	-6.106928000
C	-2.654853000	-2.237203000	-7.372454000
C	-0.557331000	-1.655721000	-8.146663000
O	1.783615000	1.934704000	-4.910920000
O	0.050930000	3.933430000	-4.211935000
O	-0.100660000	0.604465000	-2.959717000
H	1.014864000	-0.353586000	-4.391375000
H	1.850873000	2.896736000	-4.817128000
H	0.092977000	1.597125000	-6.069828000
H	-0.332109000	4.390585000	-4.969941000
H	-1.483098000	2.555509000	-4.487960000
H	0.651524000	2.428402000	-2.336716000
H	-2.375869000	1.881766000	-2.142728000
H	-1.457666000	3.301098000	-1.442365000
H	-4.501046000	-2.919652000	-6.821376000
H	-3.984521000	-3.387902000	-8.404656000
H	-2.412759000	-0.373757000	-3.222758000
H	0.146413000	-1.712898000	-8.970571000

12A-TS- Ado

N	-2.053545000	-0.061990000	0.185586000
N	-2.444584000	-1.576535000	1.793807000
N	-5.619241000	-1.888472000	-0.091129000
N	-4.141052000	-0.260123000	-1.061371000
N	-5.114641000	-3.104513000	1.818858000
C	-1.403902000	0.979133000	-0.609883000
C	-1.943489000	2.379643000	-0.296040000
C	-0.921541000	2.890597000	0.733980000
C	0.386489000	2.277897000	0.214095000
C	1.474017000	2.107660000	1.217859000
C	-1.593316000	-0.702099000	1.315476000
C	-3.527940000	-1.510100000	0.940510000
C	-3.302807000	-0.575977000	-0.067605000
C	-4.761884000	-2.187089000	0.901467000
C	-5.268382000	-0.965247000	-0.993919000
O	-1.883998000	3.149356000	-1.483249000

O	-0.812304000	4.301750000	0.752669000
O	-0.023362000	0.987726000	-0.309037000
H	-1.566945000	0.736892000	-1.660645000
H	-1.705872000	4.063817000	-1.216923000
H	-2.962157000	2.337919000	0.097005000
H	-1.454641000	4.662651000	1.375085000
H	-1.156796000	2.493719000	1.724519000
H	0.736054000	2.895349000	-0.620715000
H	1.271819000	1.383612000	2.003118000
H	1.871561000	3.050393000	1.584212000
H	-4.465665000	-3.387352000	2.531952000
H	-5.980676000	-3.605419000	1.717910000
H	-0.612112000	-0.511064000	1.717891000
H	-6.001444000	-0.768954000	-1.769274000
O	5.332593000	-0.900643000	-1.067686000
H	2.568706000	1.597125000	0.507548000
N	3.748734000	-2.192941000	-2.015473000
C	3.026727000	-0.213250000	-0.744217000
C	3.889336000	-1.322531000	1.978256000
H	4.597535000	3.156159000	-0.810689000
C	2.459278000	-1.295113000	1.500545000
N	2.179368000	-0.908277000	0.227494000
H	4.066540000	-0.413543000	2.557830000
C	4.146986000	-1.132094000	-1.289033000
H	1.191653000	-0.766135000	0.067386000
H	2.354163000	-0.005668000	-1.578446000
H	4.501236000	-2.792190000	-2.321189000
H	4.007567000	-2.171380000	2.648760000
H	4.384604000	1.021281000	0.458692000
O	1.539177000	-1.608121000	2.255833000
H	4.628624000	-1.370935000	1.184225000
C	3.547957000	1.117246000	-0.226032000
C	2.389941000	-2.600612000	-2.346433000
H	1.863118000	-2.995320000	-1.477242000
H	1.815404000	-1.770490000	-2.757871000
H	2.447002000	-3.375622000	-3.106706000
S	3.886821000	2.284155000	-1.542869000

12B-TS- Ado

O	0.916180000	-1.799878000	0.010522000
H	-0.997713000	1.938378000	0.461462000
N	2.720160000	-0.457718000	-0.121346000
C	0.483982000	0.526381000	-0.471984000
C	-2.185239000	-0.976208000	0.035908000
H	0.789183000	2.083964000	2.323311000
C	-1.793968000	-0.353615000	-1.280586000

N	-0.564404000	0.201372000	-1.430186000
H	-2.639659000	-0.209601000	0.667334000
C	1.394792000	-0.684093000	-0.184463000
H	-0.457230000	0.666208000	-2.318703000
H	1.058342000	1.311821000	-0.958058000
H	3.267932000	-1.279346000	0.088649000
H	-2.938156000	-1.735780000	-0.161935000
H	-0.460089000	0.443608000	1.533492000
O	-2.587192000	-0.325900000	-2.224248000
H	-1.339010000	-1.417069000	0.553904000
O	0.990883000	1.924112000	1.394063000
C	-0.018837000	1.144778000	0.826743000
C	3.447015000	0.771545000	-0.425040000
H	3.354009000	1.044013000	-1.478331000
H	3.101335000	1.596018000	0.194311000
H	4.498690000	0.597084000	-0.211451000
N	-1.198141000	3.501933000	-4.108790000
N	-2.665301000	2.228708000	-5.231458000
N	-1.348875000	4.235667000	-8.054144000
N	-0.325056000	4.827711000	-5.961437000
N	-2.988191000	2.608121000	-8.267354000
C	-0.415239000	4.077478000	-3.012976000
C	-0.947331000	5.445867000	-2.571282000
C	-1.857596000	5.064780000	-1.391349000
C	-1.094262000	3.890462000	-0.762817000
C	-1.910026000	2.926988000	0.029170000
C	-2.145723000	2.503910000	-4.059658000
C	-2.031138000	3.091056000	-6.103336000
C	-1.112813000	3.888697000	-5.424470000
C	-2.133458000	3.298688000	-7.492171000
C	-0.509705000	4.929189000	-7.275942000
O	0.151214000	6.220956000	-2.125112000
O	-1.996756000	6.105142000	-0.440233000
O	-0.493500000	3.217445000	-1.898569000
H	0.614986000	4.165878000	-3.360469000
H	-0.175148000	6.781721000	-1.405391000
H	-1.482594000	5.949539000	-3.379879000
H	-2.735493000	6.671082000	-0.693507000
H	-2.829772000	4.729573000	-1.760712000
H	-0.293300000	4.307240000	-0.142558000
H	-2.665647000	2.388396000	-0.537855000
H	-2.278342000	3.335256000	0.966317000
H	-3.534274000	1.858667000	-7.880340000
H	-2.981267000	2.744559000	-9.263585000
H	-2.389807000	1.997502000	-3.140678000
H	0.096473000	5.669403000	-7.787570000

13A-TS- Ado

H	-2.566423000	-1.505689000	1.965260000
H	-3.892377000	-5.951164000	-2.362607000
H	-2.933495000	-5.114713000	-3.535897000
C	-3.004181000	2.361842000	0.902285000
O	1.148629000	0.109916000	2.437572000
O	-0.192423000	-2.388432000	1.857110000
C	-2.386029000	1.094168000	1.473609000
O	-1.224649000	-1.239519000	-1.634650000
H	-3.593078000	-3.223364000	1.459649000
H	-4.212054000	-5.067859000	-0.075087000
C	-1.932956000	-2.181909000	-1.287541000
N	-2.434004000	-2.230477000	0.048080000
O	-2.778927000	3.453627000	1.382366000
O	-3.810028000	2.164748000	-0.132752000
C	-2.075781000	-1.216557000	1.029254000
O	-0.626169000	2.329413000	2.667225000
C	-0.574082000	-1.140832000	1.292240000
C	-0.253308000	0.008306000	2.249385000
C	-3.038750000	-4.194345000	-1.722646000
C	-0.890061000	1.301346000	1.777953000
O	-2.592050000	0.023377000	0.578879000
N	-3.316006000	-5.165304000	-2.606617000
N	-2.265902000	-3.195059000	-2.123145000
C	-3.240537000	-3.257068000	0.438926000
C	-3.574478000	-4.260070000	-0.398734000
H	-2.909583000	0.916242000	2.428330000
H	-0.382123000	1.583580000	0.579267000
H	-0.666087000	-0.233400000	3.237149000
H	-0.060777000	-0.965708000	0.349379000
H	-1.207744000	3.075329000	2.436337000
H	0.728563000	-2.307833000	2.137172000
H	1.541952000	0.335220000	1.572897000
H	-4.166114000	3.024460000	-0.416850000
N	2.572882000	-1.652764000	-0.760019000
N	1.548821000	-3.633978000	-1.022183000
N	3.732058000	-4.487497000	1.847704000
N	4.015821000	-2.210670000	1.132939000
N	2.266829000	-5.974239000	0.833948000
C	2.871889000	-0.243243000	-0.884757000
C	2.947317000	0.282783000	-2.324496000
C	1.602206000	1.012280000	-2.495045000
C	1.324762000	1.560566000	-1.088860000
C	-0.118225000	1.812469000	-0.787830000
C	1.641697000	-2.403704000	-1.451057000

C	2.453953000	-3.709595000	0.020631000
C	3.096896000	-2.489581000	0.204336000
C	2.808922000	-4.746248000	0.903998000
C	4.271281000	-3.264778000	1.905791000
O	4.023882000	1.202137000	-2.393731000
O	1.672463000	2.079441000	-3.424106000
O	1.848637000	0.511671000	-0.229132000
H	3.823764000	-0.085289000	-0.379965000
H	3.764539000	1.884734000	-3.031427000
H	3.083535000	-0.527383000	-3.045307000
H	1.469067000	1.747626000	-4.306579000
H	0.818336000	0.300019000	-2.763130000
H	1.925102000	2.462288000	-0.938911000
H	-0.801473000	1.080752000	-1.208551000
H	-0.432452000	2.842606000	-0.926260000
H	1.524049000	-6.165583000	0.184677000
H	2.497283000	-6.662279000	1.530168000
H	1.038875000	-1.977021000	-2.234723000
H	5.009066000	-3.116095000	2.687028000

13B-TS- Ado

H	-0.159376000	-1.807155000	-0.449715000
H	5.660323000	1.044860000	-1.500148000
H	5.943099000	-0.615015000	-1.098887000
C	-2.105382000	1.846473000	-0.300641000
O	-2.544417000	0.073465000	2.386541000
O	0.326246000	-1.165175000	2.156504000
C	-2.083297000	0.411896000	-0.834137000
O	1.934417000	-2.530890000	0.299355000
H	1.005233000	1.546381000	-0.875408000
H	3.415759000	2.060841000	-1.315188000
C	2.331259000	-1.462103000	-0.192235000
N	1.386346000	-0.441808000	-0.431446000
O	-3.357797000	2.315512000	-0.256294000
O	-1.132778000	2.487985000	0.005866000
C	-0.036425000	-0.746124000	-0.228924000
O	-2.878332000	-1.844764000	-0.520337000
C	-0.466866000	-0.463102000	1.215532000
C	-1.965079000	-0.781943000	1.403069000
C	4.006410000	-0.017012000	-0.902847000
C	-2.728177000	-0.605283000	0.103353000
O	-0.754769000	0.026836000	-1.175102000
N	5.304344000	0.156468000	-1.194700000
N	3.621669000	-1.223503000	-0.496954000
C	1.787576000	0.807222000	-0.789205000
C	3.091866000	1.073355000	-1.025217000

H	-2.644264000	0.421684000	-1.770834000
H	-3.956890000	-0.194214000	0.374128000
H	-2.053207000	-1.831061000	1.699171000
H	-0.328171000	0.605448000	1.397700000
H	-3.534544000	-1.733656000	-1.231034000
H	0.786232000	-1.894940000	1.700669000
H	-2.027563000	-0.007605000	3.198261000
H	-3.344334000	3.227348000	0.079059000
N	-6.096834000	-2.522008000	-3.044718000
N	-6.476959000	-4.625813000	-2.360995000
N	-6.288490000	-5.223299000	-6.012830000
N	-5.975825000	-2.906790000	-5.452910000
N	-6.677612000	-6.882191000	-4.439430000
C	-5.903214000	-1.081441000	-3.002093000
C	-7.203801000	-0.280721000	-2.844585000
C	-7.238889000	0.007292000	-1.332013000
C	-5.752746000	0.189243000	-1.001100000
C	-5.344005000	-0.070526000	0.408871000
C	-6.313462000	-3.382135000	-1.990167000
C	-6.369677000	-4.592387000	-3.738071000
C	-6.132704000	-3.294198000	-4.183175000
C	-6.446625000	-5.590598000	-4.728572000
C	-6.066270000	-3.934477000	-6.294462000
O	-7.064245000	0.923606000	-3.576227000
O	-7.945685000	1.191654000	-1.013662000
O	-5.092454000	-0.767534000	-1.879597000
H	-5.404095000	-0.803745000	-3.930088000
H	-7.561881000	1.603233000	-3.096869000
H	-8.068768000	-0.853836000	-3.188278000
H	-8.878838000	0.981966000	-0.888481000
H	-7.644595000	-0.853235000	-0.794774000
H	-5.455746000	1.196275000	-1.303200000
H	-5.642440000	-1.037316000	0.808220000
H	-5.513509000	0.758942000	1.086299000
H	-6.758364000	-7.186180000	-3.485181000
H	-6.686796000	-7.567062000	-5.175614000
H	-6.315434000	-3.029932000	-0.972126000
H	-5.945799000	-3.701141000	-7.347089000

13C-TS- Ado

H	-0.543136000	-0.351642000	-1.625989000
H	-6.102616000	-1.279115000	1.269844000
H	-5.428953000	-0.742505000	2.771190000
C	2.705960000	-2.190491000	-0.084186000
O	1.999049000	2.680749000	-0.882027000
O	-0.818244000	2.125056000	-1.093571000

C	1.776856000	-1.097473000	-0.676164000
O	-0.944909000	0.298107000	2.147780000
H	-2.483873000	-1.014617000	-1.725576000
H	-4.744102000	-1.418294000	-0.790158000
C	-1.883560000	-0.100627000	1.463807000
N	-1.685615000	-0.355069000	0.075339000
O	3.888630000	-2.139233000	-0.542682000
O	2.257517000	-2.997185000	0.740853000
C	-0.388179000	-0.150957000	-0.558715000
O	3.659790000	0.366639000	-1.204254000
C	0.132418000	1.285287000	-0.445107000
C	1.495173000	1.366330000	-1.115424000
C	-4.113803000	-0.759912000	1.215343000
C	2.417218000	0.288700000	-0.594551000
O	0.515255000	-1.088871000	-0.018739000
N	-5.312762000	-0.944286000	1.792429000
N	-3.123797000	-0.313668000	1.973657000
C	-2.710891000	-0.827649000	-0.685755000
C	-3.940403000	-1.046284000	-0.174168000
H	1.637514000	-1.352764000	-1.740551000
H	2.529039000	0.523971000	0.694232000
H	1.361750000	1.213520000	-2.198604000
H	0.232955000	1.552402000	0.605373000
H	4.046768000	-0.542495000	-1.068064000
H	-0.442892000	3.013860000	-1.127138000
H	2.871502000	2.738238000	-1.291176000
N	6.570563000	1.248663000	3.369806000
N	6.914287000	3.461203000	3.525607000
N	10.096956000	2.266654000	4.999225000
N	8.662450000	0.453163000	4.341818000
N	9.534101000	4.503753000	4.754168000
C	5.914757000	-0.031413000	3.088364000
C	5.251121000	-0.634356000	4.333211000
C	3.800780000	-0.144965000	4.183817000
C	3.601262000	-0.186670000	2.661522000
C	2.553608000	0.715422000	2.110240000
C	6.088788000	2.516818000	3.145267000
C	8.003294000	2.780624000	4.033339000
C	7.808473000	1.403628000	3.944088000
C	9.221987000	3.205184000	4.595958000
C	9.775124000	0.975921000	4.852120000
O	5.315605000	-2.046139000	4.228517000
O	2.861623000	-1.001432000	4.811923000
O	4.902781000	0.182495000	2.134324000
H	6.680493000	-0.706805000	2.703467000
H	4.499034000	-2.392379000	4.619078000

H	5.729742000	-0.287375000	5.252634000
H	2.758005000	-0.737487000	5.733714000
H	3.710598000	0.880229000	4.551170000
H	3.391221000	-1.224852000	2.383892000
H	2.749757000	1.778320000	2.235107000
H	1.538835000	0.426706000	2.367848000
H	8.925057000	5.220426000	4.400504000
H	10.441753000	4.760719000	5.102408000
H	5.129551000	2.670550000	2.681677000
H	10.521673000	0.267474000	5.195549000

13D-TS- Ado

H	0.115955000	-1.818201000	0.787821000
H	-5.986410000	0.599989000	0.963092000
H	-6.091279000	-1.096431000	0.637425000
C	1.634474000	2.134509000	0.594105000
O	2.646428000	0.030607000	-1.944948000
O	-0.063597000	-1.345796000	-1.878558000
C	1.752467000	0.708689000	1.224949000
O	-1.810967000	-2.748845000	-0.163815000
H	-1.321821000	1.441046000	0.838504000
H	-3.817150000	1.786841000	0.965551000
C	-2.340897000	-1.689934000	0.213975000
N	-1.514428000	-0.587976000	0.502766000
O	2.701571000	2.784445000	0.613215000
O	0.514592000	2.500851000	0.171377000
C	-0.049846000	-0.775853000	0.507079000
O	2.927628000	-1.412864000	1.211066000
C	0.533806000	-0.521195000	-0.885519000
C	2.057032000	-0.705517000	-0.870074000
C	-4.194360000	-0.351444000	0.630259000
C	2.642167000	-0.254754000	0.460147000
O	0.478512000	0.076786000	1.493555000
N	-5.529472000	-0.270809000	0.758458000
N	-3.675002000	-1.543357000	0.349711000
C	-2.044357000	0.642455000	0.726584000
C	-3.386092000	0.813971000	0.786087000
H	2.182580000	0.865886000	2.216564000
H	3.795369000	0.322999000	0.218574000
H	2.275837000	-1.771484000	-0.982403000
H	0.325491000	0.518992000	-1.142157000
H	3.134932000	-1.158481000	2.118827000
H	-0.523436000	-2.084717000	-1.438616000
H	2.190011000	-0.230917000	-2.755063000
N	6.485189000	-1.677322000	-2.875846000
N	5.672346000	-0.718147000	-4.734709000

N	8.448369000	-2.654384000	-6.242069000
N	8.309468000	-2.967345000	-3.862841000
N	7.024062000	-1.269572000	-7.440881000
C	6.595055000	-2.076077000	-1.463078000
C	7.892667000	-1.573561000	-0.828920000
C	7.459851000	-0.196490000	-0.300929000
C	6.001617000	-0.437254000	0.128235000
C	5.108106000	0.752587000	0.028534000
C	5.540325000	-0.847664000	-3.435693000
C	6.756904000	-1.511351000	-5.052513000
C	7.271041000	-2.123487000	-3.910413000
C	7.402956000	-1.808728000	-6.267064000
C	8.831364000	-3.173943000	-5.069586000
O	8.220524000	-2.442580000	0.241606000
O	8.220378000	0.231925000	0.817154000
O	5.536413000	-1.501249000	-0.746233000
H	6.533091000	-3.164342000	-1.416655000
H	8.617221000	-1.893698000	0.934540000
H	8.707726000	-1.517628000	-1.553614000
H	9.009296000	0.691651000	0.506055000
H	7.499735000	0.537609000	-1.109188000
H	6.010152000	-0.826533000	1.150821000
H	5.052676000	1.208716000	-0.955649000
H	5.227719000	1.474138000	0.829719000
H	6.190543000	-0.710762000	-7.495053000
H	7.455919000	-1.582663000	-8.293456000
H	4.772850000	-0.394469000	-2.828619000
H	9.677806000	-3.851297000	-5.114133000

14A-TS- Ado

O	5.819356000	0.368950000	-1.991984000
H	2.311829000	-0.189456000	0.858273000
C	4.251681000	0.116743000	-0.195652000
N	3.752729000	1.447220000	-0.521177000
C	5.297162000	-0.409668000	-1.224025000
H	4.553175000	2.058658000	-0.627505000
H	4.831120000	0.205911000	0.730377000
H	2.478510000	-1.069138000	-0.781260000
C	3.111737000	-0.851130000	0.072088000
C	3.333193000	-2.070450000	0.870360000
O	2.690501000	-3.094323000	0.754440000
O	4.279191000	-1.918997000	1.825157000
H	4.326034000	-2.741770000	2.337854000
C	5.677440000	-1.864462000	-1.190334000
H	5.932118000	-2.169171000	-0.173958000
H	4.827847000	-2.475069000	-1.506581000

H	6.518066000	-2.043520000	-1.856866000
C	2.932943000	1.536857000	-1.734148000
H	2.730839000	2.589162000	-1.934149000
H	3.407353000	1.104427000	-2.623070000
H	1.973417000	1.044289000	-1.580431000
N	-2.274577000	-0.082423000	-0.148224000
N	-3.103361000	-2.020300000	0.622171000
N	-6.149352000	-0.684627000	-1.011451000
N	-4.274080000	0.803397000	-1.228842000
N	-6.056203000	-2.714431000	0.106547000
C	-1.332997000	1.001786000	-0.437090000
C	-1.584711000	2.238110000	0.432373000
C	-0.613433000	2.003122000	1.603344000
C	0.579716000	1.346257000	0.892473000
C	1.439048000	0.479728000	1.742088000
C	-2.044901000	-1.252415000	0.538166000
C	-4.089489000	-1.321277000	-0.045527000
C	-3.592511000	-0.115135000	-0.534470000
C	-5.445007000	-1.593353000	-0.313135000
C	-5.538611000	0.433660000	-1.420082000
O	-1.203710000	3.381013000	-0.311513000
O	-0.197021000	3.203013000	2.227657000
O	-0.027427000	0.551430000	-0.153693000
H	-1.432099000	1.252204000	-1.494229000
H	-0.866452000	4.031029000	0.322938000
H	-2.627892000	2.302826000	0.750865000
H	-0.815478000	3.425888000	2.933502000
H	-1.058217000	1.310943000	2.322480000
H	1.180524000	2.136154000	0.434777000
H	0.942340000	-0.362061000	2.218204000
H	2.133714000	1.010790000	2.384205000
H	-5.541502000	-3.424902000	0.596147000
H	-7.016330000	-2.884086000	-0.139121000
H	-1.070465000	-1.480035000	0.934338000
H	-6.159214000	1.126157000	-1.979022000

14B-TS- Ado

O	5.778929000	-0.235484000	-1.953253000
H	2.180775000	0.153131000	0.784325000
C	4.207003000	-0.143575000	-0.136461000
N	4.239551000	1.312560000	-0.269936000
C	5.026806000	-0.864376000	-1.234262000
H	5.208890000	1.590269000	-0.374044000
H	4.731680000	-0.409537000	0.789845000
H	2.195869000	-0.636410000	-0.895000000
C	2.801263000	-0.688646000	0.005329000

C	2.568905000	-1.970546000	0.787074000
O	1.470484000	-2.550397000	0.569998000
O	3.444159000	-2.317646000	1.621265000
C	4.902086000	-2.359503000	-1.342314000
H	4.944201000	-2.814454000	-0.352282000
H	3.920729000	-2.606667000	-1.756420000
H	5.679732000	-2.755253000	-1.992601000
C	3.486425000	1.847271000	-1.407747000
H	3.671356000	2.920097000	-1.475128000
H	3.754844000	1.393429000	-2.370529000
H	2.417896000	1.703223000	-1.253442000
N	-2.019243000	0.034099000	-0.272825000
N	-2.395943000	-2.105117000	0.288803000
N	-5.843222000	-1.137808000	-0.662870000
N	-4.286428000	0.675673000	-0.918578000
N	-5.240955000	-3.250544000	0.084186000
C	-1.298796000	1.282398000	-0.570742000
C	-1.738879000	2.428565000	0.341159000
C	-0.771008000	2.266935000	1.524454000
C	0.522965000	1.785999000	0.846927000
C	1.383690000	0.890620000	1.673727000
C	-1.492659000	-1.159584000	0.172835000
C	-3.576600000	-1.511496000	-0.109272000
C	-3.361523000	-0.183215000	-0.471149000
C	-4.897295000	-1.985016000	-0.219756000
C	-5.490970000	0.113321000	-0.982205000
O	-1.497190000	3.645632000	-0.343674000
O	-0.523401000	3.485150000	2.207705000
O	0.070932000	1.085187000	-0.347066000
H	-1.474014000	1.528636000	-1.619019000
H	-1.228981000	4.293757000	0.324681000
H	-2.787687000	2.342271000	0.632030000
H	-1.198197000	3.611153000	2.885411000
H	-1.149109000	1.502699000	2.207355000
H	1.084268000	2.665835000	0.521974000
H	0.861065000	0.075037000	2.168033000
H	2.099146000	1.401002000	2.309914000
H	-4.568460000	-3.872110000	0.497962000
H	-6.209452000	-3.520720000	0.068509000
H	-0.437065000	-1.284595000	0.370031000
H	-6.296065000	0.748047000	-1.337529000

15-TS- Ado

P	3.020468000	-3.183518000	-1.626013000
O	3.016093000	-4.746296000	-1.497216000
O	4.301744000	-2.737787000	-2.422648000

O	2.810834000	-2.547844000	-0.314672000
O	1.871804000	-2.892759000	-2.693995000
P	1.151113000	-1.582390000	-3.295944000
O	2.305020000	-0.672574000	-3.856585000
O	0.080826000	-1.970237000	-4.205450000
O	0.775223000	-0.729612000	-2.017693000
P	-0.221167000	-0.993268000	-0.750165000
O	0.779140000	-1.114394000	0.443496000
O	-1.169264000	-2.079927000	-0.992429000
O	-0.914272000	0.395510000	-0.554378000
C	-0.192664000	1.624513000	-0.277437000
C	-1.190936000	2.757252000	-0.249944000
O	-1.681614000	2.995936000	-1.598593000
C	-2.430888000	2.539111000	0.599141000
O	-2.821541000	3.711711000	1.239138000
C	-3.467273000	1.998084000	-0.371137000
O	-4.769596000	2.333358000	0.043021000
C	-3.042647000	2.668156000	-1.701265000
N	-3.239469000	1.779144000	-2.845199000
C	-2.318402000	1.342341000	-3.775562000
N	-2.848067000	0.557610000	-4.677750000
C	-4.181200000	0.466204000	-4.329932000
C	-5.259375000	-0.254731000	-4.925087000
O	-5.267598000	-0.973384000	-5.916816000
N	-6.458012000	-0.052692000	-4.196007000
C	-6.606550000	0.707255000	-3.067291000
N	-7.822838000	0.735125000	-2.485809000
N	-5.604281000	1.371601000	-2.525807000
C	-4.436004000	1.218776000	-3.191000000
H	0.534559000	1.797762000	-1.070595000
H	0.313483000	1.542136000	0.681658000
H	-0.668840000	3.656037000	0.080465000
H	-2.239164000	1.615146000	1.522734000
H	-3.788010000	3.690705000	1.322234000
H	-3.340722000	0.917012000	-0.469026000
H	-5.365473000	2.065702000	-0.686321000
H	-3.642128000	3.568462000	-1.865654000
H	-1.286117000	1.639841000	-3.715100000
H	-8.638511000	0.400168000	-2.969436000
H	-7.972250000	1.405654000	-1.750764000
H	-7.259114000	-0.546596000	-4.566315000
H	1.579400000	-1.687379000	0.247485000
H	2.491637000	-0.805029000	-4.797345000
H	5.097717000	-2.613345000	-1.885269000
H	3.261621000	-5.242820000	-2.291823000
N	-0.245606000	3.449758000	4.828023000

N	-1.834378000	4.979285000	5.245822000
N	0.439772000	5.712414000	8.077165000
N	1.268332000	3.939058000	6.681874000
N	-1.552913000	6.832309000	7.681940000
C	0.505348000	2.394516000	4.130134000
C	0.641980000	1.130147000	4.979080000
C	-0.632986000	0.361815000	4.593418000
C	-0.807464000	0.712478000	3.107874000
C	-2.215910000	0.750060000	2.611085000
C	-1.439845000	4.018911000	4.445076000
C	-0.844280000	5.058380000	6.204710000
C	0.157427000	4.121553000	5.957340000
C	-0.667490000	5.881992000	7.332824000
C	1.324156000	4.775238000	7.715870000
O	1.798097000	0.438437000	4.540597000
O	-0.496192000	-1.042514000	4.732864000
O	-0.196864000	2.031264000	2.970850000
H	1.483773000	2.795551000	3.862733000
H	1.607120000	-0.507770000	4.623803000
H	0.697665000	1.355968000	6.045767000
H	-0.722863000	-1.294662000	5.635842000
H	-1.477975000	0.735423000	5.176235000
H	-0.209993000	0.011366000	2.521018000
H	-2.925516000	1.249172000	3.267708000
H	-2.585790000	-0.190205000	2.214344000
H	-2.417380000	6.931818000	7.179510000
H	-1.416302000	7.355327000	8.529823000
H	-1.953109000	3.691672000	3.555601000
H	2.198376000	4.689040000	8.352656000

16-TS- Ado

C	1.521221000	0.138612000	-1.597341000
C	0.295144000	-0.698593000	-1.975293000
C	-0.735808000	-0.628158000	-0.848431000
C	-0.112175000	-1.047522000	0.469059000
C	1.157998000	-0.232988000	0.757424000
O	2.056261000	-0.294593000	-0.351967000
N	-0.350862000	-0.331641000	-3.230073000
O	-1.834883000	-1.491722000	-1.115554000
O	-1.006909000	-0.810692000	1.563249000
C	1.934795000	-0.754033000	1.947204000
O	1.229914000	-0.793421000	3.150108000
O	1.136810000	1.484011000	-1.576697000
C	2.217336000	2.406470000	-1.443053000
H	2.339276000	-0.016898000	-2.308694000
H	0.630795000	-1.734787000	-2.058113000

H	-1.087540000	0.406269000	-0.747824000
H	0.145429000	-2.111714000	0.415329000
H	0.855209000	0.804934000	0.943744000
H	0.198215000	-0.631991000	-4.026391000
H	-0.447008000	0.676807000	-3.288592000
H	-2.032068000	-1.377025000	-2.058177000
H	-1.778313000	-1.381074000	1.457957000
H	2.453920000	-1.691687000	1.730253000
H	2.921537000	0.094532000	2.116885000
H	0.277371000	-0.761146000	2.952093000
H	1.805789000	3.400082000	-1.606902000
H	2.652119000	2.358369000	-0.442256000
H	2.999009000	2.203161000	-2.180924000
N	6.359226000	-0.255025000	-0.611792000
N	5.353049000	0.575211000	-2.437896000
N	8.759303000	0.097669000	-3.815002000
N	8.605484000	-0.583950000	-1.514955000
N	6.980090000	0.980731000	-5.014513000
C	6.523252000	-0.781626000	0.753496000
C	7.470730000	0.082187000	1.586098000
C	6.496854000	1.107528000	2.189424000
C	5.219777000	0.280458000	2.414065000
C	3.937599000	1.039369000	2.303928000
C	5.201845000	0.218354000	-1.184895000
C	6.681380000	0.315415000	-2.712359000
C	7.322723000	-0.209067000	-1.591045000
C	7.467720000	0.468284000	-3.869717000
C	9.242095000	-0.396534000	-2.668801000
O	8.031019000	-0.736577000	2.597544000
O	6.944621000	1.635124000	3.427236000
O	5.278160000	-0.763798000	1.399549000
H	6.890062000	-1.806006000	0.676959000
H	8.133749000	-0.179272000	3.383413000
H	8.249929000	0.541825000	0.974456000
H	7.517013000	2.393177000	3.259230000
H	6.308544000	1.904936000	1.466758000
H	5.296264000	-0.204772000	3.391066000
H	3.850675000	1.660395000	1.415638000
H	3.641526000	1.555144000	3.212945000
H	5.998732000	1.178420000	-5.102801000
H	7.554118000	0.988238000	-5.840255000
H	4.281661000	0.248919000	-0.626613000
H	10.289151000	-0.680203000	-2.687800000

17A-TS- Ado

O	5.679185000	0.962559000	1.586749000
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O	3.654736000	-0.055147000	0.644876000
H	2.160154000	-1.719280000	-2.959237000
O	3.691066000	0.282155000	3.141320000
C	2.440908000	-2.147964000	-0.875289000
O	1.517097000	0.813017000	-2.961674000
H	-0.208402000	-0.766673000	-2.221760000
H	1.994096000	-1.843604000	0.074778000
C	3.543282000	0.377094000	-1.723879000
H	4.576094000	2.046383000	-1.784921000
H	0.013887000	-2.359690000	-2.517539000
C	2.336333000	-3.648142000	-1.039184000
H	4.799027000	-2.131466000	2.477666000
O	5.301151000	-1.424051000	2.050255000
H	1.844641000	1.721829000	-2.910624000
C	4.160055000	-0.505152000	-0.634682000
H	6.363335000	1.059751000	2.263236000
P	4.511103000	-0.042491000	1.969061000
O	3.706794000	1.767367000	-1.475713000
O	3.856153000	-1.841750000	-0.838073000
H	2.793402000	-3.961726000	-1.980020000
C	1.742503000	-1.369739000	-2.001688000
H	4.045706000	0.097442000	-2.659207000
H	5.246752000	-0.420863000	-0.640299000
H	1.290513000	-3.954099000	-1.036753000
C	2.066191000	0.103062000	-1.887884000
N	0.296594000	-1.592399000	-1.922005000
H	1.463061000	0.534444000	-0.797365000
H	2.844521000	-4.153401000	-0.217599000
N	-3.161108000	0.068479000	-0.264056000
N	-3.298901000	-2.025118000	0.532828000
N	-6.871773000	-1.074664000	0.770252000
N	-5.517158000	0.698676000	-0.123168000
N	-6.022366000	-3.128773000	1.435825000
C	-2.592146000	1.284567000	-0.865768000
C	-2.691871000	2.485756000	0.075606000
C	-1.367164000	2.379877000	0.847439000
C	-0.392915000	1.855478000	-0.221622000
C	0.735927000	1.034552000	0.302746000
C	-2.504142000	-1.100674000	0.048978000
C	-4.549903000	-1.441123000	0.532160000
C	-4.486750000	-0.142015000	0.031384000
C	-5.822550000	-1.903006000	0.917150000
C	-6.664029000	0.148741000	0.269043000
O	-2.719754000	3.659323000	-0.717973000
O	-0.907846000	3.629365000	1.335090000
O	-1.227039000	1.073430000	-1.118803000

H	-3.120638000	1.475433000	-1.800710000
H	-2.248778000	4.344484000	-0.220644000
H	-3.569422000	2.426561000	0.722487000
H	-1.293719000	3.792433000	2.204029000
H	-1.467993000	1.652822000	1.656717000
H	-0.014021000	2.716775000	-0.780720000
H	0.440866000	0.133671000	0.834827000
H	1.494856000	1.608969000	0.823516000
H	-5.269352000	-3.793604000	1.467223000
H	-6.960116000	-3.447569000	1.610181000
H	-1.447890000	-1.212087000	-0.137764000
H	-7.548862000	0.769012000	0.171368000

17B-TS- Ado

O	5.877639000	-0.529321000	1.796468000
O	3.703310000	0.064449000	0.586628000
H	2.224543000	-1.661184000	-2.991265000
O	3.875725000	0.643562000	3.001618000
C	2.538295000	-2.068505000	-0.908447000
O	1.547419000	0.856763000	-3.017176000
H	-0.152001000	-0.746354000	-2.258179000
H	2.096660000	-1.766059000	0.044494000
C	3.581520000	0.468848000	-1.769067000
H	4.596648000	2.148782000	-1.833074000
H	0.095540000	-2.340575000	-2.521078000
C	2.450106000	-3.572221000	-1.059672000
H	2.889492000	-1.737989000	2.653993000
O	3.792389000	-1.810865000	2.321500000
H	1.878009000	1.765231000	-2.981992000
C	4.206992000	-0.373667000	-0.650395000
P	4.415788000	-0.332069000	2.010610000
O	3.711675000	1.874585000	-1.567719000
O	3.938417000	-1.736029000	-0.900428000
H	2.902779000	-3.888567000	-2.002187000
C	1.809887000	-1.312232000	-2.031670000
H	4.090959000	0.177904000	-2.697731000
H	5.294797000	-0.284800000	-0.660366000
H	1.409013000	-3.894882000	-1.044733000
C	2.110346000	0.166313000	-1.934065000
N	0.366687000	-1.557138000	-1.941165000
H	1.497365000	0.596955000	-0.852428000
H	2.974057000	-4.063171000	-0.239151000
N	-3.104722000	0.048652000	-0.254179000
N	-3.170504000	-2.037486000	0.571150000
N	-6.754236000	-1.163103000	0.913024000
N	-5.469295000	0.628115000	-0.045413000

N	-5.837247000	-3.188975000	1.575914000
C	-2.579677000	1.268639000	-0.889327000
C	-2.693478000	2.482195000	0.034086000
C	-1.357273000	2.415410000	0.789765000
C	-0.384122000	1.892608000	-0.281380000
C	0.761047000	1.094806000	0.242130000
C	-2.412225000	-1.102011000	0.050815000
C	-4.433459000	-1.480958000	0.604071000
C	-4.415315000	-0.187129000	0.086010000
C	-5.682247000	-1.965809000	1.035846000
C	-6.590216000	0.058019000	0.390315000
O	-2.756001000	3.642509000	-0.777237000
O	-0.917606000	3.682345000	1.251101000
O	-1.215424000	1.090177000	-1.165510000
H	-3.130686000	1.428288000	-1.817130000
H	-2.286953000	4.342693000	-0.299319000
H	-3.561589000	2.415540000	0.692747000
H	-1.296866000	3.852021000	2.121629000
H	-1.433569000	1.700807000	1.612645000
H	-0.022707000	2.752765000	-0.853654000
H	0.485297000	0.194288000	0.784962000
H	1.516502000	1.683696000	0.750426000
H	-5.068553000	-3.836190000	1.590901000
H	-6.761295000	-3.526489000	1.784718000
H	-1.360078000	-1.192909000	-0.169142000
H	-7.491511000	0.657209000	0.313639000

17C-TS- Ado

O	6.096163000	-0.330148000	1.560692000
O	3.737970000	-0.054143000	0.593109000
H	2.192105000	-1.623053000	-3.042328000
O	4.226253000	0.837516000	2.881512000
C	2.515469000	-2.098597000	-0.976140000
O	1.555270000	0.901651000	-2.991958000
H	-0.168539000	-0.704770000	-2.286162000
H	2.089382000	-1.809285000	-0.011365000
C	3.581083000	0.446834000	-1.748510000
H	4.636836000	2.101926000	-1.696590000
H	0.058015000	-2.297318000	-2.575498000
C	2.390185000	-3.596860000	-1.164156000
O	4.158707000	-1.693002000	2.535569000
H	1.913858000	1.798289000	-2.936193000
C	4.202792000	-0.426396000	-0.646448000
P	4.643927000	-0.344684000	2.019915000
O	3.722919000	1.850969000	-1.522238000
O	3.914380000	-1.791402000	-0.981713000

H	2.823653000	-3.899920000	-2.120411000
C	1.786245000	-1.300012000	-2.069463000
H	4.085534000	0.176401000	-2.687260000
H	5.293619000	-0.362525000	-0.684619000
H	1.343242000	-3.900600000	-1.142241000
C	2.107836000	0.169987000	-1.926882000
N	0.339061000	-1.527460000	-1.982110000
H	1.496305000	0.580415000	-0.839463000
H	2.916315000	-4.119034000	-0.364034000
N	-3.105616000	0.064625000	-0.258021000
N	-3.173459000	-2.032745000	0.538370000
N	-6.750593000	-1.149525000	0.922086000
N	-5.466671000	0.649919000	-0.022391000
N	-5.835348000	-3.187267000	1.550600000
C	-2.578829000	1.290009000	-0.882822000
C	-2.687048000	2.494396000	0.052876000
C	-1.351736000	2.412456000	0.808561000
C	-0.379154000	1.891503000	-0.264495000
C	0.754025000	1.073469000	0.254546000
C	-2.415529000	-1.093234000	0.024577000
C	-4.433598000	-1.471460000	0.589840000
C	-4.414398000	-0.170592000	0.089510000
C	-5.680504000	-1.957479000	1.025398000
C	-6.586156000	0.077926000	0.414422000
O	-2.742936000	3.663496000	-0.746535000
O	-0.904738000	3.673296000	1.280627000
O	-1.216528000	1.111702000	-1.164549000
H	-3.131802000	1.459824000	-1.807677000
H	-2.264709000	4.354048000	-0.263677000
H	-3.556017000	2.425951000	0.710189000
H	-1.284595000	3.838520000	2.151754000
H	-1.433782000	1.692387000	1.626056000
H	-0.004808000	2.754240000	-0.824376000
H	0.464320000	0.169639000	0.784224000
H	1.512665000	1.646800000	0.775702000
H	-5.068790000	-3.837202000	1.550170000
H	-6.758891000	-3.524742000	1.761639000
H	-1.365867000	-1.185843000	-0.207145000
H	-7.485891000	0.681200000	0.352752000

18-TS- Ado

H	1.500273000	-0.444554000	-2.396116000
C	-4.759271000	-0.810384000	0.701043000
C	-1.992814000	-0.335815000	-1.423803000
C	1.807103000	-0.139688000	-1.388063000
C	-0.784838000	1.735639000	-0.520767000

N	-1.861779000	0.725257000	-0.563293000
N	-3.039717000	-1.086243000	-1.169460000
O	1.839421000	3.199617000	0.354693000
N	-3.188236000	1.435117000	1.359032000
C	-2.910510000	0.641185000	0.316038000
C	1.429061000	1.327621000	-1.202212000
C	-3.629731000	-0.487707000	-0.074662000
O	5.288499000	-1.323547000	-0.353120000
O	3.200815000	-0.293793000	-1.244757000
O	3.058829000	-2.576776000	-0.087081000
C	-4.273308000	1.027948000	2.014059000
H	1.258689000	-0.766369000	-0.679841000
H	-5.287970000	-2.517881000	-0.291157000
H	-0.221806000	2.224885000	1.570124000
N	-5.057025000	-0.024790000	1.751157000
H	2.208988000	1.190032000	0.814875000
C	0.079833000	1.628276000	0.717746000
O	0.058157000	1.551892000	-1.629996000
H	2.065798000	1.943326000	-1.839677000
O	3.517934000	-0.481780000	1.298281000
H	-1.280145000	2.709378000	-0.591082000
H	-0.056273000	0.381213000	1.200841000
C	1.498995000	1.800751000	0.250849000
H	-4.552990000	1.613022000	2.883262000
H	-1.282209000	-0.493373000	-2.216654000
N	-5.551036000	-1.863188000	0.424609000
H	-6.284501000	-2.113586000	1.065635000
P	3.815779000	-1.257876000	0.015533000
H	2.788804000	3.282495000	0.202831000
N	-0.908108000	0.506144000	5.546107000
N	-3.088001000	1.038567000	5.477678000
N	-2.689211000	0.682885000	9.143484000
N	-0.634296000	0.280304000	7.962569000
N	-4.691958000	1.205032000	8.094422000
C	0.472859000	0.263199000	5.092102000
C	0.908532000	-1.181526000	5.342485000
C	0.465374000	-1.867299000	4.038686000
C	0.700505000	-0.776902000	2.983539000
C	-0.243255000	-0.802651000	1.827056000
C	-1.999529000	0.834253000	4.775478000
C	-2.694440000	0.843723000	6.786566000
C	-1.340304000	0.518999000	6.850437000
C	-3.379501000	0.919496000	8.013894000
C	-1.387189000	0.385427000	9.055013000
O	2.319975000	-1.198761000	5.463904000
O	1.248300000	-3.008006000	3.722251000

O	0.545960000	0.480049000	3.710654000
H	1.122542000	0.964062000	5.618160000
H	2.626666000	-2.009792000	5.030902000
H	0.433502000	-1.603852000	6.230555000
H	0.876432000	-3.779121000	4.166759000
H	-0.594623000	-2.125603000	4.101635000
H	1.731038000	-0.831360000	2.622500000
H	-1.298919000	-0.782840000	2.086801000
H	-0.007086000	-1.554959000	1.080529000
H	-5.204767000	1.466949000	7.270823000
H	-5.119821000	1.331012000	8.995735000
H	-1.922085000	0.920042000	3.705136000
H	-0.884503000	0.208066000	10.000040000

19-TS- Ado

H	1.357294000	-1.465295000	-1.804090000
C	-0.356295000	-2.163091000	0.992548000
H	-1.344300000	-1.754690000	0.772071000
H	-0.475578000	-3.142875000	1.447097000
H	0.155534000	-1.498397000	1.683824000
C	0.415926000	-2.330515000	-0.292169000
H	-0.233279000	1.885539000	-0.010395000
H	1.219954000	0.687528000	-1.493117000
H	3.254393000	1.718017000	1.310763000
H	-0.663492000	0.441643000	0.889845000
O	0.620506000	-3.445661000	-0.768789000
C	2.037755000	0.391922000	0.479700000
C	0.931617000	0.169210000	-0.579372000
N	0.838404000	-1.226818000	-0.971794000
S	-1.743849000	0.504444000	-1.261284000
C	-0.375535000	0.809265000	-0.092205000
O	2.388436000	-0.521642000	1.220180000
N	2.584164000	1.621137000	0.561073000
C	-2.991950000	1.469078000	-0.457924000
H	-3.264078000	0.938460000	0.711912000
H	-2.697427000	2.494236000	-0.237258000
H	-3.927529000	1.410939000	-1.007885000
C	2.298557000	2.819257000	-0.215448000
H	1.531902000	3.437038000	0.257216000
H	3.211884000	3.405563000	-0.296788000
H	1.975790000	2.568409000	-1.222970000
N	-7.517138000	-1.023835000	1.335166000
N	-7.330430000	-3.140554000	0.613039000
N	-10.985776000	-3.042887000	1.211666000
N	-9.923220000	-0.950044000	1.730634000
N	-9.845899000	-4.900880000	0.418947000

C	-7.154466000	0.337629000	1.737184000
C	-7.093903000	0.497681000	3.260646000
C	-5.600415000	0.259214000	3.541511000
C	-4.936221000	0.891782000	2.309404000
C	-3.591601000	0.362797000	1.945672000
C	-6.693390000	-2.026959000	0.880182000
C	-8.649957000	-2.860884000	0.908925000
C	-8.786212000	-1.548996000	1.357942000
C	-9.830784000	-3.625006000	0.842231000
C	-10.966710000	-1.769625000	1.622997000
O	-7.456559000	1.829843000	3.577250000
O	-5.145588000	0.908377000	4.715376000
O	-5.871766000	0.631544000	1.233463000
H	-7.900598000	1.011138000	1.313291000
H	-6.938658000	2.084529000	4.355560000
H	-7.744628000	-0.219215000	3.767513000
H	-5.282195000	0.327550000	5.473250000
H	-5.393388000	-0.813418000	3.574312000
H	-4.887817000	1.973283000	2.476633000
H	-3.558680000	-0.702400000	1.726077000
H	-2.794041000	0.690723000	2.606546000
H	-8.989056000	-5.372390000	0.188670000
H	-10.704420000	-5.424009000	0.436393000
H	-5.637307000	-1.862161000	0.753979000
H	-11.929307000	-1.356775000	1.906001000

20-TS- Ado

N	-0.626301000	0.670870000	-0.816904000
H	-4.640607000	2.270879000	-0.861176000
H	4.008531000	-2.361003000	-0.721018000
O	-2.839654000	-2.288618000	-0.978579000
H	-4.396090000	-1.964504000	0.481821000
C	-2.192697000	-1.202220000	-0.332604000
C	4.715410000	-0.002046000	-0.207863000
H	5.015556000	-0.635032000	0.914367000
C	-3.835468000	0.507386000	-0.736579000
N	3.298038000	0.123921000	-0.339893000
H	-1.695735000	2.438012000	-0.241913000
O	3.425542000	2.205582000	0.660126000
N	0.397982000	2.409569000	0.155292000
O	-4.256185000	-1.176286000	1.027056000
H	-1.402705000	-1.542590000	0.336706000
C	2.543398000	-0.912002000	-0.870148000
H	-2.197739000	-2.983015000	-1.163817000
H	-2.827451000	0.251263000	1.132289000
C	1.317244000	1.410414000	-0.111373000

C	0.694940000	0.326998000	-0.710909000
C	-1.681037000	-0.185845000	-1.364827000
C	2.715806000	1.356218000	0.134143000
N	3.193285000	-2.046625000	-1.236589000
H	-1.274333000	-0.684659000	-2.243617000
C	-0.742252000	1.937188000	-0.274408000
O	-4.124023000	1.770656000	-0.217218000
H	-4.714625000	0.069641000	-1.214907000
O	-2.797732000	0.587198000	-1.732655000
H	5.165733000	-0.591262000	-0.998558000
H	2.573383000	-2.788062000	-1.523799000
C	-3.282589000	-0.394530000	0.379860000
N	1.245275000	-0.839577000	-1.080565000
H	5.176573000	0.966516000	-0.068983000
N	6.416816000	-5.121124000	0.085991000
N	8.622573000	-5.382750000	-0.238290000
N	7.372385000	-7.608448000	-2.924096000
N	5.585308000	-6.586065000	-1.683915000
N	9.617793000	-7.246140000	-2.469896000
C	5.170162000	-4.647953000	0.646049000
C	4.913499000	-5.062226000	2.106841000
C	5.185214000	-3.762037000	2.890466000
C	4.748124000	-2.684452000	1.890788000
C	5.345291000	-1.330857000	2.065872000
C	7.698370000	-4.793305000	0.473614000
C	7.920302000	-6.146514000	-1.151727000
C	6.548267000	-5.996061000	-0.969901000
C	8.325735000	-7.005633000	-2.191192000
C	6.088215000	-7.368907000	-2.636207000
O	3.550952000	-5.432545000	2.220186000
O	4.415426000	-3.662865000	4.073750000
O	5.174970000	-3.220644000	0.616644000
H	4.377598000	-5.045839000	0.012318000
H	3.262953000	-5.170721000	3.108093000
H	5.568666000	-5.882917000	2.409391000
H	4.907438000	-4.047563000	4.808648000
H	6.252067000	-3.662472000	3.102300000
H	3.653438000	-2.631359000	1.912389000
H	6.432631000	-1.308107000	2.056063000
H	4.899525000	-0.740088000	2.860130000
H	10.346779000	-6.780917000	-1.958387000
H	9.862156000	-7.841695000	-3.242282000
H	7.881127000	-4.100650000	1.278990000
H	5.366109000	-7.881930000	-3.262585000

21A-TS- Ado

N	-0.028133000	0.046185000	0.251915000
N	-1.180892000	1.909925000	-0.233570000
N	-3.987797000	-0.506258000	-0.154633000
N	-1.875867000	-1.551354000	0.320542000
N	-4.223054000	1.750825000	-0.638808000
C	1.103494000	-0.821887000	0.618007000
C	1.357985000	-1.900917000	-0.434890000
C	2.328191000	-1.178860000	-1.383702000
C	3.157575000	-0.303686000	-0.428870000
C	3.649691000	0.983598000	-1.006778000
C	0.001942000	1.403413000	0.021015000
C	-2.041706000	0.833456000	-0.156857000
C	-1.345428000	-0.333357000	0.153669000
C	-3.434522000	0.708568000	-0.317302000
C	-3.195684000	-1.541337000	0.149376000
O	1.997635000	-2.990774000	0.206165000
O	3.186459000	-2.067523000	-2.080014000
O	2.267939000	-0.044071000	0.695374000
H	0.886984000	-1.265844000	1.590586000
H	2.621472000	-3.364564000	-0.433986000
H	0.437100000	-2.219029000	-0.927492000
H	2.746141000	-2.366609000	-2.884544000
H	1.764077000	-0.551898000	-2.078213000
H	3.992805000	-0.902291000	-0.055647000
H	2.905599000	1.558628000	-1.553925000
H	4.603169000	0.915390000	-1.522184000
H	-3.842951000	2.680478000	-0.674048000
H	-5.221660000	1.632604000	-0.653290000
H	0.924627000	1.957784000	0.079869000
H	-3.700079000	-2.494173000	0.271494000
H	3.891008000	1.834557000	0.068687000
C	5.083992000	3.657299000	0.625277000
P	5.171798000	5.131319000	1.658820000
O	2.662536000	3.343116000	0.956252000
O	6.339137000	6.069154000	1.099919000
H	6.029531000	3.116411000	0.682115000
H	2.747004000	4.288735000	1.178903000
O	3.858258000	5.810770000	1.778545000
H	4.960464000	4.014926000	-0.401242000
O	5.802040000	4.574183000	3.008609000
H	4.090929000	2.175070000	1.916363000
C	3.929074000	2.751436000	1.002444000
H	5.778686000	5.195563000	3.750473000
H	6.028245000	6.731931000	0.467386000

21B-TS- Ado

N	0.001887000	0.038032000	0.277766000
N	-1.101304000	1.941757000	-0.165494000
N	-3.970318000	-0.401444000	-0.147390000
N	-1.887306000	-1.512285000	0.305994000
N	-4.145166000	1.871844000	-0.580349000
C	1.112429000	-0.865726000	0.626193000
C	1.337712000	-1.928850000	-0.449208000
C	2.315873000	-1.206695000	-1.388755000
C	3.170179000	-0.364143000	-0.426132000
C	3.679126000	0.926699000	-0.978647000
C	0.067969000	1.399208000	0.079524000
C	-1.989702000	0.886388000	-0.116073000
C	-1.324328000	-0.305098000	0.168168000
C	-3.384806000	0.801733000	-0.280981000
C	-3.205995000	-1.463744000	0.133420000
O	1.959103000	-3.044750000	0.165368000
O	3.152913000	-2.098769000	-2.108082000
O	2.295224000	-0.120935000	0.718006000
H	0.884205000	-1.323295000	1.589854000
H	2.579212000	-3.410295000	-0.483155000
H	0.407362000	-2.219019000	-0.941292000
H	2.698547000	-2.379878000	-2.911243000
H	1.759846000	-0.556373000	-2.068207000
H	3.998424000	-0.984963000	-0.074171000
H	2.948260000	1.512294000	-1.532678000
H	4.641259000	0.859526000	-1.477769000
H	-3.741295000	2.792161000	-0.584432000
H	-5.146788000	1.781494000	-0.589757000
H	1.004277000	1.929343000	0.155615000
H	-3.735414000	-2.405606000	0.232822000
H	3.913182000	1.787349000	0.122735000
C	5.091743000	3.628048000	0.661805000
P	5.110679000	5.159417000	1.678044000
O	2.692715000	3.285942000	1.047119000
O	6.154253000	6.137453000	0.876833000
H	6.048881000	3.111547000	0.750565000
H	2.825716000	4.257764000	1.171414000
O	3.717511000	5.741515000	1.559075000
H	4.970169000	3.935475000	-0.381973000
O	5.710906000	4.905992000	3.022250000
H	4.147046000	2.115402000	1.953612000
C	3.962403000	2.698215000	1.045640000
H	5.722540000	6.562605000	0.125302000

21C-TS- Ado

N	0.295867000	-0.252363000	-0.297497000
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N	-0.869561000	1.567126000	-0.919431000
N	-2.071479000	1.278984000	2.570572000
N	-0.511413000	-0.457980000	1.998621000
N	-2.749402000	2.934144000	1.089556000
C	1.294625000	-1.315621000	-0.273529000
C	1.698886000	-1.816118000	-1.662258000
C	2.976779000	-1.002915000	-1.942865000
C	3.604758000	-0.883988000	-0.553324000
C	4.480669000	0.307514000	-0.347477000
C	0.010206000	0.671220000	-1.281882000
C	-1.176537000	1.239873000	0.387056000
C	-0.463741000	0.114446000	0.791927000
C	-2.007985000	1.839334000	1.350798000
C	-1.340972000	0.185104000	2.817241000
O	2.006762000	-3.195938000	-1.548637000
O	3.870611000	-1.671287000	-2.819123000
O	2.478558000	-0.851687000	0.356537000
H	0.867088000	-2.124070000	0.318193000
H	2.733082000	-3.368627000	-2.166865000
H	0.917197000	-1.662370000	-2.409729000
H	3.642009000	-1.455783000	-3.731137000
H	2.723653000	-0.012035000	-2.327164000
H	4.156096000	-1.817516000	-0.365854000
H	5.202220000	0.459574000	-1.146981000
H	4.927911000	0.376770000	0.641433000
H	-2.573711000	3.458249000	0.249177000
H	-3.194598000	3.409914000	1.856700000
H	0.472500000	0.628761000	-2.253987000
H	-1.435932000	-0.223124000	3.817911000
H	3.652105000	1.515307000	-0.381046000
C	2.305365000	2.674172000	1.003827000
P	1.742071000	4.381040000	1.510422000
O	4.061321000	3.617093000	-0.412438000
O	1.216594000	4.249771000	2.936813000
H	1.454240000	1.995905000	0.955757000
H	3.835388000	4.316185000	0.285236000
O	3.068562000	5.185156000	1.414926000
H	2.961495000	2.315383000	1.804661000
O	0.700848000	4.838428000	0.490848000
H	2.402395000	2.644692000	-1.187540000
C	3.056354000	2.650675000	-0.305500000

22A-TS- Ado

N	-0.544463000	-0.263948000	-0.470759000
N	-1.826403000	0.891170000	-1.907548000
N	-3.716508000	1.542629000	1.213639000

N	-1.776799000	0.175267000	1.591403000
N	-4.332434000	2.343879000	-0.873490000
C	0.571879000	-0.996698000	0.068299000
C	1.073272000	-2.173334000	-0.786719000
C	2.407507000	-1.650714000	-1.361507000
C	2.907046000	-0.722435000	-0.246568000
C	3.868341000	0.341841000	-0.635688000
C	-0.757271000	0.154653000	-1.769012000
C	-2.352236000	0.983587000	-0.631373000
C	-1.567123000	0.281515000	0.276965000
C	-3.484431000	1.637810000	-0.108140000
C	-2.870107000	0.835221000	1.969517000
O	1.302508000	-3.269624000	0.080042000
O	3.345736000	-2.684317000	-1.588415000
O	1.682218000	-0.096799000	0.211738000
H	0.263225000	-1.360592000	1.047494000
H	2.052199000	-3.762875000	-0.287089000
H	0.356454000	-2.441601000	-1.566520000
H	3.254332000	-3.007691000	-2.492437000
H	2.227194000	-1.069580000	-2.268715000
H	3.317847000	-1.346057000	0.555293000
H	3.541721000	0.984046000	-1.449905000
H	4.903515000	0.024643000	-0.705643000
H	-4.166225000	2.450502000	-1.858619000
H	-5.113764000	2.816399000	-0.452435000
H	-0.086498000	-0.119614000	-2.567446000
H	-3.108104000	0.797632000	3.027240000
H	3.939732000	1.289107000	0.452904000
H	2.062642000	0.538980000	3.353349000
H	1.684248000	2.062140000	2.843128000
C	3.667907000	1.711781000	2.681705000
N	2.246789000	1.223306000	2.621908000
C	4.085743000	2.241808000	1.323542000
C	3.680932000	2.870294000	3.743799000
O	2.577754000	3.456951000	3.880132000
H	3.376943000	2.990352000	0.967072000
H	4.297695000	0.891435000	3.013396000
O	4.766350000	3.096644000	4.298877000
C	5.488516000	2.680101000	1.166770000
C	5.786212000	3.902380000	0.557010000
C	6.563428000	1.865138000	1.549864000
C	7.097712000	4.312304000	0.352907000
H	4.977709000	4.551054000	0.242199000
C	7.875153000	2.260094000	1.351904000
H	6.374463000	0.902041000	2.006628000
C	8.148861000	3.490948000	0.753908000

H	7.304282000	5.268263000	-0.114014000
H	8.698638000	1.625094000	1.651964000
O	9.460448000	3.831713000	0.586126000
H	9.528077000	4.696950000	0.163116000
H	1.976161000	0.800873000	1.714452000

22B-TS- Ado

H	-3.624406000	-1.945190000	-0.936486000
H	-3.659259000	-0.861636000	0.259958000
C	-1.871067000	-0.928578000	-0.681801000
N	-3.344427000	-0.998729000	-0.697313000
C	-1.470695000	0.542023000	-0.588573000
C	-1.238859000	-1.823913000	0.421670000
O	-1.731681000	-1.723799000	1.574335000
H	-2.086345000	0.987492000	0.465581000
H	-1.513588000	-1.309233000	-1.644247000
H	-1.970798000	1.100174000	-1.381007000
O	-0.292460000	-2.571454000	0.072758000
C	-0.056959000	0.952581000	-0.444298000
C	0.745229000	0.532778000	0.627173000
C	0.507616000	1.867777000	-1.344605000
C	2.046429000	0.989622000	0.782860000
H	0.337554000	-0.146444000	1.362895000
C	1.807772000	2.330928000	-1.203007000
H	-0.088363000	2.226231000	-2.175756000
C	2.585049000	1.890649000	-0.134690000
H	2.643666000	0.654117000	1.623398000
H	2.228670000	3.034525000	-1.909973000
O	3.860068000	2.378195000	-0.031951000
H	4.293167000	2.007318000	0.746891000
N	-3.029174000	5.673454000	1.137146000
N	-5.142252000	6.057147000	0.485411000
N	-4.054472000	9.554739000	1.044130000
N	-2.305119000	7.973217000	1.510227000
N	-6.181620000	8.948986000	0.344697000
C	-1.803922000	4.956765000	1.502283000
C	-1.638280000	4.825648000	3.021102000
C	-2.251891000	3.439902000	3.284060000
C	-1.832665000	2.659862000	2.029744000
C	-2.679216000	1.495706000	1.656028000
C	-4.229615000	5.146686000	0.722015000
C	-4.512100000	7.254424000	0.761747000
C	-3.196931000	7.036217000	1.167509000
C	-4.935576000	8.596009000	0.707013000
C	-2.819816000	9.197258000	1.416794000
O	-0.252127000	4.822241000	3.314875000

O	-1.720152000	2.809531000	4.436850000
O	-1.869642000	3.654010000	0.973410000
H	-0.966168000	5.509608000	1.074569000
H	-0.127796000	4.226794000	4.069273000
H	-2.150995000	5.630782000	3.553537000
H	-2.230010000	3.078664000	5.210042000
H	-3.340678000	3.515217000	3.338412000
H	-0.794297000	2.341195000	2.168929000
H	-3.705901000	1.734555000	1.388005000
H	-2.574669000	0.629788000	2.300347000
H	-6.834930000	8.255383000	0.025718000
H	-6.420318000	9.922073000	0.259384000
H	-4.355126000	4.084603000	0.599639000
H	-2.156024000	10.015445000	1.675859000

22C-TS- Ado

N	0.101837000	-0.838311000	-0.225956000
N	-1.621582000	-0.280332000	-1.555341000
N	-2.683319000	1.468688000	1.534278000
N	-0.579545000	0.339205000	1.803881000
N	-3.895914000	1.461978000	-0.441126000
C	1.354987000	-1.380574000	0.268505000
C	2.039718000	-2.368792000	-0.671456000
C	2.963671000	-1.452526000	-1.501427000
C	3.419346000	-0.413616000	-0.462788000
C	3.741645000	0.943107000	-0.983723000
C	-0.487590000	-0.922008000	-1.473756000
C	-1.799458000	0.273736000	-0.302238000
C	-0.739262000	-0.053707000	0.534535000
C	-2.815545000	1.076568000	0.253135000
C	-1.601333000	1.090985000	2.218253000
O	2.804933000	-3.245119000	0.133357000
O	4.092463000	-2.132140000	-2.010724000
O	2.295018000	-0.318168000	0.452848000
H	1.160476000	-1.827844000	1.241176000
H	3.569961000	-3.517907000	-0.395154000
H	1.333292000	-2.928731000	-1.287659000
H	3.876672000	-2.510360000	-2.871633000
H	2.396535000	-0.967489000	-2.299420000
H	4.266881000	-0.835522000	0.083751000
H	2.926252000	1.448584000	-1.495197000
H	4.702800000	1.025034000	-1.481591000
H	-4.019518000	1.178585000	-1.397296000
H	-4.598006000	2.032883000	-0.002375000
H	-0.039752000	-1.479288000	-2.279232000
H	-1.545384000	1.446645000	3.241499000

H	3.977437000	1.788894000	0.154573000
H	1.393964000	1.718584000	2.695194000
H	1.594950000	2.770388000	1.445602000
C	3.421066000	2.202527000	2.324503000
N	2.002143000	1.958485000	1.910833000
C	4.250541000	2.626473000	1.116982000
C	3.505507000	3.274235000	3.404219000
O	2.515411000	4.169078000	3.289847000
H	3.876751000	3.562084000	0.700992000
H	3.784505000	1.273112000	2.754042000
O	4.390781000	3.320814000	4.215021000
C	5.718576000	2.625206000	1.274574000
C	6.473926000	3.700209000	0.793218000
C	6.408440000	1.539092000	1.833196000
C	7.858572000	3.706699000	0.876686000
H	5.969485000	4.550518000	0.350910000
C	7.789047000	1.533621000	1.922941000
H	5.865060000	0.676888000	2.198363000
C	8.522534000	2.621238000	1.446147000
H	8.423301000	4.552886000	0.503906000
H	8.314182000	0.692552000	2.356064000
O	9.878423000	2.563342000	1.562772000
H	10.280761000	3.364025000	1.202671000
H	1.975819000	1.137292000	1.265896000
H	2.621026000	4.862925000	3.962340000

22D-TS- Ado

H	-3.690728000	-1.847539000	-1.048152000
H	-3.764969000	-0.739439000	0.146872000
C	-1.929154000	-0.830215000	-0.762261000
N	-3.390668000	-0.916989000	-0.779059000
C	-1.513025000	0.615707000	-0.499715000
C	-1.290579000	-1.840613000	0.186876000
O	-1.759555000	-1.732094000	1.444455000
H	-2.086056000	0.965397000	0.627328000
H	-1.565990000	-1.113039000	-1.754108000
H	-2.038995000	1.248840000	-1.212363000
O	-0.474355000	-2.670006000	-0.137593000
C	-0.084135000	0.981999000	-0.384800000
C	0.749523000	0.472086000	0.619793000
C	0.465971000	1.937247000	-1.251602000
C	2.071851000	0.875196000	0.741418000
H	0.358919000	-0.228749000	1.345040000
C	1.784475000	2.349611000	-1.142356000
H	-0.155816000	2.366269000	-2.027995000
C	2.596433000	1.815978000	-0.143334000

H	2.693649000	0.469142000	1.530855000
H	2.195593000	3.085402000	-1.821377000
O	3.887253000	2.256530000	-0.074370000
H	4.346958000	1.826491000	0.657569000
H	-1.343832000	-2.417860000	1.992284000
N	-3.061279000	5.636125000	1.143469000
N	-5.203353000	5.999033000	0.581174000
N	-4.076335000	9.513853000	0.906301000
N	-2.310539000	7.947180000	1.360063000
N	-6.232030000	8.886852000	0.323713000
C	-1.821185000	4.935909000	1.482009000
C	-1.574833000	4.874847000	2.995312000
C	-2.140007000	3.488776000	3.352806000
C	-1.773388000	2.668278000	2.108571000
C	-2.605028000	1.463099000	1.839367000
C	-4.283759000	5.096011000	0.818289000
C	-4.555295000	7.205047000	0.761816000
C	-3.222121000	6.999892000	1.110836000
C	-4.976421000	8.544854000	0.660866000
C	-2.825375000	9.168168000	1.232391000
O	-0.175892000	4.914767000	3.215310000
O	-1.529569000	2.921037000	4.498214000
O	-1.915132000	3.608419000	1.017705000
H	-1.005009000	5.465273000	0.987876000
H	0.001011000	4.366271000	3.994392000
H	-2.079258000	5.690984000	3.518671000
H	-2.011433000	3.198949000	5.286127000
H	-3.225411000	3.542511000	3.465358000
H	-0.718260000	2.386904000	2.194368000
H	-3.654316000	1.661114000	1.633583000
H	-2.436510000	0.638822000	2.524477000
H	-6.933370000	8.181171000	0.183715000
H	-6.500741000	9.855671000	0.309970000
H	-4.420197000	4.030053000	0.757453000
H	-2.146731000	9.994249000	1.417243000

23A-TS- Ado

C	-1.271589000	1.099359000	0.133265000
N	-1.597356000	0.277949000	1.286787000
C	-0.223906000	0.384279000	-0.753422000
C	1.201569000	0.676071000	-0.350865000
C	2.225785000	-0.284492000	-0.792920000
O	3.477958000	0.217588000	-0.662841000
H	-0.842551000	2.037126000	0.494199000
H	-0.344468000	0.679066000	-1.801213000
H	-0.417092000	-0.688211000	-0.714540000

O	2.023910000	-1.419282000	-1.178872000
C	-2.488107000	1.450085000	-0.734988000
O	-3.477641000	0.745371000	-0.738561000
H	1.319775000	0.631733000	0.954732000
H	1.505283000	1.708693000	-0.506437000
H	4.108035000	-0.477381000	-0.911921000
C	-2.299403000	1.002945000	2.343065000
H	-1.628434000	1.748545000	2.768274000
H	-3.209616000	1.517995000	2.006695000
H	-2.575415000	0.307945000	3.136405000
H	-2.170182000	-0.498544000	0.972243000
C	-2.389751000	2.703427000	-1.560911000
H	-1.408011000	2.799646000	-2.026979000
H	-3.173536000	2.735253000	-2.314806000
H	-2.499374000	3.555764000	-0.884586000
N	-0.672079000	4.274479000	3.325986000
N	-2.427338000	3.856558000	4.666445000
N	-4.244147000	5.254800000	1.757517000
N	-1.866971000	5.196884000	1.404979000
N	-5.268677000	4.504891000	3.698058000
C	0.665085000	4.240494000	2.756232000
C	1.794625000	4.239825000	3.789300000
C	2.143668000	2.741766000	3.901312000
C	1.910561000	2.249768000	2.464186000
C	1.560966000	0.807719000	2.327789000
C	-1.129313000	3.784193000	4.532858000
C	-2.866669000	4.411057000	3.479777000
C	-1.794888000	4.673641000	2.632644000
C	-4.149381000	4.721825000	2.988653000
C	-3.124502000	5.460567000	1.055569000
O	2.880933000	4.958213000	3.231470000
O	3.489601000	2.517451000	4.275519000
O	0.818904000	3.055617000	1.981520000
H	0.744479000	5.107311000	2.102003000
H	3.690968000	4.552259000	3.575479000
H	1.491911000	4.679246000	4.742884000
H	3.551972000	2.482937000	5.237568000
H	1.455140000	2.241148000	4.585727000
H	2.812069000	2.482258000	1.885762000
H	0.608654000	0.510358000	2.753193000
H	2.382515000	0.121061000	2.509168000
H	-5.224116000	4.083795000	4.609199000
H	-6.166114000	4.717767000	3.297666000
H	-0.458195000	3.393754000	5.279656000
H	-3.264852000	5.894657000	0.071229000

23B-TS- Ado

C	-1.373762000	0.884964000	0.405916000
N	-2.618560000	0.305435000	0.906560000
C	-0.384950000	-0.241615000	0.056101000
C	1.027830000	0.200812000	-0.244296000
C	2.040704000	-0.867110000	-0.621754000
O	3.089345000	-0.461371000	-1.192929000
H	-0.945739000	1.506167000	1.193772000
H	-0.789343000	-0.796287000	-0.799654000
H	-0.372922000	-0.942733000	0.892006000
O	1.777477000	-2.056230000	-0.302244000
C	-1.608462000	1.756447000	-0.843050000
O	-2.322729000	1.341583000	-1.737611000
H	1.512427000	0.626559000	0.888246000
H	1.117808000	1.081895000	-0.876524000
C	-3.559970000	1.293669000	1.430573000
H	-3.122520000	1.781940000	2.302389000
H	-3.842313000	2.078438000	0.713409000
H	-4.472172000	0.789565000	1.751726000
H	-3.057023000	-0.207470000	0.147911000
C	-0.971387000	3.112683000	-0.900609000
H	-1.016393000	3.518985000	-1.909591000
H	-1.519596000	3.771858000	-0.218607000
H	0.051052000	3.086808000	-0.525612000
N	-0.736825000	4.121277000	3.227995000
N	-2.319399000	3.375931000	4.638350000
N	-4.478007000	5.271774000	2.299822000
N	-2.156714000	5.380062000	1.687541000
N	-5.259156000	4.114601000	4.152008000
C	0.540666000	4.236993000	2.547350000
C	1.740296000	4.488858000	3.471862000
C	2.386494000	3.093219000	3.580604000
C	2.084398000	2.474565000	2.206103000
C	1.998486000	0.986913000	2.168351000
C	-1.045539000	3.374559000	4.345107000
C	-2.897989000	4.156603000	3.655118000
C	-1.934369000	4.623003000	2.765881000
C	-4.232591000	4.510254000	3.380896000
C	-3.450404000	5.655162000	1.534574000
O	2.614556000	5.387290000	2.810370000
O	3.786848000	3.151138000	3.787338000
O	0.804236000	3.029897000	1.847546000
H	0.432595000	5.061537000	1.843536000
H	3.516297000	5.124354000	3.050555000
H	1.431604000	4.891160000	4.440258000
H	3.968018000	3.185428000	4.734094000

H	1.900123000	2.510800000	4.366299000
H	2.844467000	2.834938000	1.503197000
H	1.250221000	0.559985000	2.832584000
H	2.956883000	0.477338000	2.201164000
H	-5.104315000	3.501960000	4.933266000
H	-6.201811000	4.343427000	3.887138000
H	-0.285666000	2.851364000	4.902198000
H	-3.709547000	6.265235000	0.675844000

24-TS- Ado

H	-0.803835000	-0.527866000	0.400058000
C	-0.725095000	-1.943921000	2.501643000
H	-0.887908000	-1.404689000	3.437107000
H	-0.654493000	-3.005002000	2.738552000
H	0.213075000	-1.606493000	2.061877000
C	-1.928102000	-1.724284000	1.612123000
H	-2.283273000	0.617835000	-0.822009000
H	-5.927028000	-0.103720000	0.652885000
O	-3.019493000	-2.234823000	1.863191000
C	-3.989547000	-0.027746000	0.334021000
C	-2.743931000	-0.525083000	-0.391524000
N	-1.725571000	-0.921093000	0.544931000
C	-2.815105000	-1.361962000	-1.673500000
O	-3.875784000	0.980637000	1.036245000
N	-5.203280000	-0.600519000	0.154177000
H	-3.277418000	-2.322223000	-1.430300000
C	-1.411745000	-1.666534000	-2.211971000
H	-0.860790000	-0.747073000	-2.421391000
H	-0.827230000	-2.256995000	-1.506915000
H	-1.488918000	-2.231008000	-3.142463000
C	-3.652423000	-0.663487000	-2.751169000
H	-3.147480000	0.239820000	-3.099862000
H	-3.785149000	-1.322663000	-3.610059000
H	-4.638675000	-0.372419000	-2.391199000
C	-5.517950000	-1.978055000	-0.209731000
H	-6.490425000	-2.218881000	0.215157000
H	-5.579619000	-2.117395000	-1.289405000
H	-4.780808000	-2.658893000	0.210450000
N	2.593955000	0.814393000	-0.073053000
N	4.132888000	0.301199000	-1.625442000
N	4.562933000	-2.622196000	0.613258000
N	2.860478000	-1.117677000	1.395564000
N	5.802857000	-2.263771000	-1.313479000
C	1.463696000	1.439905000	0.561726000
C	1.456129000	2.983356000	0.575708000
C	0.233679000	3.338602000	-0.304950000

C	-0.670064000	2.112484000	-0.122669000
C	-1.690270000	1.867935000	-1.176860000
C	3.215340000	1.154695000	-1.257044000
C	4.113102000	-0.673983000	-0.644176000
C	3.157426000	-0.379806000	0.322739000
C	4.844262000	-1.863742000	-0.461882000
C	3.609626000	-2.216652000	1.459140000
O	1.254845000	3.411090000	1.910720000
O	-0.427647000	4.511485000	0.130929000
O	0.282032000	1.029243000	-0.132117000
H	1.440526000	1.075262000	1.589162000
H	0.705456000	4.209149000	1.865173000
H	2.385401000	3.399780000	0.180049000
H	-0.090517000	5.271116000	-0.357998000
H	0.536029000	3.415269000	-1.351557000
H	-1.151220000	2.178204000	0.860365000
H	-1.290829000	1.708100000	-2.174513000
H	-2.552298000	2.524397000	-1.136557000
H	6.012645000	-1.727938000	-2.137104000
H	6.280111000	-3.135153000	-1.158724000
H	2.944620000	2.047528000	-1.797688000
H	3.424462000	-2.871806000	2.303742000

25-TS- Ado

H	2.357974000	3.464301000	-0.419055000
H	-2.737141000	0.692056000	0.615184000
H	-2.427922000	2.119929000	-0.382349000
H	-1.633169000	-2.478600000	-0.674092000
H	0.991876000	-3.123848000	-0.580246000
H	3.385502000	-0.111429000	-0.255174000
H	3.531096000	-0.115079000	1.393224000
H	-0.592093000	0.877149000	-1.544959000
H	-1.082725000	-1.111170000	0.968220000
H	1.210631000	-1.040007000	-1.279482000
H	1.243097000	-0.500877000	1.724311000
H	1.618331000	1.859999000	1.194846000
C	1.832049000	2.877516000	-1.177037000
O	1.829989000	1.489053000	-0.822986000
O	-3.177439000	0.542940000	-1.420513000
C	-2.369555000	1.031554000	-0.359755000
O	-1.403672000	-1.648306000	-1.137444000
O	1.093014000	-2.521114000	0.166026000
N	3.016381000	-0.518916000	0.609202000
O	-0.159697000	1.408727000	0.422115000
C	-0.905676000	0.626445000	-0.522999000
C	-0.656911000	-0.849192000	-0.269039000

C	0.821760000	-1.192777000	-0.264834000
C	1.230373000	1.205549000	0.407636000
H	-2.993601000	-0.404333000	-1.505164000
H	2.353720000	2.952726000	-2.127409000
H	0.811982000	3.249151000	-1.285557000
C	1.540585000	-0.265393000	0.704862000
H	3.186717000	-1.528983000	0.601240000
N	-1.527841000	-5.639348000	1.255230000
N	0.552053000	-6.321788000	1.745685000
N	-1.088783000	-9.627289000	1.407636000
N	-2.616249000	-7.810662000	1.027608000
N	1.149739000	-9.333968000	1.938618000
C	-2.661900000	-4.761448000	0.968966000
C	-3.659531000	-4.696143000	2.127798000
C	-3.143299000	-3.484765000	2.925428000
C	-2.662146000	-2.541609000	1.815294000
C	-1.577637000	-1.583505000	2.181760000
C	-0.228801000	-5.288149000	1.549180000
C	-0.271755000	-7.416655000	1.572375000
C	-1.568457000	-7.012982000	1.262913000
C	-0.049821000	-8.805587000	1.642393000
C	-2.282695000	-9.096445000	1.119909000
O	-4.938705000	-4.429534000	1.584361000
O	-4.156083000	-2.846919000	3.680027000
O	-2.176750000	-3.448006000	0.779740000
H	-3.146628000	-5.120662000	0.061179000
H	-5.421796000	-3.905764000	2.240869000
H	-3.659567000	-5.620130000	2.710689000
H	-4.216934000	-3.264160000	4.547593000
H	-2.304113000	-3.786346000	3.556957000
H	-3.530910000	-2.009972000	1.417709000
H	-0.702419000	-2.037244000	2.639937000
H	-1.922006000	-0.692747000	2.697867000
H	1.948441000	-8.741360000	2.081273000
H	1.271321000	-10.332068000	1.942162000
H	0.075698000	-4.255362000	1.574590000
H	-3.079406000	-9.810426000	0.939634000

26-TS- Ado

N	0.703816000	0.308246000	0.436989000
N	2.019135000	-1.419542000	-0.129307000
N	4.626321000	1.163856000	0.378923000
N	2.413466000	2.015044000	0.774763000
N	5.066834000	-1.020298000	-0.265471000
C	-0.493710000	1.095277000	0.735495000
C	-0.869036000	2.045603000	-0.408558000

C	-1.892728000	1.204719000	-1.191342000
C	-2.607361000	0.461336000	-0.062720000
C	0.789140000	-1.015753000	0.072052000
C	2.792667000	-0.301943000	0.114694000
C	1.993131000	0.781823000	0.470765000
C	4.180695000	-0.068172000	0.074251000
C	3.739454000	2.111504000	0.704323000
O	-1.487916000	3.188083000	0.154795000
O	-2.828234000	1.988402000	-1.909056000
O	-1.580494000	0.211634000	0.916989000
H	-0.299221000	1.658014000	1.649300000
H	-2.171199000	3.477685000	-0.468251000
H	0.003235000	2.322703000	-1.004654000
H	-2.477895000	2.179098000	-2.787228000
H	-1.373350000	0.502404000	-1.848464000
H	-3.350912000	1.136916000	0.369755000
H	4.762307000	-1.962290000	-0.437335000
H	6.052141000	-0.823632000	-0.225120000
H	-0.093275000	-1.626802000	-0.009099000
H	4.160717000	3.083098000	0.940145000
C	-3.256636000	-0.834836000	-0.492163000
H	-3.971784000	-0.607741000	-1.283512000
H	-2.511312000	-1.526252000	-0.887314000
S	-4.165618000	-1.624504000	0.884989000
C	-5.301642000	-2.635919000	-0.023499000
H	-6.164793000	-1.887288000	-0.674610000
H	-4.836030000	-3.248316000	-0.794100000
H	-5.906154000	-3.222622000	0.664253000
N	-7.439305000	1.838751000	1.189060000
N	-5.423004000	2.811174000	1.010360000
N	-7.380518000	5.747687000	2.131363000
N	-8.736081000	3.770348000	1.946776000
N	-5.114229000	5.799719000	1.629522000
C	-8.443449000	0.758887000	1.221163000
C	-9.605169000	1.032755000	0.267907000
C	-9.068960000	0.438122000	-1.045211000
C	-8.231896000	-0.764908000	-0.570262000
C	-7.029724000	-1.059688000	-1.408948000
C	-6.104150000	1.698268000	0.891914000
C	-6.356884000	3.741309000	1.421170000
C	-7.615845000	3.155013000	1.548960000
C	-6.265844000	5.110797000	1.731784000
C	-8.523722000	5.056615000	2.215484000
O	-10.726558000	0.301917000	0.732108000
O	-10.099016000	-0.013046000	-1.909158000
O	-7.840621000	-0.432781000	0.792439000

H	-8.789933000	0.645942000	2.248940000
H	-11.209036000	0.002154000	-0.052840000
H	-9.832660000	2.097546000	0.191001000
H	-10.392575000	0.721606000	-2.461115000
H	-8.431997000	1.171138000	-1.545104000
H	-8.887715000	-1.637688000	-0.516977000
H	-6.394503000	-0.198845000	-1.609346000
H	-7.242080000	-1.640628000	-2.302234000
H	-4.254716000	5.318533000	1.429155000
H	-5.074349000	6.751255000	1.952819000
H	-5.701994000	0.737243000	0.622756000
H	-9.387416000	5.623232000	2.547283000

27-TS- Ado

H	-0.132478000	0.684135000	-0.197120000
C	-1.059299000	3.467409000	-1.820462000
H	-1.746955000	4.026389000	-1.182097000
H	-0.366408000	4.173681000	-2.271175000
H	-1.629306000	2.968727000	-2.599843000
C	-0.260805000	2.500533000	-0.980632000
H	-4.110291000	0.802831000	-1.362122000
H	-1.961651000	-0.445758000	-0.374339000
H	-2.445014000	-1.045477000	-4.007681000
H	-3.299266000	2.330163000	-1.204551000
O	0.860906000	2.799950000	-0.573401000
C	-1.788028000	0.137037000	-2.563006000
C	-1.975517000	0.635502000	-1.136266000
N	-0.808726000	1.303829000	-0.627075000
C	-3.316479000	1.310081000	-0.818814000
O	-0.878431000	0.584448000	-3.262703000
N	-2.623094000	-0.811744000	-3.041553000
C	-3.644693000	1.328602000	0.655671000
C	-4.544897000	0.405256000	1.188904000
C	-3.035950000	2.241111000	1.519377000
C	-4.820153000	0.380722000	2.552220000
H	-5.035414000	-0.304071000	0.532814000
C	-3.307187000	2.219917000	2.883098000
H	-2.342167000	2.971933000	1.125103000
C	-4.197694000	1.286239000	3.405248000
H	-5.520828000	-0.344700000	2.946317000
H	-2.824450000	2.934659000	3.537862000
H	-4.409334000	1.269287000	4.466858000
C	-3.715944000	-1.524156000	-2.399001000
H	-3.608888000	-1.514185000	-1.320405000
H	-4.686894000	-1.095668000	-2.658238000
H	-3.698166000	-2.563358000	-2.724674000

N	2.562941000	-1.069633000	0.506045000
N	3.365481000	0.161058000	2.205831000
N	4.969083000	1.951308000	-0.614095000
N	3.613593000	0.110713000	-1.356139000
N	5.248889000	2.518014000	1.617864000
C	1.726784000	-1.982927000	-0.243430000
C	1.496452000	-3.347750000	0.417071000
C	0.088365000	-3.202833000	1.031479000
C	-0.610179000	-2.266698000	0.033449000
C	-1.711802000	-1.435977000	0.598347000
C	2.602979000	-0.843903000	1.867167000
C	3.850982000	0.646928000	1.005693000
C	3.359903000	-0.097716000	-0.061571000
C	4.699669000	1.723171000	0.683633000
C	4.424376000	1.151057000	-1.537290000
O	1.487184000	-4.323215000	-0.610145000
O	-0.606906000	-4.432397000	1.107993000
O	0.439549000	-1.392584000	-0.424472000
H	2.204695000	-2.112037000	-1.213263000
H	0.864155000	-5.013089000	-0.335213000
H	2.261026000	-3.577826000	1.163174000
H	-0.421946000	-4.852651000	1.956343000
H	0.149370000	-2.723089000	2.010905000
H	-0.968300000	-2.872683000	-0.805852000
H	-1.432549000	-0.816356000	1.446999000
H	-2.658165000	-1.948452000	0.730933000
H	5.010162000	2.405259000	2.587428000
H	5.796783000	3.313469000	1.338046000
H	2.054241000	-1.460834000	2.560023000
H	4.677166000	1.385629000	-2.565869000

28-TS- Ado

H	0.923513000	0.245780000	2.140723000
C	2.698848000	0.152091000	-0.695367000
H	2.468423000	1.081320000	-1.216594000
H	3.760860000	-0.056991000	-0.792153000
H	2.124155000	-0.647067000	-1.161262000
C	2.368877000	0.280732000	0.771463000
H	-1.044601000	0.357458000	1.204449000
H	-1.471704000	-2.857486000	-0.591912000
O	3.253395000	0.353070000	1.624072000
C	-0.291009000	-1.430329000	0.109659000
C	-0.104639000	0.065626000	0.344989000
N	1.060254000	0.345695000	1.141792000
O	0.591095000	-2.227826000	0.431028000
N	-1.448478000	-1.860376000	-0.437599000

C	-0.314444000	0.942911000	-0.867672000
C	-1.385056000	2.013309000	-0.918425000
C	0.058044000	2.400192000	-0.830363000
H	-0.143048000	0.439351000	-1.812107000
H	-1.999812000	2.156205000	-0.040980000
H	-1.905176000	2.145966000	-1.857355000
H	0.539909000	2.817429000	-1.704380000
H	0.418448000	2.786901000	0.113391000
C	-2.613167000	-1.104087000	-0.872967000
H	-2.803824000	-0.263944000	-0.213022000
H	-2.500158000	-0.726014000	-1.890452000
H	-3.478023000	-1.763521000	-0.838186000
N	0.760658000	0.018531000	5.649499000
N	1.775129000	1.943321000	6.198777000
N	3.334381000	-0.281188000	8.718400000
N	1.779900000	-1.453062000	7.308344000
N	3.786008000	1.985560000	8.525184000
C	-0.119331000	-0.929890000	4.980825000
C	-1.517845000	-1.028481000	5.609842000
C	-2.362224000	-0.128644000	4.687193000
C	-1.700705000	-0.369453000	3.321837000
C	-1.878764000	0.713562000	2.315566000
C	0.917472000	1.363366000	5.397947000
C	2.208699000	0.930580000	7.032008000
C	1.590450000	-0.274209000	6.706217000
C	3.125398000	0.895187000	8.100464000
C	2.667273000	-1.361533000	8.296706000
O	-1.943227000	-2.375498000	5.515646000
O	-3.722778000	-0.510801000	4.635290000
O	-0.298447000	-0.503337000	3.641625000
H	0.372140000	-1.902535000	5.017136000
H	-2.906282000	-2.360898000	5.408797000
H	-1.514659000	-0.685687000	6.647631000
H	-4.213624000	-0.040081000	5.319202000
H	-2.251336000	0.918162000	4.979457000
H	-2.071976000	-1.323217000	2.931655000
H	-1.469128000	1.681723000	2.592406000
H	-2.875418000	0.764607000	1.889935000
H	3.676215000	2.866082000	8.053830000
H	4.459701000	1.906381000	9.267418000
H	0.385927000	1.847132000	4.596514000
H	2.879620000	-2.279836000	8.833965000

Cartesian coordinates of all reactant and products complexes of **substrates 1-28** with 5'-dAdo.

1A-RC-complex

N	-2.803414000	1.001473000	-0.395961000
N	-1.870811000	2.523311000	-1.757121000
N	-0.404346000	3.641410000	1.455744000
N	-1.856882000	1.746138000	1.729393000
N	0.002447000	4.658582000	-0.588576000
C	-3.557016000	-0.159492000	0.039352000
C	-5.082945000	0.028198000	0.041249000
C	-5.523911000	-0.719843000	-1.230741000
C	-4.489957000	-1.865462000	-1.302492000
C	-4.288844000	-2.462116000	-2.631832000
C	-2.652618000	1.477349000	-1.680053000
C	-1.478910000	2.757581000	-0.452910000
C	-2.047062000	1.822700000	0.408758000
C	-0.614479000	3.704513000	0.128730000
C	-1.022905000	2.688672000	2.162803000
O	-5.600434000	-0.608563000	1.195898000
O	-6.829064000	-1.254746000	-1.132278000
O	-3.272322000	-1.230519000	-0.859348000
H	-3.209685000	-0.403859000	1.043607000
H	-6.478032000	-0.945784000	0.960254000
H	-5.353964000	1.087016000	0.021627000
H	-7.464087000	-0.613518000	-1.472147000
H	-5.422547000	-0.073367000	-2.104939000
H	-4.797505000	-2.625118000	-0.573937000
H	-3.648402000	-1.966044000	-3.347976000
H	-4.874520000	-3.315803000	-2.937482000
H	-0.108601000	4.700479000	-1.586285000
H	0.644301000	5.288288000	-0.138562000
H	-3.129504000	0.993272000	-2.516108000
H	-0.813269000	2.687245000	3.227189000
H	10.254995000	0.419050000	-1.465322000
H	7.755940000	0.030724000	0.907716000
H	7.096260000	1.156092000	-0.247455000
H	5.805310000	-0.716646000	-1.338346000
H	6.463937000	-1.844592000	-0.173284000
H	5.380473000	-0.556844000	1.688006000
H	4.726116000	0.576260000	0.521068000
H	3.452007000	-1.280979000	-0.566407000
H	4.092671000	-2.413376000	0.604538000
H	3.015788000	-1.166164000	2.459280000
H	2.387022000	0.023837000	1.339231000
H	1.576683000	0.031561000	-0.993718000
H	0.293341000	0.424651000	0.158247000
H	-0.111370000	-0.205245000	-1.442419000
H	0.553394000	-1.863488000	3.200659000

H	1.745352000	-2.955969000	1.277427000
H	1.007434000	-2.376437000	-0.854851000
H	-1.513244000	-2.012607000	-0.223825000
O	8.532130000	-1.049908000	-1.895738000
O	9.548442000	0.646833000	-0.839106000
C	8.508570000	-0.187635000	-1.049083000
C	7.367018000	0.104566000	-0.112414000
C	6.159480000	-0.803172000	-0.307576000
C	5.022537000	-0.469824000	0.656131000
C	3.800970000	-1.366615000	0.467321000
C	2.664188000	-1.029052000	1.431778000
C	0.600296000	-0.275111000	-0.618551000
O	-1.897035000	-2.061209000	2.342717000
C	-0.847320000	-1.968067000	1.710156000
N	0.388627000	-1.659338000	2.227546000
C	1.435761000	-1.903547000	1.232249000
C	0.631176000	-1.704890000	-0.083249000
N	-0.696221000	-2.144473000	0.360304000

1B-PC-complex

N	1.523885000	-1.361722000	-0.423277000
N	-0.314656000	-2.133943000	-1.454441000
N	-1.268702000	-2.861083000	2.049737000
N	0.909095000	-1.859112000	1.890348000
N	-2.606308000	-3.314650000	0.209515000
C	2.798610000	-0.704321000	-0.247238000
C	4.033737000	-1.464698000	-0.797352000
C	4.695130000	-0.416702000	-1.734764000
C	4.082279000	0.904744000	-1.271589000
C	4.056510000	2.008788000	-2.299287000
C	0.849897000	-1.557660000	-1.608863000
C	-0.421804000	-2.333468000	-0.091481000
C	0.709942000	-1.858979000	0.567189000
C	-1.453497000	-2.844874000	0.716894000
C	-0.125671000	-2.381020000	2.548426000
O	4.889175000	-1.824804000	0.270434000
O	6.108426000	-0.381275000	-1.599670000
O	2.739617000	0.534452000	-0.934471000
H	2.940592000	-0.552892000	0.823852000
H	5.780385000	-1.536179000	0.015375000
H	3.726159000	-2.359379000	-1.343708000
H	6.509534000	-0.939630000	-2.275715000
H	4.406245000	-0.612356000	-2.769122000
H	4.601534000	1.233694000	-0.362972000
H	3.496639000	1.694485000	-3.182070000
H	5.076760000	2.252970000	-2.598338000

H	-2.809903000	-3.197459000	-0.768011000
H	-3.357878000	-3.556609000	0.832926000
H	1.270480000	-1.236258000	-2.547759000
H	-0.036075000	-2.410849000	3.628851000
H	-8.800784000	-0.083265000	-1.766013000
H	-5.832729000	-0.852498000	-0.149017000
H	-5.343451000	-0.340888000	-1.740539000
H	-4.772503000	1.942232000	-0.838953000
H	-5.272205000	1.434399000	0.760046000
H	-3.503341000	-0.346144000	0.746795000
H	-3.001710000	0.163373000	-0.850179000
H	-2.406168000	2.420266000	0.051248000
H	-2.908941000	1.915070000	1.654924000
H	-1.212113000	0.091616000	1.623642000
H	-0.683049000	0.589527000	0.026795000
H	-0.442829000	3.369586000	-1.337738000
H	1.020534000	2.217934000	-1.198355000
H	3.592830000	2.906776000	-1.890616000
H	1.222817000	0.343312000	2.336512000
H	-0.560104000	2.324419000	2.526158000
H	-0.203447000	4.007609000	0.996367000
H	2.418085000	3.792299000	0.672494000
O	-7.567448000	1.628390000	-0.839250000
O	-7.914219000	-0.448248000	-1.610813000
C	-7.145993000	0.518417000	-1.065367000
C	-5.749431000	0.027794000	-0.793632000
C	-4.833255000	1.075877000	-0.174864000
C	-3.433799000	0.526846000	0.088729000
C	-2.486996000	1.551572000	0.711845000
C	-1.104798000	0.957608000	0.964780000
C	0.330969000	2.911424000	-0.738537000
O	3.402080000	1.777125000	1.950772000
C	2.226637000	2.056641000	1.723300000
N	1.148511000	1.263291000	1.928787000
C	-0.114516000	1.912128000	1.612765000
C	0.377032000	3.124216000	0.730779000
N	1.762129000	3.260609000	1.224574000

1B-RC-complex

7	-3.053715000	1.047093000	-0.647082000
7	-1.792224000	2.283620000	-2.035056000
7	-0.635260000	3.677593000	1.195699000
7	-2.307935000	1.976812000	1.483926000
7	0.133144000	4.378649000	-0.877786000
6	-3.903130000	-0.018743000	-0.162802000
6	-5.180128000	-0.251353000	-0.982123000

6	-4.834865000	-1.499525000	-1.817876000
6	-3.910623000	-2.285959000	-0.862551000
6	-2.976107000	-3.222199000	-1.507641000
6	-2.675841000	1.325688000	-1.945139000
6	-1.554160000	2.659046000	-0.726018000
6	-2.321924000	1.900338000	0.151353000
6	-0.670158000	3.588353000	-0.145906000
6	-1.438925000	2.887677000	1.916837000
8	-6.227809000	-0.538890000	-0.073543000
8	-5.970209000	-2.278222000	-2.137706000
8	-3.171512000	-1.247576000	-0.186730000
1	-4.158381000	0.235425000	0.864839000
1	-6.826806000	-1.154601000	-0.522714000
1	-5.429462000	0.613579000	-1.602300000
1	-6.334485000	-1.981776000	-2.980265000
1	-4.281952000	-1.216610000	-2.715893000
1	-4.555338000	-2.807203000	-0.145059000
1	-2.059628000	-2.844194000	-1.939393000
1	-3.253917000	-4.254825000	-1.655082000
1	0.174739000	4.276741000	-1.876678000
1	0.802120000	4.972786000	-0.418681000
1	-3.091126000	0.788632000	-2.782193000
1	-1.365598000	3.003929000	2.992765000
1	7.825466000	0.103379000	0.429570000
1	7.052255000	1.091561000	-0.779815000
1	5.550928000	-0.828266000	-1.393261000
1	6.318973000	-1.817127000	-0.175928000
1	5.568751000	-0.205249000	1.602945000
1	4.789058000	0.773695000	0.376300000
1	3.314547000	-1.160906000	-0.221627000
1	4.080059000	-2.129859000	1.018278000
1	3.318707000	-0.545168000	2.775130000
1	2.560200000	0.473175000	1.569665000
1	1.423945000	0.137727000	-0.587184000
1	0.303043000	0.764057000	0.630877000
1	-0.309848000	-0.116366000	-0.773854000
1	0.977373000	-1.008959000	3.959464000
1	1.853259000	-2.443862000	2.102013000
1	0.824029000	-2.193174000	0.029197000
1	-1.563876000	-1.599228000	0.919567000
8	8.053053000	-1.364606000	-2.338626000
8	9.432260000	0.243065000	-1.600946000
6	8.351446000	-0.404488000	-1.585219000
6	7.313365000	0.055208000	-0.536980000
6	6.047736000	-0.785247000	-0.419852000
6	5.069536000	-0.255819000	0.628178000

6	3.804448000	-1.102526000	0.755558000
6	2.825466000	-0.562157000	1.797881000
6	0.500466000	-0.067373000	-0.045666000
8	-1.571596000	-1.237934000	3.506143000
6	-0.628533000	-1.286093000	2.719874000
7	0.676743000	-0.948696000	2.999299000
6	1.562453000	-1.400215000	1.922842000
6	0.579200000	-1.385733000	0.719426000
7	-0.680589000	-1.681827000	1.410358000

1B-PC-complex

N	1.491495000	-1.357698000	-0.434605000
N	-0.342452000	-2.120030000	-1.481234000
N	-1.314095000	-2.875824000	2.011890000
N	0.865249000	-1.874381000	1.871648000
N	-2.642647000	-3.315153000	0.161180000
C	2.765948000	-0.703216000	-0.246835000
C	4.002982000	-1.460575000	-0.796808000
C	4.669094000	-0.406682000	-1.724074000
C	4.056529000	0.912040000	-1.252879000
C	4.036743000	2.024361000	-2.271756000
C	0.823128000	-1.543225000	-1.625077000
C	-0.456507000	-2.330836000	-0.120498000
C	0.672380000	-1.862713000	0.547659000
C	-1.492586000	-2.847858000	0.678450000
C	-0.173085000	-2.401141000	2.520198000
O	4.853651000	-1.827937000	0.272398000
O	6.082057000	-0.374587000	-1.584083000
O	2.711968000	0.541160000	-0.924385000
H	2.902643000	-0.560480000	0.826133000
H	5.746655000	-1.541161000	0.021403000
H	3.697348000	-2.351457000	-1.350436000
H	6.484469000	-0.928046000	-2.263363000
H	4.383303000	-0.594013000	-2.760846000
H	4.572584000	1.232834000	-0.339533000
H	3.480499000	1.717900000	-3.159576000
H	5.058627000	2.269745000	-2.564180000
H	-2.847091000	-3.171159000	-0.812795000
H	-3.401847000	-3.543949000	0.780592000
H	1.248499000	-1.214289000	-2.559185000
H	-0.088690000	-2.440372000	3.600759000
H	-5.895251000	-0.838309000	-0.104203000
H	-5.364643000	-0.396564000	-1.703994000
H	-4.802460000	1.912369000	-0.881075000
H	-5.309773000	1.460051000	0.728046000
H	-3.553776000	-0.342622000	0.769200000

H	-3.036935000	0.134066000	-0.831700000
H	-2.441378000	2.408848000	0.040800000
H	-2.945736000	1.920286000	1.648789000
H	-1.254772000	0.083657000	1.623542000
H	-0.717920000	0.585518000	0.030916000
H	-0.472216000	3.372007000	-1.319338000
H	0.993892000	2.223793000	-1.181490000
H	3.572175000	2.919540000	-1.857957000
H	1.179429000	0.326064000	2.339200000
H	-0.602608000	2.310122000	2.537546000
H	-0.239578000	4.000486000	1.018167000
H	2.383477000	3.784831000	0.703775000
O	-7.486377000	1.707270000	-1.103823000
O	-8.036135000	-0.435480000	-1.474800000
C	-7.232126000	0.477418000	-1.146351000
C	-5.804006000	0.012622000	-0.786571000
C	-4.872948000	1.064311000	-0.194638000
C	-3.476548000	0.518869000	0.095990000
C	-2.524971000	1.545969000	0.709056000
C	-1.143777000	0.951775000	0.967841000
C	0.301692000	2.913762000	-0.720382000
O	3.361234000	1.761841000	1.973330000
C	2.186533000	2.043663000	1.743841000
N	1.107135000	1.250440000	1.941249000
C	-0.154550000	1.901895000	1.623496000
C	0.341630000	3.118261000	0.750223000
N	1.724825000	3.251215000	1.250789000

2A-RC-complex

O	-0.746488000	-0.642135000	-4.303662000
P	-1.440804000	-0.504785000	-2.890544000
O	-1.002372000	-1.832048000	-2.126960000
O	-0.571688000	0.666781000	-2.288074000
O	-2.901465000	-0.296089000	-2.895428000
C	-1.703619000	-2.290772000	-0.952120000
C	-1.135038000	-1.644841000	0.295029000
C	-1.864529000	-2.053323000	1.577958000
O	-1.284617000	-0.199078000	0.189800000
C	-1.869554000	0.307904000	1.389000000
C	-2.761250000	-0.834583000	1.870644000
N	-2.502042000	1.566722000	1.138003000
O	-0.904485000	-2.218670000	2.611468000
O	-3.043012000	-0.669475000	3.246659000
C	-3.560295000	1.870459000	0.292162000
C	-3.783102000	3.212820000	0.464244000
N	-2.900188000	3.735573000	1.392297000

C	-2.146103000	2.736171000	1.765396000
N	-4.225033000	0.896211000	-0.446068000
H	-1.299228000	-1.084773000	-4.961976000
H	-0.641096000	0.657358000	-1.309587000
H	-2.769626000	-2.085649000	-1.059764000
H	-1.546615000	-3.366999000	-0.907622000
H	-0.071167000	-1.867049000	0.375758000
H	-2.449823000	-2.967634000	1.445242000
H	-1.095587000	0.495491000	2.134854000
H	-3.669870000	-0.872386000	1.270265000
H	-1.360022000	-2.055074000	3.450599000
H	-3.889865000	-1.082734000	3.449703000
H	-4.528884000	3.817372000	-0.025714000
H	-1.318369000	2.769727000	2.454550000
H	-3.659458000	0.453461000	-1.168647000
H	-5.057214000	1.276143000	-0.876864000
N	2.412827000	0.270047000	0.258033000
N	1.045716000	1.764045000	1.225329000
N	1.443709000	3.386803000	-2.084670000
N	2.702194000	1.349212000	-1.911436000
N	0.094851000	4.222936000	-0.395709000
C	3.201026000	-0.928289000	0.061953000
C	4.356453000	-1.112603000	1.063925000
C	3.844288000	-2.241994000	1.977303000
C	2.977953000	-3.072957000	1.006120000
C	1.957924000	-3.923071000	1.640946000
C	1.690575000	0.636880000	1.372364000
C	1.347832000	2.173629000	-0.061680000
C	2.204121000	1.260460000	-0.676593000
C	0.943188000	3.274481000	-0.841966000
C	2.275361000	2.443512000	-2.537262000
O	5.499570000	-1.536995000	0.342382000
O	4.886976000	-3.039901000	2.504030000
O	2.347227000	-2.062392000	0.192232000
H	3.604957000	-0.863075000	-0.948436000
H	5.991208000	-2.134765000	0.926223000
H	4.562900000	-0.189267000	1.611326000
H	5.166418000	-2.680729000	3.354306000
H	3.215634000	-1.833467000	2.771275000
H	3.662001000	-3.671767000	0.392286000
H	1.045641000	-3.477548000	2.013638000
H	2.176363000	-4.959660000	1.850085000
H	-0.467663000	4.049472000	0.422226000
H	-0.260852000	4.886161000	-1.064789000
H	1.663806000	0.017133000	2.254113000
H	2.643231000	2.590047000	-3.547242000

2A-PC-complex

O	4.009434000	-0.974523000	2.531472000
P	3.158109000	-0.633769000	1.250373000
O	2.369028000	0.698922000	1.704233000
O	4.292581000	-0.162321000	0.267245000
O	2.246806000	-1.677940000	0.753283000
C	1.468281000	1.348354000	0.888713000
C	2.021916000	2.222947000	-0.162182000
C	0.993346000	3.033411000	-0.938423000
O	2.712305000	1.394271000	-1.190642000
C	2.085182000	1.546631000	-2.463578000
C	0.709577000	2.152805000	-2.166695000
N	2.076008000	0.300788000	-3.179004000
O	1.593797000	4.259655000	-1.326457000
O	0.281181000	2.892451000	-3.295241000
C	1.406398000	-0.880793000	-2.880892000
C	1.674948000	-1.719516000	-3.929996000
N	2.486082000	-1.093444000	-4.857853000
C	2.717472000	0.098870000	-4.375965000
N	0.602844000	-1.013622000	-1.746264000
H	3.591709000	-1.622925000	3.114905000
H	3.908191000	0.356769000	-0.481238000
H	0.436943000	1.032708000	0.962103000
H	3.225269000	4.536976000	2.555755000
H	2.795018000	2.864229000	0.257102000
H	0.089587000	3.212632000	-0.349339000
H	2.661792000	2.251321000	-3.065434000
H	0.007186000	1.361833000	-1.906472000
H	1.155568000	4.543401000	-2.142326000
H	-0.682439000	2.914310000	-3.313477000
H	1.326029000	-2.731427000	-4.059155000
H	3.334342000	0.861197000	-4.824348000
H	1.137860000	-1.113448000	-0.885147000
H	-0.005630000	-1.816883000	-1.834297000
N	5.760503000	2.666652000	-0.997283000
N	4.922921000	3.413023000	-2.941084000
N	6.846502000	0.516139000	-4.213520000
N	7.035761000	0.756435000	-1.829284000
N	5.591220000	1.939757000	-5.551927000
C	6.065705000	2.584149000	0.428031000
C	7.244078000	3.472799000	0.851418000
C	6.528454000	4.721205000	1.399184000
C	5.269315000	4.123374000	2.024471000
C	4.085854000	5.055262000	2.132007000
C	4.977680000	3.594928000	-1.645573000

C	5.711122000	2.301343000	-3.167317000
C	6.239046000	1.820290000	-1.970266000
C	6.053825000	1.594197000	-4.333271000
C	7.280783000	0.165596000	-2.996884000
O	7.945588000	2.806978000	1.887283000
O	7.281156000	5.402574000	2.388756000
O	4.934224000	3.021550000	1.155648000
H	6.282099000	1.537732000	0.639697000
H	8.271517000	3.492405000	2.489962000
H	7.904100000	3.692106000	0.008304000
H	7.864643000	6.041350000	1.962256000
H	6.261667000	5.390509000	0.576932000
H	5.533434000	3.727853000	3.010996000
H	3.810035000	5.447532000	1.151672000
H	4.339024000	5.891986000	2.784685000
H	5.129231000	2.824297000	-5.677073000
H	5.961641000	1.475834000	-6.364504000
H	4.441578000	4.355249000	-1.104129000
H	7.916860000	-0.712449000	-2.963521000

2B-RC-complex

O	0.441288000	0.722233000	-3.797166000
P	1.213406000	-0.676996000	-3.443601000
O	0.478349000	-1.146489000	-2.069772000
O	0.832473000	-1.681870000	-4.471179000
O	2.647038000	-0.345558000	-3.150642000
C	0.612137000	-0.359600000	-0.889781000
C	0.859098000	-1.271940000	0.293624000
C	0.916924000	-0.521143000	1.624447000
O	2.137952000	-1.939003000	0.137951000
C	2.966103000	-1.664176000	1.251616000
C	2.427507000	-0.360936000	1.848317000
N	4.349686000	-1.633248000	0.852569000
O	0.346563000	-1.330982000	2.650193000
O	2.790715000	-0.282249000	3.216848000
C	4.969572000	-0.793933000	-0.061152000
C	6.303491000	-1.109467000	0.009297000
N	6.516560000	-2.113773000	0.935565000
C	5.335053000	-2.410122000	1.409016000
N	4.271556000	0.177721000	-0.772264000
H	0.954585000	1.479347000	-3.491610000
H	1.434299000	0.352753000	-0.984592000
H	-0.310552000	0.200736000	-0.728935000
H	0.079349000	-2.032699000	0.330670000
H	0.399471000	0.440011000	1.578207000

H	2.884287000	-2.453916000	2.006168000
H	2.806950000	0.487291000	1.278641000
H	0.854272000	-1.156036000	3.457124000
H	2.782844000	0.641512000	3.493332000
H	7.107671000	-0.667906000	-0.557144000
H	5.107602000	-3.167320000	2.142555000
H	3.605572000	-0.187586000	-1.458980000
H	4.913435000	0.792040000	-1.255489000
N	-2.788249000	0.501849000	0.254064000
N	-2.575804000	-1.720913000	0.031951000
N	-3.132456000	-0.836824000	-3.520159000
N	-3.185777000	1.089957000	-2.084627000
N	-2.781888000	-2.998948000	-2.753779000
C	-2.780607000	1.823821000	0.863261000
C	-4.027204000	2.132435000	1.702572000
C	-3.550844000	1.821828000	3.131844000
C	-2.066871000	2.252112000	3.076229000
C	-1.181283000	1.588465000	4.046969000
C	-2.558503000	-0.711824000	0.864683000
C	-2.828918000	-1.150494000	-1.200402000
C	-2.964427000	0.230554000	-1.085260000
C	-2.906855000	-1.682558000	-2.500652000
C	-3.256757000	0.469504000	-3.260392000
O	-4.314283000	3.512529000	1.563713000
O	-4.228566000	2.575416000	4.118460000
O	-1.661119000	1.919170000	1.729664000
H	-2.697377000	2.537341000	0.043529000
H	-4.692634000	3.807139000	2.405859000
H	-4.879012000	1.519064000	1.397161000
H	-5.013967000	2.093943000	4.404398000
H	-3.625429000	0.750563000	3.330748000
H	-2.043610000	3.340481000	3.204218000
H	-0.820589000	0.590327000	3.840187000
H	-1.000085000	2.037366000	5.012017000
H	-2.464366000	-3.616336000	-2.026281000
H	-2.696454000	-3.305029000	-3.708562000
H	-2.338357000	-0.781140000	1.917000000
H	-3.433643000	1.102328000	-4.123489000

2B-PC-complex

O	4.619576000	0.715005000	1.464297000
P	3.888297000	-0.301769000	0.423635000
O	3.084485000	0.761523000	-0.573726000
O	4.938355000	-0.908459000	-0.429577000
O	2.856710000	-1.098768000	1.151218000
C	2.027017000	1.475203000	-0.109075000

C	1.056340000	1.919961000	-1.120572000
C	0.023417000	2.899019000	-0.574160000
O	0.264548000	0.762580000	-1.620059000
C	-1.090150000	0.906509000	-1.244271000
C	-1.117298000	1.969791000	-0.140003000
N	-1.652508000	-0.371278000	-0.874691000
O	-0.403203000	3.752682000	-1.631392000
O	-2.388166000	2.597722000	-0.120356000
C	-1.260547000	-1.231510000	0.138242000
C	-2.147160000	-2.278225000	0.087880000
N	-3.067177000	-2.083486000	-0.925737000
C	-2.737330000	-0.949584000	-1.485687000
N	-0.228856000	-0.928639000	1.021344000
H	4.072699000	0.880230000	2.241897000
H	1.753726000	1.361510000	0.932968000
H	3.708146000	3.993785000	2.722129000
H	1.571696000	2.337009000	-1.985294000
H	0.425196000	3.485602000	0.255394000
H	-1.689167000	1.267725000	-2.086153000
H	-0.880543000	1.510095000	0.820118000
H	-1.289880000	4.066248000	-1.401728000
H	-2.550623000	2.953615000	0.760660000
H	-2.165668000	-3.147848000	0.724886000
H	-3.220379000	-0.484721000	-2.330449000
H	0.686964000	-0.800552000	0.599396000
H	-0.147272000	-1.632564000	1.742100000
N	2.286917000	6.954083000	-0.697649000
N	2.355330000	9.033104000	0.145421000
N	0.683858000	9.762084000	-3.079648000
N	1.190973000	7.425984000	-2.826235000
N	1.206234000	11.369886000	-1.491059000
C	2.482294000	5.509122000	-0.828776000
C	3.750202000	5.152668000	-1.617812000
C	4.768085000	4.902765000	-0.490881000
C	3.897889000	4.285678000	0.600702000
C	4.406358000	4.439827000	2.013133000
C	2.656420000	7.772869000	0.343070000
C	1.756550000	9.051226000	-1.098723000
C	1.704281000	7.767465000	-1.638555000
C	1.209426000	10.083552000	-1.884240000
C	0.704156000	8.482747000	-3.472489000
O	3.504117000	3.961304000	-2.344238000
O	5.788115000	3.987311000	-0.858627000
O	2.623663000	4.956260000	0.463099000
H	1.598916000	5.112533000	-1.329545000
H	4.309596000	3.424970000	-2.289310000

H	4.044532000	5.962735000	-2.289701000
H	6.496315000	4.464307000	-1.307394000
H	5.193055000	5.852407000	-0.154623000
H	3.758635000	3.226951000	0.367225000
H	4.545593000	5.491576000	2.269661000
H	5.363955000	3.925939000	2.109312000
H	1.524317000	11.620939000	-0.571591000
H	0.740262000	12.061886000	-2.052510000
H	3.124379000	7.370943000	1.225315000
H	0.265236000	8.286935000	-4.445411000

2C-RC-complex

O	4.206535000	3.510613000	-1.430905000
P	3.148050000	2.564073000	-1.981226000
O	2.032624000	2.348585000	-0.731862000
O	2.274821000	3.134796000	-3.084431000
O	3.687311000	1.157494000	-2.269002000
C	2.484353000	1.760206000	0.466273000
C	1.415192000	0.830792000	1.013604000
C	1.822375000	0.140487000	2.311192000
O	1.137863000	-0.233415000	0.063937000
C	1.456782000	-1.492650000	0.623496000
C	2.374630000	-1.202982000	1.813186000
N	2.000176000	-2.375633000	-0.380913000
O	0.667499000	-0.061057000	3.124197000
O	2.258869000	-2.252121000	2.764454000
C	3.195910000	-2.287882000	-1.082513000
C	3.241942000	-3.427051000	-1.849223000
N	2.114950000	-4.201351000	-1.643380000
C	1.392888000	-3.541194000	-0.775378000
N	4.101636000	-1.248621000	-0.895446000
H	3.410477000	1.200393000	0.307246000
H	2.683821000	2.531334000	1.223768000
H	0.489330000	1.385821000	1.155052000
H	2.574756000	0.712081000	2.862562000
H	0.553274000	-1.984140000	0.993523000
H	3.401136000	-1.083178000	1.468985000
H	0.827097000	-0.862492000	3.644142000
H	3.069677000	-2.296542000	3.283623000
H	4.025197000	-3.719705000	-2.530423000
H	0.425539000	-3.831083000	-0.397235000
H	3.807032000	-0.338918000	-1.300993000
H	4.990807000	-1.490629000	-1.313934000
N	-2.389057000	0.042285000	0.127229000
N	-1.905454000	-1.939950000	1.060030000
N	-2.866305000	-3.108470000	-2.319552000

N	-3.030905000	-0.720040000	-2.102585000
N	-2.175509000	-4.510232000	-0.600727000
C	-2.625978000	1.478395000	-0.007662000
C	-4.021917000	1.890293000	0.469834000
C	-3.760226000	2.252024000	1.941924000
C	-2.351156000	2.887690000	1.868518000
C	-1.543075000	2.800233000	3.097310000
C	-1.961198000	-0.643738000	1.240502000
C	-2.312717000	-2.125046000	-0.246716000
C	-2.615286000	-0.902988000	-0.845281000
C	-2.457984000	-3.269647000	-1.049458000
C	-3.121964000	-1.872001000	-2.764017000
O	-4.416050000	3.035401000	-0.263185000
O	-4.679884000	3.197110000	2.454165000
O	-1.698124000	2.182417000	0.789215000
H	-2.489828000	1.723585000	-1.060668000
H	-4.963423000	3.574103000	0.327605000
H	-4.744077000	1.077383000	0.354798000
H	-5.438885000	2.732411000	2.826048000
H	-3.739148000	1.348203000	2.553969000
H	-2.495107000	3.934152000	1.573233000
H	-0.903856000	1.944802000	3.269179000
H	-1.669739000	3.542430000	3.871765000
H	-2.036761000	-4.662595000	0.383664000
H	-2.415694000	-5.301548000	-1.174166000
H	-1.650045000	-0.131476000	2.134614000
H	-3.447817000	-1.805325000	-3.796573000

2C-PC-complex

O	2.936813000	-2.016085000	-0.425806000
P	2.880920000	-0.871113000	-1.417751000
O	2.998398000	0.562322000	-0.443185000
O	4.087069000	-0.708246000	-2.316018000
O	1.530859000	-0.696742000	-2.107668000
C	2.100384000	0.770397000	0.533426000
C	1.674454000	2.167302000	0.738965000
C	0.768195000	2.369271000	1.946102000
O	0.864728000	2.652817000	-0.422490000
C	-0.468012000	2.879287000	-0.026262000
C	-0.633876000	2.211867000	1.342928000
N	-1.397517000	2.431425000	-1.042037000
O	0.948968000	3.686060000	2.461301000
O	-1.646947000	2.889410000	2.075151000
C	-1.652231000	1.146518000	-1.501054000
C	-2.664066000	1.290207000	-2.419542000
N	-3.029399000	2.617970000	-2.539947000

C	-2.247623000	3.269527000	-1.717235000
N	-1.003731000	0.023238000	-0.994568000
H	1.445568000	-0.052871000	0.802582000
H	4.845478000	3.075545000	2.122236000
H	2.532569000	2.835032000	0.771701000
H	0.962293000	1.627790000	2.726201000
H	-0.650877000	3.951241000	0.088258000
H	-0.868760000	1.155457000	1.215539000
H	0.102859000	3.952661000	2.849447000
H	-2.012690000	2.288460000	2.734134000
H	-3.138751000	0.507999000	-2.990476000
H	-2.228059000	4.337366000	-1.566444000
H	-0.015566000	-0.071141000	-1.283544000
H	-1.484061000	-0.814196000	-1.298385000
N	2.477436000	5.621641000	-1.097242000
N	0.453325000	6.119378000	-0.266264000
N	-0.252179000	6.650077000	-3.861758000
N	2.022920000	5.978646000	-3.471414000
N	-1.820951000	6.915302000	-2.168428000
C	3.894160000	5.275717000	-1.149206000
C	4.814919000	6.462708000	-0.832235000
C	5.106193000	6.252065000	0.664291000
C	5.141855000	4.728377000	0.775079000
C	4.810239000	4.165290000	2.137455000
C	1.672920000	5.733407000	0.013610000
C	0.442703000	6.261237000	-1.639942000
C	1.692097000	5.953041000	-2.176271000
C	-0.560546000	6.624912000	-2.554061000
C	0.992739000	6.331709000	-4.237242000
O	6.001257000	6.316785000	-1.593778000
O	6.353400000	6.793314000	1.068076000
O	4.163526000	4.277491000	-0.185185000
H	4.087440000	4.906226000	-2.156494000
H	6.726571000	6.655620000	-1.047924000
H	4.326792000	7.417290000	-1.044943000
H	6.233961000	7.718493000	1.313081000
H	4.289130000	6.658753000	1.266005000
H	6.132515000	4.388799000	0.454302000
H	3.813284000	4.474442000	2.455350000
H	5.540385000	4.522492000	2.865490000
H	-2.018763000	7.063475000	-1.193474000
H	-2.461789000	7.294247000	-2.845516000
H	2.022293000	5.463598000	0.995268000
H	1.182397000	6.369787000	-5.304682000

3-RC-complex

N	0.726871000	-1.994846000	1.255077000
N	2.108724000	-1.749508000	3.005419000
N	4.615412000	-1.776430000	0.276662000
N	2.370603000	-2.011296000	-0.548046000
N	5.146383000	-1.597798000	2.526048000
C	-0.494556000	-2.180640000	0.483425000
C	-0.868582000	-3.654509000	0.243594000
C	-2.012515000	-3.876480000	1.250810000
C	-2.681112000	-2.484428000	1.278999000
C	-3.481143000	-2.179436000	2.475029000
C	0.862731000	-1.876116000	2.619636000
C	2.840478000	-1.793095000	1.833669000
C	1.998111000	-1.942355000	0.733852000
C	4.219237000	-1.714959000	1.559543000
C	3.691606000	-1.912079000	-0.680727000
O	-1.344308000	-3.775459000	-1.085009000
O	-2.941700000	-4.853793000	0.823713000
O	-1.557821000	-1.585718000	1.197958000
H	-0.338251000	-1.688444000	-0.478250000
H	-2.029110000	-4.461333000	-1.075841000
H	-0.017422000	-4.317668000	0.418533000
H	-2.673913000	-5.717889000	1.158125000
H	-1.607421000	-4.110842000	2.237542000
H	-3.291476000	-2.396362000	0.371650000
H	-2.987450000	-1.858846000	3.381843000
H	-4.541677000	-2.379757000	2.485069000
H	4.869828000	-1.471608000	3.483702000
H	6.109460000	-1.452858000	2.275380000
H	0.000672000	-1.869423000	3.264461000
H	4.073137000	-1.948091000	-1.695460000
H	-4.408879000	1.408822000	-1.457094000
H	5.033295000	1.531787000	1.247511000
H	1.570162000	2.621503000	1.770661000
H	1.575230000	0.895674000	1.996886000
H	0.765607000	0.570771000	-0.350450000
H	0.737696000	2.299651000	-0.589051000
H	-0.965005000	2.559699000	1.202846000
H	-0.862219000	0.848847000	1.576846000
H	-1.667057000	0.300008000	-0.729554000
H	-1.876024000	2.010178000	-1.056261000
H	-3.554633000	2.171124000	0.770931000
H	-3.248211000	0.501243000	1.217670000
O	3.363154000	1.601969000	-0.507555000
C	-5.736578000	0.601337000	0.042146000
C	-4.359024000	0.720003000	-0.606806000
C	3.110823000	1.618473000	0.697877000

C	1.692814000	1.672810000	1.236288000
C	0.617635000	1.521719000	0.168557000
C	-0.789911000	1.572467000	0.760069000
C	-1.887026000	1.261721000	-0.255448000
C	-3.279605000	1.189722000	0.366789000
H	-4.065802000	-0.252139000	-1.018417000
H	-6.489773000	0.260495000	-0.671533000
H	-5.714321000	-0.111007000	0.871282000
H	-6.066243000	1.564012000	0.441917000
N	4.099006000	1.596898000	1.620735000
C	3.935952000	1.603465000	3.065523000
H	3.406101000	2.495317000	3.404581000
H	3.394100000	0.722556000	3.415271000
H	4.923452000	1.599615000	3.520226000

3-PC-complex

N	0.882392000	-2.104591000	1.164254000
N	2.172440000	-1.752872000	2.966171000
N	4.810315000	-1.843491000	0.366218000
N	2.614586000	-2.171703000	-0.554163000
N	5.221125000	-1.521409000	2.623937000
C	-0.301690000	-2.343305000	0.351476000
C	-0.742428000	-3.818979000	0.296184000
C	-1.954023000	-3.836543000	1.248763000
C	-2.535123000	-2.438081000	1.052993000
C	-3.386880000	-1.909149000	2.180707000
C	0.949701000	-1.922338000	2.526806000
C	2.960977000	-1.831976000	1.833862000
C	2.176633000	-2.049879000	0.702974000
C	4.349049000	-1.729933000	1.623551000
C	3.937866000	-2.048484000	-0.627078000
O	-1.148821000	-4.110078000	-1.030340000
O	-2.915040000	-4.819914000	0.901628000
O	-1.370035000	-1.607521000	0.911841000
H	-0.063538000	-1.997820000	-0.656316000
H	-1.891636000	-4.729386000	-0.963996000
H	0.061091000	-4.488421000	0.613680000
H	-2.697503000	-5.648917000	1.344211000
H	-1.616879000	-3.959567000	2.281184000
H	-3.100786000	-2.430557000	0.113708000
H	-2.831929000	-1.919588000	3.120387000
H	-4.277224000	-2.529660000	2.289947000
H	4.903882000	-1.445255000	3.574293000
H	6.204789000	-1.456557000	2.427488000
H	0.058147000	-1.900918000	3.130077000
H	4.370754000	-2.127408000	-1.618694000

H	-4.644904000	1.142950000	-1.491152000
H	4.918514000	1.441523000	1.284707000
H	1.465149000	2.565687000	1.745267000
H	1.441664000	0.844338000	2.004061000
H	0.629392000	0.478604000	-0.328705000
H	0.679888000	2.197632000	-0.632112000
H	-1.030586000	2.590020000	1.136814000
H	-1.030893000	0.877294000	1.532288000
H	-1.828700000	0.334239000	-0.767634000
H	-1.845371000	2.038427000	-1.169677000
H	-3.585200000	2.163262000	0.960040000
H	-3.699499000	-0.886589000	1.968767000
O	3.268053000	1.436483000	-0.489216000
C	-5.829456000	0.830187000	0.284558000
C	-4.506505000	0.734898000	-0.475195000
C	3.003386000	1.518390000	0.710698000
C	1.579372000	1.605325000	1.230304000
C	0.515669000	1.454350000	0.151617000
C	-0.898041000	1.587954000	0.713261000
C	-1.982803000	1.328718000	-0.334648000
C	-3.370061000	1.424106000	0.193738000
H	-4.246223000	-0.319771000	-0.638966000
H	-6.631322000	0.316547000	-0.249296000
H	-5.743576000	0.380357000	1.276306000
H	-6.127773000	1.872740000	0.417402000
N	3.982023000	1.547007000	1.643689000
C	3.803776000	1.600130000	3.085589000
H	3.250161000	2.491549000	3.385927000
H	3.279220000	0.719335000	3.460884000
H	4.786323000	1.636959000	3.549138000

4-RC-complex

C	2.067873000	1.911480000	-1.638593000
C	0.619802000	1.730555000	-1.254563000
O	-0.305618000	2.054231000	-1.998807000
N	0.390872000	1.215774000	-0.026670000
C	-0.946488000	1.041692000	0.504752000
C	-1.864543000	0.112743000	-0.296686000
O	-3.019991000	0.458320000	-0.538065000
H	2.731383000	1.219255000	-1.121205000
H	-1.464672000	1.997204000	0.559068000
H	-0.855003000	0.649888000	1.518427000
N	-1.387774000	-1.087495000	-0.680907000
H	-2.041301000	-1.637619000	-1.218158000
H	1.175569000	0.954783000	0.545624000
H	2.358446000	2.931443000	-1.381458000

H	2.170266000	1.785614000	-2.714103000
C	-0.105566000	-1.700970000	-0.364203000
H	0.681649000	-1.386777000	-1.051230000
H	0.201361000	-1.463699000	0.653098000
H	-0.219624000	-2.780883000	-0.433897000
N	1.882828000	5.655731000	-2.926618000
N	1.240352000	4.575375000	-4.784330000
N	3.899941000	6.709565000	-6.235371000
N	3.636410000	7.064429000	-3.872649000
N	2.620199000	5.211784000	-7.459824000
C	1.952239000	6.087518000	-1.528751000
C	1.270023000	7.440373000	-1.306097000
C	-0.147086000	7.013329000	-0.891180000
C	0.135576000	5.737562000	-0.065426000
C	-0.971212000	4.771506000	0.009954000
C	1.046458000	4.721759000	-3.495874000
C	2.256977000	5.460298000	-5.085567000
C	2.671996000	6.139351000	-3.942328000
C	2.924450000	5.784241000	-6.282009000
C	4.193553000	7.282020000	-5.062109000
O	1.929756000	8.093860000	-0.237324000
O	-0.799931000	7.968967000	-0.077694000
O	1.281698000	5.143791000	-0.722962000
H	3.006887000	6.142335000	-1.256210000
H	1.261843000	8.620877000	0.226173000
H	1.281831000	8.051906000	-2.211754000
H	-1.272135000	8.595358000	-0.638932000
H	-0.739937000	6.767523000	-1.774903000
H	0.433452000	6.067846000	0.936664000
H	-1.101528000	4.039206000	-0.773946000
H	-1.717115000	4.871586000	0.784524000
H	1.919602000	4.493658000	-7.513178000
H	3.145696000	5.448634000	-8.283610000
H	0.347589000	4.155421000	-2.902814000
H	4.989205000	8.019158000	-5.089066000

4-PC-complex

C	2.273429000	1.979657000	-2.905566000
C	1.042047000	1.839044000	-2.047675000
O	-0.075515000	1.672473000	-2.508267000
N	1.275754000	1.875264000	-0.686396000
C	0.340193000	1.770056000	0.312392000
C	-0.905787000	1.008967000	0.292594000
O	-1.891105000	1.484573000	0.885800000
H	2.689486000	0.985927000	-3.087877000
H	-1.999733000	3.894698000	0.175985000

H	0.516477000	2.371025000	1.191518000
N	-0.969748000	-0.207376000	-0.296729000
H	-1.889864000	-0.620094000	-0.282658000
H	2.178061000	2.230661000	-0.404743000
H	3.047843000	2.588890000	-2.439946000
H	1.989931000	2.414062000	-3.860815000
C	0.114833000	-1.004434000	-0.843182000
H	0.255840000	-0.825763000	-1.910464000
H	1.045904000	-0.786640000	-0.323694000
H	-0.117427000	-2.057519000	-0.692710000
N	1.433518000	5.358565000	-2.711948000
N	0.836249000	4.814691000	-4.805531000
N	4.431691000	5.499416000	-5.381442000
N	3.800556000	5.823984000	-3.084747000
N	2.947129000	4.847962000	-7.040404000
C	1.333179000	5.645340000	-1.282362000
C	0.927847000	7.095854000	-0.983642000
C	-0.590106000	6.964069000	-0.764635000
C	-0.704872000	5.590154000	-0.105480000
C	-2.028267000	4.884574000	-0.280517000
C	0.432206000	4.961604000	-3.568423000
C	2.179525000	5.136019000	-4.769733000
C	2.569991000	5.476294000	-3.476533000
C	3.185978000	5.154785000	-5.753991000
C	4.662165000	5.806180000	-4.099680000
O	1.570880000	7.494368000	0.214832000
O	-1.113639000	7.959603000	0.099277000
O	0.339864000	4.812054000	-0.726711000
H	2.312087000	5.431551000	-0.851363000
H	0.956018000	8.081985000	0.679599000
H	1.186755000	7.764143000	-1.808864000
H	-1.349971000	8.738031000	-0.418889000
H	-1.108055000	6.967850000	-1.727610000
H	-0.472949000	5.703407000	0.959167000
H	-2.270072000	4.775542000	-1.339608000
H	-2.816713000	5.469066000	0.197046000
H	2.034837000	4.544619000	-7.332420000
H	3.705220000	4.830529000	-7.700760000
H	-0.563121000	4.766503000	-3.208117000
H	5.686044000	6.074177000	-3.861189000

5-RC-complex

N	0.515608	1.215290	0.574767
N	1.956065	1.094464	-1.139056
N	3.659346	-1.201118	1.218018
N	1.632545	-0.292042	2.136652

N	4.458471	-0.676358	-0.896431
C	-0.610124	1.625153	1.413244
C	-0.257080	2.804472	2.344859
C	-0.697269	3.987345	1.476539
C	-1.995290	3.446642	0.841458
C	-2.416717	4.099304	-0.407836
C	0.841475	1.629986	-0.699205
C	2.393343	0.291956	-0.104694
C	1.511236	0.354680	0.971219
C	3.519126	-0.536944	0.056473
C	2.730061	-1.045068	2.168249
O	-1.046653	2.779865	3.519235
O	-0.953148	5.201116	2.142910
O	-1.676566	2.050504	0.593912
H	-0.901467	0.751828	1.999032
H	-0.718164	2.082214	4.098484
H	0.810284	2.823917	2.577278
H	-0.125266	5.547918	2.496616
H	0.049837	4.118191	0.686681
H	-2.780861	3.505301	1.602353
H	-1.890565	3.881884	-1.328446
H	-3.138663	4.901976	-0.375437
H	4.341357	-0.239419	-1.793636
H	5.214537	-1.325571	-0.762739
H	0.228847	2.317272	-1.267568
H	2.898287	-1.606032	3.081608
C	3.343091	4.195537	-2.770501
N	2.513220	5.085547	-3.113999
C	1.276917	5.198833	-2.349608
C	0.106303	4.701075	-3.264949
O	-0.315992	5.487849	-4.138725
C	1.083699	6.641886	-1.884479
C	-0.181022	6.805072	-1.047030
C	-0.332551	8.195885	-0.434731
C	-1.593139	8.262821	0.409163
N	-1.719425	9.604183	1.088354
O	-0.298776	3.532620	-3.035405
H	3.183439	3.512664	-1.929106
H	1.305598	4.539351	-1.472256
H	1.044337	7.292870	-2.759938
H	-1.054805	6.580425	-1.663649
H	-0.179591	6.073867	-0.237266
H	-0.370261	8.954843	-1.221898
H	0.537860	8.419185	0.190063
H	-2.491086	8.136942	-0.192587
H	-1.589004	7.510415	1.196407

H	-2.577171	9.669186	1.638437
H	-0.935246	9.774717	1.720228
H	-1.733880	10.364765	0.406766
H	1.957252	6.936954	-1.293548
H	4.266587	4.081363	-3.336100

5-PC-complex

N	0.600815	1.105249	0.576943
N	2.025205	0.924724	-1.145399
N	3.643850	-1.443966	1.198805
N	1.664939	-0.448501	2.131953
N	4.449984	-0.952585	-0.921023
C	-0.497343	1.570099	1.419039
C	-0.143088	2.835475	2.235097
C	-0.722931	3.930998	1.331284
C	-1.997325	3.274089	0.809523
C	-2.544970	3.840306	-0.477883
C	0.937340	1.506552	-0.698258
C	2.434546	0.104195	-0.113517
C	1.562639	0.204023	0.968100
C	3.523787	-0.773730	0.038716
C	2.729073	-1.247947	2.155756
O	-0.831219	2.851557	3.473307
O	-1.023499	5.162712	1.947685
O	-1.603905	1.896989	0.604472
H	-0.739800	0.746743	2.092938
H	-0.405663	2.225288	4.070647
H	0.936038	2.926948	2.377022
H	-0.204772	5.576289	2.245913
H	-0.031727	4.071410	0.492465
H	-2.752637	3.312989	1.601685
H	-1.804468	3.770168	-1.275459
H	-3.444025	3.301872	-0.780715
H	4.335885	-0.522880	-1.822177
H	5.168328	-1.645419	-0.798058
H	0.350968	2.219123	-1.262665
H	2.879398	-1.815991	3.067873
C	3.218994	4.286977	-2.383964
N	2.443955	5.188179	-2.814078
C	1.137602	5.325728	-2.183777
C	0.080011	4.673429	-3.195500
O	-0.428832	5.425281	-4.048970
C	0.835499	6.741632	-1.878342
C	-0.367278	7.079733	-1.069722
C	-0.376662	8.493077	-0.474938

C	-0.479434	9.567471	-1.543237
N	-0.534572	10.937663	-0.913913
O	-0.118735	3.449489	-3.023648
H	2.970126	3.620177	-1.552118
H	1.073854	4.719588	-1.268620
H	1.297127	7.496269	-2.503664
H	-1.275603	6.947437	-1.680428
H	-0.475142	6.368889	-0.246396
H	0.530330	8.648544	0.115894
H	-1.228023	8.585136	0.204611
H	0.378171	9.575590	-2.210998
H	-1.385853	9.462405	-2.136435
H	-0.581058	11.673877	-1.619970
H	-1.352835	11.037881	-0.310373
H	0.292434	11.114869	-0.340782
H	-2.809263	4.888513	-0.328734
H	4.188073	4.146659	-2.859889

6A-RC-complex

C	1.769164000	-2.210008000	-0.923093000
N	0.812070000	-1.500178000	-0.507371000
C	0.990439000	-0.058079000	-0.520938000
C	0.767118000	0.576539000	0.843960000
O	0.176667000	-0.219465000	1.745846000
C	0.036311000	0.601230000	-1.543176000
C	-1.446176000	0.393503000	-1.260793000
O	1.082828000	1.719017000	1.083439000
H	2.725305000	-1.796850000	-1.265490000
H	2.015883000	0.222363000	-0.798077000
H	0.290875000	0.199186000	-2.525103000
H	-1.680805000	-0.669218000	-1.192329000
H	-1.713751000	0.821116000	-0.288225000
H	0.268950000	1.665154000	-1.570094000
H	1.658207000	-3.291778000	-0.952027000
C	-2.401119000	1.028176000	-2.294529000
O	-1.908907000	1.828371000	-3.136805000
O	-3.609480000	0.711240000	-2.195388000
N	1.091003000	4.134445000	-4.180500000
N	1.790450000	2.118323000	-4.874122000
N	4.654158000	4.157958000	-6.047474000
N	2.983942000	5.484609000	-4.939987000
N	4.487322000	1.859698000	-6.324627000
C	0.296262000	5.142858000	-3.526593000
C	-1.210282000	5.073041000	-3.815066000
C	-1.760478000	5.872257000	-2.634296000

C	-0.840622000	5.409691000	-1.472051000
C	-1.384342000	4.289507000	-0.677155000
C	0.837747000	2.778985000	-4.264386000
C	2.727189000	3.079510000	-5.208465000
C	2.314084000	4.338537000	-4.781173000
C	3.964641000	3.016099000	-5.873928000
C	4.136376000	5.299726000	-5.579916000
O	-1.576469000	5.559417000	-5.084510000
O	-1.566752000	7.248693000	-2.955352000
O	0.406184000	5.002832000	-2.116220000
H	0.695812000	6.105762000	-3.855734000
H	-1.567056000	6.526240000	-5.033960000
H	-1.552801000	4.040797000	-3.735504000
H	-2.132187000	7.790934000	-2.395004000
H	-2.811209000	5.661424000	-2.436057000
H	-0.626950000	6.275642000	-0.840827000
H	-1.427798000	3.305363000	-1.120423000
H	-1.855553000	4.473229000	0.277709000
H	3.945938000	1.013723000	-6.290862000
H	5.328665000	1.876756000	-6.875114000
H	-0.067205000	2.348973000	-3.850017000
H	4.737301000	6.187512000	-5.747369000
H	0.065850000	0.290070000	2.566339000

6A-PC-complex

C	2.796374000	-0.053775000	-2.355669000
N	1.725417000	-0.260038000	-1.720700000
C	1.143956000	0.882109000	-1.019644000
C	0.925890000	0.574218000	0.463434000
O	0.445511000	-0.658773000	0.689827000
C	-0.189808000	1.273834000	-1.582189000
C	-1.188400000	0.299047000	-2.076044000
O	1.105194000	1.385139000	1.343091000
H	3.303134000	0.916518000	-2.391699000
H	1.804308000	1.757265000	-1.036187000
H	-0.417740000	2.326427000	-1.589448000
H	-0.816292000	-0.189533000	-2.990602000
H	-1.334752000	-0.518737000	-1.363376000
H	-1.095622000	4.029625000	0.267740000
H	3.252653000	-0.870493000	-2.910768000
C	-2.558168000	0.919168000	-2.444806000
O	-2.545746000	2.068343000	-2.963284000
O	-3.569250000	0.211425000	-2.228887000
N	0.863480000	3.724898000	-3.965540000
N	1.142418000	1.706778000	-4.910570000
N	4.650530000	2.891096000	-5.036706000

N	3.174924000	4.516590000	-4.057939000
N	3.938118000	0.825726000	-5.822762000
C	0.241973000	4.857304000	-3.327157000
C	-1.226062000	5.094899000	-3.705661000
C	-1.663570000	6.005910000	-2.556971000
C	-0.899130000	5.425335000	-1.355706000
C	-1.729171000	4.505917000	-0.481316000
C	0.286940000	2.533714000	-4.365267000
C	2.354087000	2.370462000	-4.858068000
C	2.203322000	3.624237000	-4.272075000
C	3.656072000	2.010176000	-5.246777000
C	4.358568000	4.068247000	-4.471459000
O	-1.416686000	5.628691000	-4.994300000
O	-1.223946000	7.321629000	-2.903746000
O	0.216903000	4.676561000	-1.917904000
H	0.845355000	5.730119000	-3.593956000
H	-1.242171000	6.579386000	-4.935566000
H	-1.772666000	4.154846000	-3.637126000
H	-1.673242000	7.965402000	-2.345678000
H	-2.743443000	5.989595000	-2.403107000
H	-0.485788000	6.249181000	-0.768270000
H	-2.203356000	3.728206000	-1.082634000
H	-2.500029000	5.081355000	0.034890000
H	3.226990000	0.119464000	-5.897418000
H	4.896512000	0.569150000	-5.986970000
H	-0.760520000	2.334323000	-4.187791000
H	5.199402000	4.739158000	-4.329880000
H	0.269923000	-0.743837000	1.641808000

6B-RC-complex

C	2.166993000	-1.716711000	-0.020953000
N	1.344340000	-0.767208000	0.104660000
C	1.500689000	0.391022000	-0.760905000
C	1.788033000	1.697799000	0.051108000
O	1.163380000	1.880502000	1.121989000
C	0.241720000	0.577107000	-1.628233000
C	-1.051005000	0.682666000	-0.826811000
O	2.608301000	2.479295000	-0.488659000
H	2.990028000	-1.710296000	-0.747085000
H	2.351184000	0.255819000	-1.441078000
H	0.170386000	-0.262114000	-2.325304000
H	-1.299165000	-0.269048000	-0.350458000
H	-0.943720000	1.395542000	-0.008599000
H	0.374505000	1.477202000	-2.229952000
H	2.075850000	-2.596873000	0.613468000
C	-2.234596000	1.093309000	-1.652862000

O	-2.262905000	1.224393000	-2.856046000
O	-3.324341000	1.314056000	-0.885938000
H	-4.059209000	1.566458000	-1.468502000
N	-0.731693000	4.634423000	-5.127530000
N	-2.884907000	4.200357000	-5.589776000
N	-2.065112000	6.283538000	-8.541127000
N	-0.178541000	5.996872000	-7.079216000
N	-4.161934000	5.382077000	-8.122670000
C	0.573943000	4.582640000	-4.449138000
C	1.014990000	5.962478000	-3.961031000
C	0.401967000	5.999950000	-2.552744000
C	0.544736000	4.543915000	-2.077650000
C	-0.484503000	4.099171000	-1.121270000
C	-1.895478000	4.003305000	-4.751803000
C	-2.344808000	4.996663000	-6.579634000
C	-1.003826000	5.269991000	-6.315485000
C	-2.876791000	5.549465000	-7.759689000
C	-0.792489000	6.459287000	-8.165721000
O	2.430390000	5.970226000	-3.894523000
O	1.105222000	6.855847000	-1.667476000
O	0.471492000	3.758927000	-3.317371000
H	1.299254000	4.165057000	-5.149207000
H	2.671251000	6.521953000	-3.135376000
H	0.647474000	6.762739000	-4.606544000
H	0.762904000	7.753233000	-1.756763000
H	-0.652827000	6.278540000	-2.617263000
H	1.539397000	4.393772000	-1.657224000
H	-1.529597000	4.141612000	-1.399618000
H	-0.204195000	3.694337000	-0.160598000
H	-4.758503000	4.764262000	-7.600759000
H	-4.474017000	5.719786000	-9.017064000
H	-1.936693000	3.395304000	-3.863880000
H	-0.186456000	7.057199000	-8.838364000

6B-PC-complex

C	1.520811000	-1.867144000	-2.036314000
N	0.947090000	-0.995613000	-1.324614000
C	1.048904000	0.397965000	-1.743359000
C	1.958877000	1.178394000	-0.679289000
O	1.556298000	1.184631000	0.503009000
C	-0.278312000	1.054916000	-1.831103000
C	-1.295384000	0.847317000	-0.770922000
O	2.975678000	1.726471000	-1.155660000
H	2.070628000	-1.630484000	-2.955504000
H	1.569145000	0.488974000	-2.704032000
H	-0.345614000	1.942165000	-2.444133000

H	-1.536125000	-0.210214000	-0.631603000
H	-0.882628000	1.157103000	0.203432000
H	0.506476000	3.506548000	-0.266568000
H	1.479784000	-2.913997000	-1.740326000
C	-2.576625000	1.608837000	-0.960701000
O	-2.777911000	2.494708000	-1.760296000
O	-3.523264000	1.204779000	-0.089049000
H	-4.317460000	1.745869000	-0.229063000
N	-0.453780000	4.629436000	-4.847139000
N	-2.461831000	3.802947000	-5.401535000
N	-1.370894000	4.972210000	-8.739397000
N	0.275867000	5.397332000	-7.044501000
N	-3.373731000	3.860250000	-8.337680000
C	0.694658000	5.043377000	-4.043650000
C	0.625770000	6.518042000	-3.617778000
C	0.080810000	6.409647000	-2.183203000
C	0.716032000	5.109840000	-1.693856000
C	-0.007360000	4.420748000	-0.562211000
C	-1.609292000	4.015056000	-4.427470000
C	-1.840282000	4.308389000	-6.524030000
C	-0.589697000	4.824788000	-6.199416000
C	-2.221443000	4.397440000	-7.876488000
C	-0.194280000	5.427174000	-8.289700000
O	1.943522000	7.040559000	-3.612262000
O	0.485201000	7.487606000	-1.354294000
O	0.720889000	4.265464000	-2.866209000
H	1.586883000	4.872398000	-4.648269000
H	1.989549000	7.671900000	-2.878350000
H	-0.021628000	7.096883000	-4.281285000
H	-0.150061000	8.208472000	-1.437156000
H	-1.008068000	6.312445000	-2.203053000
H	1.752490000	5.322806000	-1.409762000
H	-1.027378000	4.170306000	-0.855057000
H	-0.039916000	5.091819000	0.298228000
H	-4.197130000	3.829516000	-7.634787000
H	-3.779794000	4.338124000	-9.228752000
H	-1.757907000	3.721279000	-3.400897000
H	0.447322000	5.879919000	-9.037154000

6C-RC-complex

C	2.032204000	-1.869296000	-1.018833000
N	1.402914000	-0.916143000	-0.480860000
C	1.430295000	0.371631000	-1.158484000
C	1.972489000	1.470425000	-0.251090000
O	1.587255000	1.360123000	1.028928000
C	0.022010000	0.746921000	-1.670137000

C	-1.060410000	0.746480000	-0.596904000
O	2.658599000	2.377737000	-0.656265000
H	2.605193000	-1.769587000	-1.947601000
H	2.101133000	0.366109000	-2.025275000
H	-0.235154000	0.025208000	-2.447907000
H	-1.179113000	-0.238430000	-0.145497000
H	-0.805133000	1.421043000	0.224659000
H	0.080373000	1.724250000	-2.147618000
H	2.014401000	-2.850180000	-0.549275000
C	-2.396054000	1.202353000	-1.116202000
O	-2.597714000	1.750200000	-2.176079000
O	-3.381824000	0.955769000	-0.233281000
H	-4.214141000	1.299218000	-0.598016000
N	-0.506756000	4.620655000	-4.843961000
N	-2.586175000	4.012852000	-5.427844000
N	-1.645136000	5.887671000	-8.481785000
N	0.125758000	5.849145000	-6.856917000
N	-3.713160000	4.888872000	-8.151956000
C	0.737656000	4.729420000	-4.072809000
C	1.005711000	6.163883000	-3.613220000
C	0.338555000	6.176710000	-2.228729000
C	0.633242000	4.752170000	-1.711873000
C	-0.334132000	4.230513000	-0.732661000
C	-1.660514000	3.952684000	-4.500602000
C	-2.012967000	4.753949000	-6.441926000
C	-0.716822000	5.135044000	-6.100737000
C	-2.475521000	5.169743000	-7.704708000
C	-0.421253000	6.178171000	-8.025013000
O	2.407423000	6.330214000	-3.496985000
O	0.906146000	7.127881000	-1.347630000
O	0.625941000	3.937197000	-2.915077000
H	1.552972000	4.366223000	-4.700312000
H	2.557369000	6.951717000	-2.769106000
H	0.576250000	6.897981000	-4.298452000
H	0.455039000	7.973058000	-1.459788000
H	-0.738436000	6.324073000	-2.336436000
H	1.644450000	4.744786000	-1.297152000
H	-1.313698000	3.916516000	-1.064891000
H	-0.112359000	4.254736000	0.323437000
H	-4.316464000	4.281624000	-7.625408000
H	-3.969484000	5.133503000	-9.093156000
H	-1.746074000	3.425194000	-3.565555000
H	0.202333000	6.757214000	-8.698080000
H	1.947528000	2.117783000	1.519916000

6C-PC-complex

C	-0.303303	1.219100	-3.304977
N	-1.297763	1.065802	-2.540936
C	-1.281870	1.814368	-1.285324
C	-1.286431	0.851905	-0.089266
O	-2.198552	-0.125584	-0.206933
C	-2.477401	2.701317	-1.142650
C	-3.799534	2.335143	-1.703498
O	-0.584688	0.994212	0.883029
H	0.540103	1.876952	-3.076545
H	-0.376907	2.417825	-1.171903
H	-2.404701	3.532729	-0.456945
H	-3.735866	2.087833	-2.764398
H	-4.187001	1.418590	-1.229860
H	1.428518	3.631782	0.273517
H	-0.277678	0.683360	-4.250461
C	-4.853820	3.391172	-1.491353
O	-4.857741	4.221769	-0.617090
O	-5.860566	3.271221	-2.384289
H	-6.533265	3.940786	-2.176989
N	-0.916179	4.995928	-3.708083
N	-3.155466	4.919477	-3.552935
N	-2.690887	2.545263	-6.356444
N	-0.607756	3.459886	-5.582842
N	-4.749804	3.064145	-5.409972
C	0.467067	5.231550	-3.344900
C	0.791354	6.686588	-2.972926
C	0.861369	6.635295	-1.434438
C	1.392605	5.226988	-1.174650
C	1.041862	4.646166	0.174931
C	-2.055269	5.418461	-3.055839
C	-2.730357	4.100830	-4.582161
C	-1.343461	4.137224	-4.698091
C	-3.412431	3.229693	-5.451135
C	-1.362896	2.701889	-6.376059
O	2.063048	7.001345	-3.514978
O	1.748591	7.598354	-0.890867
O	0.793682	4.428943	-2.211698
H	1.062608	4.925737	-4.204296
H	2.494334	7.596596	-2.882825
H	0.032201	7.379878	-3.343286
H	1.269009	8.419976	-0.731528
H	-0.138846	6.741412	-1.006741
H	2.479833	5.242971	-1.312933
H	-0.040684	4.623832	0.310672
H	1.482743	5.259887	0.961958
H	-5.258425	3.380736	-4.598663

H	-5.150986	2.313045	-5.947432
H	-2.009195	6.094879	-2.218160
H	-0.835218	2.126049	-7.128781
H	-2.183312	-0.658281	0.605694

6D-RC-complex

C	1.932595000	-0.937912000	0.907125000
N	0.742569000	-0.545638000	0.763801000
C	0.518709000	0.786353000	0.219582000
C	-0.138217000	1.750945000	1.257201000
O	-0.595692000	1.279172000	2.320774000
C	-0.334576000	0.688367000	-1.059215000
C	-1.762103000	0.203020000	-0.839358000
O	-0.141465000	2.960932000	0.907690000
H	2.806039000	-0.322541000	0.652708000
H	1.477590000	1.252207000	-0.053588000
H	0.176264000	0.023065000	-1.761256000
H	-1.765011000	-0.758735000	-0.323002000
H	-2.293802000	0.900202000	-0.185513000
H	-0.355636000	1.673636000	-1.522900000
H	2.131698000	-1.933210000	1.302439000
C	-2.628265000	0.062832000	-2.106989000
O	-2.195560000	0.542976000	-3.187412000
O	-3.737977000	-0.514070000	-1.950164000
N	-4.292249000	4.240892000	1.237025000
N	-3.132427000	4.506248000	3.138842000
N	-6.552353000	4.975452000	4.481291000
N	-6.555765000	4.541924000	2.116621000
N	-4.616758000	5.120545000	5.755062000
C	-4.567732000	4.037910000	-0.177005000
C	-4.468361000	5.321920000	-1.033482000
C	-4.053637000	4.745377000	-2.387485000
C	-3.073339000	3.646273000	-1.953913000
C	-1.685913000	4.133156000	-1.771108000
C	-3.058936000	4.263714000	1.851707000
C	-4.482109000	4.652983000	3.389496000
C	-5.222620000	4.485049000	2.220176000
C	-5.211862000	4.913816000	4.563512000
C	-7.133155000	4.786874000	3.289720000
O	-5.637256000	6.102399000	-1.048209000
O	-5.243868000	4.223155000	-2.973725000
O	-3.624544000	3.135985000	-0.705007000
H	-5.582262000	3.635257000	-0.238887000
H	-6.260083000	5.674804000	-1.653630000
H	-3.661827000	5.944799000	-0.644499000

H	-5.075639000	4.000315000	-3.895830000
H	-3.585940000	5.487065000	-3.036672000
H	-3.100376000	2.808725000	-2.662521000
H	-1.109837000	3.820475000	-0.910320000
H	-1.200754000	4.643661000	-2.593086000
H	-3.629995000	4.958808000	5.856607000
H	-5.182785000	5.185080000	6.584052000
H	-2.148479000	4.037352000	1.313713000
H	-8.217019000	4.842384000	3.286008000

6D-PC-complex

C	1.875071000	-0.911748000	1.028759000
N	0.679072000	-0.586483000	0.789885000
C	0.437227000	0.732579000	0.207686000
C	-0.362231000	1.655860000	1.224118000
O	-1.227411000	1.113703000	1.942083000
C	-0.343744000	0.632482000	-1.057984000
C	-1.594798000	-0.158679000	-1.162273000
O	-0.063442000	2.873288000	1.165687000
H	2.733239000	-0.260134000	0.818675000
H	1.383201000	1.252900000	0.011500000
H	-0.108181000	1.321845000	-1.855833000
H	-1.384179000	-1.237903000	-1.118452000
H	-2.228320000	0.020043000	-0.284855000
H	-1.032687000	3.459310000	-1.089826000
H	2.092320000	-1.885300000	1.466235000
C	-2.449602000	0.063692000	-2.432184000
O	-1.923417000	0.639274000	-3.417888000
O	-3.627668000	-0.376489000	-2.373659000
N	-4.282380000	4.261385000	1.288122000
N	-3.096604000	4.664162000	3.149806000
N	-6.501213000	5.168332000	4.516876000
N	-6.535817000	4.585847000	2.184642000
N	-4.547638000	5.426074000	5.745215000
C	-4.573530000	3.965608000	-0.109831000
C	-4.564004000	5.210450000	-1.031982000
C	-4.056738000	4.611702000	-2.346827000
C	-3.035790000	3.588998000	-1.859761000
C	-1.645780000	4.165068000	-1.647576000
C	-3.040479000	4.338911000	1.880143000
C	-4.444025000	4.809303000	3.412405000
C	-5.200183000	4.555698000	2.268476000
C	-5.158861000	5.133016000	4.579650000
C	-7.098125000	4.895639000	3.349671000
O	-5.799265000	5.876127000	-1.124079000
O	-5.195411000	4.003101000	-2.957816000

O	-3.588907000	3.093854000	-0.604633000
H	-5.563697000	3.502687000	-0.128738000
H	-6.346871000	5.374758000	-1.745490000
H	-3.840278000	5.929338000	-0.648544000
H	-4.959930000	3.702821000	-3.842503000
H	-3.614156000	5.362562000	-3.004655000
H	-2.985389000	2.732210000	-2.531409000
H	-1.674448000	5.101932000	-1.087482000
H	-1.176384000	4.359175000	-2.614009000
H	-3.557894000	5.278106000	5.840725000
H	-5.101265000	5.525651000	6.579133000
H	-2.137221000	4.082897000	1.344795000
H	-8.182525000	4.933267000	3.361281000

7A-RC-complex

C	1.530078000	-0.700077000	0.215247000
C	1.092225000	0.604091000	0.047302000
C	2.038543000	1.646831000	-0.042248000
N	0.628562000	-1.707749000	0.312066000
C	-0.803198000	-1.464526000	0.369060000
C	-1.075832000	-0.023857000	0.811980000
N	-0.293630000	0.891084000	-0.017068000
C	-2.557588000	0.282514000	0.763233000
O	-2.800056000	1.600878000	0.695840000
O	-3.429828000	-0.549144000	0.832040000
O	1.791915000	2.857781000	-0.157181000
N	5.057929000	-0.384071000	0.242223000
H	-0.798283000	0.050013000	1.873140000
H	4.074793000	1.931689000	-0.060185000
H	0.979970000	-2.607819000	0.592336000
H	-1.252872000	-2.151678000	1.082762000
H	-1.265331000	-1.636060000	-0.606337000
H	-0.462429000	1.863435000	0.210583000
H	5.272600000	-1.299244000	0.605868000
H	5.705027000	0.336582000	0.521502000
N	2.845038000	-1.047710000	0.309013000
C	3.727082000	-0.088649000	0.202508000
N	3.372555000	1.208986000	0.012410000
H	-3.760963000	1.743482000	0.707603000
N	2.513806000	-0.317704000	3.618173000
N	2.928124000	1.877729000	3.411321000
N	6.410977000	0.613973000	3.355189000
N	4.804710000	-1.157186000	3.600470000
N	5.832592000	2.851850000	3.158047000
C	1.789139000	-1.588535000	3.694358000
C	1.867838000	-2.219581000	5.086672000

C	0.581638000	-1.691953000	5.745177000
C	-0.406099000	-1.694537000	4.557812000
C	-1.533681000	-0.754019000	4.659819000
C	2.003311000	0.956026000	3.519646000
C	4.117546000	1.176403000	3.431830000
C	3.880307000	-0.190679000	3.559106000
C	5.464093000	1.569923000	3.317712000
C	6.036567000	-0.663124000	3.496531000
O	1.811708000	-3.625892000	4.932640000
O	0.096656000	-2.536151000	6.771068000
O	0.426815000	-1.352987000	3.421247000
H	2.220234000	-2.250231000	2.942081000
H	1.363349000	-3.978061000	5.715913000
H	2.772480000	-1.914960000	5.618501000
H	0.498356000	-2.280823000	7.610079000
H	0.736007000	-0.671653000	6.103996000
H	-0.766649000	-2.721102000	4.435651000
H	-1.367776000	0.303404000	4.505808000
H	-2.501564000	-1.093723000	4.995904000
H	5.142984000	3.581771000	3.124077000
H	6.806423000	3.089492000	3.079898000
H	0.941972000	1.130541000	3.522188000
H	6.845025000	-1.385988000	3.520983000

7A-PC-complex

C	1.638719000	-0.812229000	0.215965000
C	0.956688000	0.393678000	0.360348000
C	1.678159000	1.605438000	0.480179000
N	0.934164000	-1.968485000	0.211495000
C	-0.499327000	-1.969349000	-0.078995000
C	-1.155576000	-0.739743000	0.474422000
N	-0.420347000	0.398310000	0.518185000
C	-2.515257000	-0.758841000	0.863675000
O	-2.977409000	0.465377000	1.288631000
O	-3.255173000	-1.746605000	0.843358000
O	1.196498000	2.726814000	0.676206000
N	5.014315000	0.197323000	0.112365000
H	-2.038235000	0.384549000	3.646294000
H	3.618145000	2.275852000	0.489990000
H	1.453318000	-2.806298000	-0.001840000
H	-0.955104000	-2.850598000	0.366854000
H	-0.662866000	-2.028457000	-1.164350000
H	-0.841802000	1.254200000	0.850984000
H	5.458328000	-0.703577000	0.172187000
H	5.571532000	0.997638000	0.358229000
N	2.987555000	-0.895047000	0.136608000

C	3.667991000	0.225127000	0.220703000
N	3.066523000	1.435977000	0.383881000
H	-3.908302000	0.352163000	1.528757000
N	2.648667000	-0.099237000	3.629803000
N	3.495879000	1.976306000	3.724524000
N	6.647351000	0.074524000	3.302665000
N	4.720660000	-1.361428000	3.367856000
N	6.531061000	2.386154000	3.455960000
C	1.675903000	-1.194180000	3.592892000
C	1.577734000	-1.949747000	4.924101000
C	0.363210000	-1.273007000	5.583901000
C	-0.525478000	-0.955955000	4.382037000
C	-1.480797000	0.199239000	4.563949000
C	2.405719000	1.249258000	3.752111000
C	4.517853000	1.059286000	3.576971000
C	4.010615000	-0.237492000	3.516482000
C	5.913822000	1.191706000	3.452691000
C	6.024075000	-1.109538000	3.270470000
O	1.296661000	-3.309166000	4.637426000
O	-0.326505000	-2.126635000	6.482763000
O	0.406375000	-0.649374000	3.324042000
H	1.983263000	-1.871442000	2.795213000
H	0.712260000	-3.627852000	5.341770000
H	2.494457000	-1.854271000	5.511027000
H	0.072630000	-2.056060000	7.357953000
H	0.674763000	-0.348775000	6.077890000
H	-1.074664000	-1.864276000	4.111490000
H	-0.940224000	1.107213000	4.837775000
H	-2.189700000	-0.037482000	5.359168000
H	6.009402000	3.228446000	3.623816000
H	7.534988000	2.430513000	3.418972000
H	1.400566000	1.625711000	3.828369000
H	6.669402000	-1.972724000	3.146669000

8A-RC-complex

N	1.153279000	0.828202000	-0.762939000
N	-0.251258000	-0.672006000	-1.639053000
N	2.958068000	-2.285462000	-2.544027000
N	3.273216000	-0.205618000	-1.384057000
N	0.877697000	-3.181239000	-3.037112000
C	1.635077000	1.988141000	-0.006114000
C	1.947514000	3.181254000	-0.909648000
C	0.602421000	3.927229000	-0.917316000
C	0.101751000	3.703743000	0.529020000
C	-1.360103000	3.740969000	0.705302000
C	-0.145819000	0.452799000	-0.971346000

C	1.049598000	-1.065358000	-1.884448000
C	1.939750000	-0.137750000	-1.348036000
C	1.616986000	-2.196690000	-2.499909000
C	3.692278000	-1.309128000	-1.999837000
O	2.948598000	3.956754000	-0.277969000
O	0.737171000	5.313379000	-1.162336000
O	0.622253000	2.396782000	0.884671000
H	2.521392000	1.666675000	0.541625000
H	2.784800000	4.880907000	-0.518280000
H	2.261285000	2.862821000	-1.907449000
H	0.706745000	5.473045000	-2.113173000
H	-0.080569000	3.460578000	-1.630833000
H	0.587298000	4.456863000	1.158064000
H	-1.965590000	2.893940000	0.412568000
H	-1.846502000	4.655985000	1.008541000
H	-0.123491000	-3.176843000	-2.952645000
H	1.331427000	-4.001630000	-3.401283000
H	-0.981472000	1.012526000	-0.590945000
H	4.766717000	-1.441571000	-2.062458000
O	-2.899539000	-1.557720000	-1.549861000
O	-6.146265000	-0.820895000	1.213181000
C	-3.051425000	0.095805000	1.951284000
C	-2.045698000	-1.043320000	1.772404000
C	-0.701665000	-0.773977000	2.411277000
C	2.869451000	-1.633918000	1.560709000
C	1.478943000	-3.454831000	0.810923000
O	-0.558640000	0.061078000	3.285637000
H	-6.733286000	0.091116000	-0.676675000
O	4.199086000	0.252122000	2.068946000
O	-6.063566000	0.094808000	-1.376205000
H	-4.667346000	1.098779000	0.967446000
C	0.478184000	-1.544598000	1.904370000
O	5.245713000	-1.581545000	1.310243000
C	1.743851000	-0.979474000	2.051208000
C	2.734557000	-2.885195000	0.954099000
H	-3.733170000	0.139511000	-2.397049000
H	-4.435011000	-1.907334000	0.755969000
H	-5.360988000	-1.861052000	-1.473896000
H	-6.572625000	-1.682950000	1.286521000
H	-1.965631000	-1.272969000	-1.699550000
C	4.220134000	-1.020076000	1.625095000
C	0.351311000	-2.780020000	1.264646000
H	-3.629395000	-0.025790000	2.869475000
H	-2.422938000	-1.978941000	2.198838000
H	-2.513825000	1.039645000	2.054100000
H	-1.891605000	-1.245379000	0.712839000

H	1.831947000	-0.015078000	2.528760000
H	3.614962000	-3.385516000	0.576533000
H	1.373302000	-4.415258000	0.325047000
H	-0.623668000	-3.225456000	1.123637000
O	-3.296656000	0.472560000	-0.439372000
C	-4.926089000	-0.968578000	0.496379000
C	-5.107259000	-0.895030000	-1.030501000
C	-3.723941000	-0.431141000	-1.464518000
C	-4.020778000	0.234668000	0.785488000
H	5.110807000	0.584517000	2.075936000

8A-PC-complex

N	1.145995000	0.727011000	-0.918678000
N	-0.351278000	-0.812630000	-1.535649000
N	2.749110000	-2.620412000	-2.453989000
N	3.192990000	-0.437243000	-1.556095000
N	0.618992000	-3.497941000	-2.709106000
C	1.701215000	1.944685000	-0.327684000
C	1.717354000	3.131943000	-1.297351000
C	0.410080000	3.859302000	-0.934033000
C	0.312419000	3.622293000	0.573124000
C	-1.086113000	3.647199000	1.144045000
C	-0.172941000	0.373565000	-1.003535000
C	0.920811000	-1.272861000	-1.816575000
C	1.867607000	-0.321723000	-1.442810000
C	1.416947000	-2.483947000	-2.334043000
C	3.542166000	-1.614210000	-2.070597000
O	2.839355000	3.938068000	-0.982956000
O	0.457989000	5.251275000	-1.199216000
O	0.894777000	2.315602000	0.771146000
H	2.711439000	1.698067000	-0.001977000
H	2.576995000	4.857490000	-1.141310000
H	1.749511000	2.801585000	-2.338709000
H	0.187080000	5.411532000	-2.111032000
H	-0.433944000	3.391510000	-1.448083000
H	0.941100000	4.364976000	1.075238000
H	-1.725507000	2.917203000	0.644888000
H	-1.517946000	4.639564000	1.005283000
H	-0.371665000	-3.459237000	-2.545794000
H	1.028845000	-4.370827000	-2.995201000
H	-0.965910000	1.001096000	-0.636996000
H	4.606401000	-1.786869000	-2.187548000
O	-3.028066000	-1.596540000	-1.580727000
O	-6.199345000	-0.582949000	1.238865000
C	-3.039744000	0.023563000	1.998935000
C	-1.951062000	-1.074687000	1.905037000

C	-0.613115000	-0.668412000	2.481685000
C	2.978795000	-1.395901000	1.591139000
C	1.686325000	-3.372737000	1.107899000
O	-0.504345000	0.250241000	3.272984000
H	-6.669861000	0.322030000	-0.551658000
O	4.207455000	0.610489000	1.819608000
O	-6.100872000	0.212761000	-1.329617000
H	-1.070296000	3.424521000	2.210930000
C	0.599219000	-1.410898000	2.011672000
O	5.340996000	-1.243349000	1.262340000
C	1.829024000	-0.754595000	2.042101000
C	2.906236000	-2.716055000	1.139269000
H	-3.768256000	0.185792000	-2.353238000
H	-4.737909000	-1.980509000	0.785077000
H	-5.503405000	-1.769868000	-1.478754000
H	-6.750843000	-1.368284000	1.347861000
H	-2.071662000	-1.351709000	-1.663355000
C	4.291866000	-0.704529000	1.536621000
C	0.532583000	-2.718331000	1.524219000
H	-3.647938000	-0.107575000	2.893562000
H	-2.276172000	-1.982838000	2.422060000
H	-2.551595000	0.995917000	2.089334000
H	-1.801817000	-1.361964000	0.863570000
H	1.866188000	0.266626000	2.390480000
H	3.805961000	-3.203779000	0.791845000
H	1.627715000	-4.388358000	0.740832000
H	-0.415057000	-3.236603000	1.475589000
O	-3.288946000	0.382202000	-0.378217000
C	-5.015101000	-0.952991000	0.520098000
C	-5.195982000	-0.829787000	-1.015365000
C	-3.790643000	-0.441272000	-1.459426000
C	-3.908437000	0.011537000	0.795180000
H	5.098869000	0.989698000	1.760416000

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N	-0.655148000	1.625527000	0.218277000
N	-0.738151000	1.125778000	2.403553000
N	-4.366564000	1.462484000	1.741277000
N	-3.043398000	1.859595000	-0.224904000
N	-3.463372000	0.898623000	3.802703000
C	-0.117783000	1.954590000	-1.106951000
C	-0.245449000	3.449450000	-1.406423000
C	1.084712000	3.986943000	-0.852822000
C	2.063216000	2.845234000	-1.214802000
C	3.254020000	2.721365000	-0.357736000
C	0.039410000	1.307141000	1.363565000

C	-2.015482000	1.330253000	1.920980000
C	-1.985599000	1.633306000	0.561871000
C	-3.288150000	1.236702000	2.511647000
C	-4.187427000	1.752672000	0.447473000
O	-0.308273000	3.611425000	-2.811295000
O	1.505359000	5.184459000	-1.477610000
O	1.254972000	1.646225000	-1.138708000
H	-0.655340000	1.357571000	-1.844250000
H	0.112432000	4.459346000	-3.017295000
H	-1.117865000	3.888919000	-0.917194000
H	1.132939000	5.937577000	-1.003849000
H	1.019319000	4.103594000	0.231038000
H	2.356551000	3.003401000	-2.259404000
H	3.223311000	2.115852000	0.536542000
H	4.133581000	3.309265000	-0.574133000
H	-2.671292000	0.807988000	4.414468000
H	-4.387179000	0.911190000	4.199806000
H	1.108152000	1.181019000	1.347390000
H	-5.094650000	1.916868000	-0.123981000
O	3.253019000	-2.380911000	2.489573000
O	5.329201000	-1.333493000	-1.191896000
C	2.028169000	-1.533675000	-1.133365000
C	1.623863000	-2.950488000	-0.687051000
C	0.261949000	-3.284489000	-1.254081000
C	-3.337865000	-2.261479000	-0.700065000
C	-2.111238000	-1.861083000	1.349540000
O	0.171452000	-3.928938000	-2.288770000
H	5.971058000	0.082993000	0.309523000
O	-4.597885000	-2.621496000	-2.686554000
O	5.549908000	0.024410000	1.179905000
H	3.379336000	0.068443000	-0.758537000
C	-0.958168000	-2.756348000	-0.573445000
O	-5.655767000	-1.767895000	-0.899742000
C	-2.164877000	-2.729473000	-1.281149000
C	-3.298994000	-1.836121000	0.629573000
H	3.643547000	-0.368357000	2.795824000
H	4.250614000	-2.762589000	-0.137419000
H	5.577016000	-1.983060000	1.718891000
H	5.996441000	-2.024363000	-1.281057000
H	2.423475000	-2.299818000	2.975904000
C	-4.645940000	-2.213034000	-1.500165000
C	-0.938929000	-2.300554000	0.749807000
H	2.342177000	-1.551886000	-2.179619000
H	2.327686000	-3.690848000	-1.065138000
H	1.170871000	-0.862574000	-1.077884000
H	1.630296000	-3.000138000	0.401065000

H	-2.188230000	-3.070468000	-2.305992000
H	-4.209809000	-1.470344000	1.082604000
H	-2.092089000	-1.520560000	2.375752000
H	-0.020925000	-2.290719000	1.318916000
O	2.665633000	-0.645262000	1.035234000
C	4.432716000	-1.687305000	-0.145537000
C	4.923455000	-1.246492000	1.245368000
C	3.603965000	-1.106668000	1.992270000
C	3.131802000	-0.895839000	-0.307698000

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N	-0.561049	1.904345	0.117935
N	-1.463921	2.019731	2.169156
N	-4.460820	0.954514	0.272731
N	-2.533232	1.203733	-1.139293
N	-4.443255	1.368645	2.557238
C	0.426912	1.952037	-0.941530
C	0.852769	3.370355	-1.374483
C	2.272397	3.490852	-0.786350
C	2.765364	2.047527	-0.834938
C	3.882849	1.701595	0.116757
C	-0.375012	2.161968	1.456934
C	-2.428158	1.645237	1.252537
C	-1.885176	1.562512	-0.027799
C	-3.788882	1.314892	1.378436
C	-3.809206	0.913867	-0.894353
O	0.898395	3.406344	-2.791702
O	3.121159	4.322309	-1.562808
O	1.593885	1.284298	-0.489661
H	-0.021723	1.442963	-1.796434
H	1.663440	3.952346	-3.030218
H	0.164496	4.127376	-0.990668
H	3.036282	5.234787	-1.262181
H	2.222623	3.837081	0.249383
H	3.062313	1.816644	-1.862611
H	3.589409	1.907079	1.147944
H	4.763715	2.298144	-0.125090
H	-3.914907	1.467484	3.407457
H	-5.355927	0.948685	2.618232
H	0.593776	2.432909	1.843155
H	-4.400552	0.602912	-1.748877
O	5.643539	-1.831817	-3.216520
O	2.797545	0.879224	-5.220336
C	1.479489	-0.967451	-3.032505
C	1.330852	-2.477241	-2.684757
C	-0.102146	-2.814434	-2.337566

C	-2.569847	-2.307686	0.484438
C	-0.422148	-1.438710	1.192506
O	-0.808950	-3.379407	-3.161545
H	4.203272	2.022353	-4.275645
O	-4.749431	-2.959654	-0.209367
O	4.932143	1.614323	-3.781324
H	4.144511	0.648102	0.022342
C	-0.649050	-2.408999	-1.008559
O	-4.430430	-2.462352	1.956464
C	-2.001642	-2.645787	-0.737286
C	-1.762073	-1.701420	1.449550
H	5.712772	-0.083917	-2.096723
H	3.584464	-1.033424	-5.294699
H	5.702762	0.015171	-4.856595
H	2.963414	0.843025	-6.171298
H	5.783575	-2.355259	-2.417635
C	-4.047485	-2.599809	0.768149
C	0.138345	-1.794329	-0.027063
H	0.869363	-0.726220	-3.903991
H	1.617158	-3.083269	-3.543304
H	1.095468	-0.385134	-2.193254
H	2.001376	-2.712715	-1.857847
H	-2.621770	-3.104067	-1.493764
H	-2.204000	-1.432434	2.398971
H	0.187621	-0.948125	1.940170
H	1.181012	-1.576690	-0.204881
O	3.793699	-0.738434	-2.305546
C	3.510952	-0.194417	-4.590478
C	4.926027	0.240853	-4.123357
C	5.114324	-0.587741	-2.856282
C	2.868857	-0.564903	-3.305721

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H	-3.034081000	-0.941796000	-0.960465000
C	-2.334284000	-0.577272000	-4.220636000
H	-1.249818000	-0.600555000	-4.149879000
H	-2.666540000	-1.229353000	-5.023978000
H	-2.628276000	0.447227000	-4.460155000
C	-3.030374000	-1.000854000	-2.949175000
H	0.237966000	-1.043789000	-2.586736000
H	-1.335578000	0.383171000	-0.417899000
H	-1.825288000	3.128515000	-2.703989000
H	-0.326144000	-1.841160000	-1.120688000
O	-4.081501000	-1.639249000	-2.982348000
C	-1.052534000	1.346329000	-2.277474000
C	-1.241269000	0.055617000	-1.455902000

N	-2.501009000	-0.623825000	-1.756621000
C	-0.027747000	-0.879527000	-1.542138000
O	-0.060661000	1.515340000	-2.984209000
N	-2.012501000	2.283618000	-2.176927000
C	1.170625000	-0.331023000	-0.777678000
H	1.453085000	0.643948000	-1.170651000
H	0.921959000	-0.220238000	0.279964000
S	2.602470000	-1.451466000	-0.920785000
C	3.801092000	-0.507800000	0.064393000
H	4.736755000	-1.065078000	0.060943000
H	3.970740000	0.476035000	-0.373876000
H	3.455641000	-0.397755000	1.092450000
C	-3.162108000	2.300794000	-1.285299000
H	-3.963279000	1.652261000	-1.639058000
H	-2.884428000	2.000569000	-0.274659000
H	-3.535899000	3.321228000	-1.239093000
N	-0.846528000	4.737905000	-0.218900000
N	-2.427405000	5.910718000	0.862631000
N	-3.303291000	6.829979000	-2.619028000
N	-1.427217000	5.332400000	-2.517735000
N	-4.417835000	7.612793000	-0.743340000
C	0.308437000	3.878690000	-0.442113000
C	1.641910000	4.517258000	-0.030164000
C	1.874757000	3.929718000	1.372867000
C	1.282694000	2.511629000	1.215611000
C	0.846619000	1.846967000	2.452867000
C	-1.413791000	5.093252000	0.985870000
C	-2.542323000	6.113794000	-0.498848000
C	-1.571919000	5.391520000	-1.187966000
C	-3.439925000	6.867665000	-1.280433000
C	-2.333972000	6.078910000	-3.148536000
O	2.636140000	4.058748000	-0.929029000
O	3.244426000	3.834870000	1.712825000
O	0.158426000	2.697397000	0.330397000
H	0.322933000	3.640499000	-1.504829000
H	3.462216000	3.993311000	-0.426442000
H	1.583010000	5.608811000	-0.029853000
H	3.522724000	4.649040000	2.148842000
H	1.319504000	4.497035000	2.122137000
H	2.051379000	1.915867000	0.711513000
H	-0.147169000	2.025999000	2.838506000
H	1.553029000	1.274473000	3.035056000
H	-4.551003000	7.643253000	0.252184000
H	-5.049619000	8.118443000	-1.340335000
H	-1.046525000	4.696777000	1.917765000
H	-2.282212000	6.074587000	-4.231882000

9-PC-complex

H	-1.872730000	-1.073442000	-0.529076000
C	-3.858341000	-0.616347000	-3.187522000
H	-3.048779000	-0.730472000	-3.907853000
H	-4.685633000	-1.271581000	-3.447755000
H	-4.202177000	0.417666000	-3.235863000
C	-3.419562000	-0.955665000	-1.788867000
H	0.417069000	-1.268879000	-2.736170000
H	-0.282221000	0.099220000	1.648891000
H	-2.483204000	2.859456000	-3.188765000
H	0.304357000	-1.059827000	-1.006958000
O	-4.150433000	-1.528459000	-0.990653000
C	-1.400180000	1.215864000	-2.919609000
C	-1.132195000	0.042595000	-2.083056000
N	-2.131461000	-0.633470000	-1.405495000
C	0.253143000	-0.514936000	-1.955385000
O	-0.758067000	1.386600000	-3.968452000
N	-2.347687000	2.108337000	-2.529581000
C	1.366578000	0.531119000	-2.000803000
H	1.515874000	0.892153000	-3.015462000
H	1.097616000	1.373934000	-1.369058000
S	2.927072000	-0.179169000	-1.376978000
C	3.990140000	1.284509000	-1.539447000
H	4.981229000	1.004071000	-1.185041000
H	4.058847000	1.595176000	-2.582119000
H	3.609455000	2.105501000	-0.931986000
C	-2.968964000	2.247379000	-1.220117000
H	-3.877320000	1.648275000	-1.124985000
H	-2.271202000	1.968133000	-0.434109000
H	-3.239109000	3.291765000	-1.080823000
N	-0.584033000	4.622197000	-0.192448000
N	-2.475229000	5.755286000	0.228859000
N	-2.200699000	6.413013000	-3.408133000
N	-0.391518000	5.059978000	-2.588465000
N	-3.906771000	7.221834000	-2.061260000
C	0.539141000	3.733537000	0.004377000
C	1.554820000	4.175959000	1.077456000
C	1.318113000	3.161664000	2.215849000
C	0.846729000	1.920753000	1.462060000
C	0.024245000	0.943894000	2.265631000
C	-1.528477000	5.007940000	0.733567000
C	-2.147679000	5.870149000	-1.109851000
C	-0.977734000	5.170397000	-1.392943000
C	-2.772408000	6.515355000	-2.194714000
C	-1.069263000	5.709909000	-3.532114000

O	2.858014000	4.025215000	0.539410000
O	2.498089000	2.872044000	2.946935000
O	0.038376000	2.461087000	0.402821000
H	1.044750000	3.670560000	-0.960189000
H	3.424382000	3.720478000	1.265453000
H	1.385113000	5.209545000	1.388417000
H	2.573365000	3.483247000	3.689139000
H	0.523436000	3.517745000	2.876341000
H	1.723927000	1.418890000	1.035113000
H	-0.867383000	1.432332000	2.662439000
H	0.619450000	0.563307000	3.096866000
H	-4.370009000	7.282807000	-1.171716000
H	-4.337889000	7.636148000	-2.869687000
H	-1.466210000	4.693755000	1.763000000
H	-0.656056000	5.662919000	-4.533995000

10A-RC-complex

C	-0.375432000	0.630114000	1.764808000
C	0.461811000	0.814709000	0.512793000
O	0.080264000	1.828929000	-0.264008000
C	-1.118722000	-0.731636000	1.660308000
C	-2.082837000	-0.834329000	0.518018000
C	-1.797179000	-1.279444000	-0.747256000
C	-3.472992000	-0.465402000	0.508593000
N	-2.918397000	-1.203338000	-1.541706000
C	-3.964615000	-0.712351000	-0.800988000
C	-4.353785000	0.037686000	1.476746000
C	-5.290739000	-0.466486000	-1.157242000
C	-5.671596000	0.280807000	1.127435000
C	-6.135382000	0.032826000	-0.178472000
O	1.391648000	0.084556000	0.229902000
H	-1.642709000	-0.891307000	2.605592000
H	-0.366947000	-1.517825000	1.576928000
H	-0.866489000	-1.647852000	-1.146902000
H	-4.007351000	0.237018000	2.482721000
H	-6.359732000	0.669690000	1.867580000
H	-5.645619000	-0.659773000	-2.161766000
H	-7.170885000	0.235404000	-0.422229000
H	0.353820000	0.522088000	2.573046000
H	-2.965209000	-1.486302000	-2.505271000
C	-1.303687000	1.798821000	2.082690000
H	-2.061251000	1.924555000	1.310578000
H	-1.810762000	1.617354000	3.031686000
H	-0.745933000	2.731649000	2.166844000
H	0.677413000	1.894355000	-1.051121000
N	3.018811000	5.430822000	-0.983759000

N	4.326601000	7.223116000	-0.649529000
N	1.713830000	8.784816000	-2.762973000
N	1.293517000	6.450459000	-2.373587000
N	3.553669000	9.917517000	-1.919850000
C	2.502278000	4.061962000	-0.918128000
C	2.745650000	3.300034000	-2.224299000
C	4.077157000	2.588786000	-1.938267000
C	3.943597000	2.252454000	-0.435673000
C	5.209808000	2.105287000	0.298744000
C	4.152728000	5.948803000	-0.401050000
C	3.248875000	7.570415000	-1.440210000
C	2.422718000	6.470221000	-1.656610000
C	2.847635000	8.780334000	-2.038867000
C	1.018212000	7.648496000	-2.885378000
O	1.705859000	2.339316000	-2.393969000
O	4.227139000	1.392612000	-2.678329000
O	3.171852000	3.360858000	0.102851000
H	1.436048000	4.129591000	-0.697317000
H	2.104697000	1.563447000	-2.821077000
H	2.784385000	3.967197000	-3.086107000
H	4.662391000	1.587373000	-3.516891000
H	4.910705000	3.273391000	-2.106249000
H	3.341559000	1.341840000	-0.359281000
H	5.754178000	2.981082000	0.623676000
H	5.658432000	1.129944000	0.413805000
H	4.381664000	9.948312000	-1.351647000
H	3.209701000	10.766886000	-2.333731000
H	4.795393000	5.334099000	0.204926000
H	0.113558000	7.717114000	-3.480340000

10A-PC-complex

C	-0.143582000	0.053099000	1.647108000
C	0.605113000	0.511472000	0.408120000
O	0.118750000	1.614464000	-0.156731000
C	-0.970107000	-1.232645000	1.242423000
C	-1.962845000	-1.017391000	0.148781000
C	-1.768582000	-1.283277000	-1.182510000
C	-3.280614000	-0.452458000	0.257955000
N	-2.879382000	-0.916188000	-1.906227000
C	-3.826637000	-0.406246000	-1.052407000
C	-4.056534000	0.008762000	1.330640000
C	-5.106223000	0.085999000	-1.308687000
C	-5.328081000	0.498053000	1.080068000
C	-5.847256000	0.537453000	-0.227627000
O	1.546672000	-0.105813000	-0.048218000
H	-1.464223000	-1.587764000	2.148664000

H	-0.248526000	-1.994924000	0.944050000
H	-0.909056000	-1.708675000	-1.674527000
H	-3.664171000	-0.014722000	2.339286000
H	-5.935935000	0.857501000	1.901000000
H	-5.504253000	0.113743000	-2.315193000
H	-6.844258000	0.926518000	-0.391943000
H	0.623824000	-0.312832000	2.335080000
H	-2.986123000	-1.027569000	-2.899625000
C	-0.961771000	1.090950000	2.318370000
H	-1.453568000	1.868917000	1.756050000
H	-1.221868000	0.959189000	3.359477000
H	5.253262000	1.899083000	0.986092000
H	0.637276000	1.834151000	-0.972924000
N	2.775971000	5.489636000	-0.769157000
N	4.032880000	7.321724000	-0.456350000
N	1.016705000	8.915293000	-1.903898000
N	0.787417000	6.529331000	-1.724623000
N	2.918909000	10.075684000	-1.259564000
C	2.354246000	4.087853000	-0.787534000
C	2.490194000	3.468652000	-2.183336000
C	3.874086000	2.803322000	-2.104513000
C	3.927450000	2.337625000	-0.649902000
C	5.310264000	2.201152000	-0.059886000
C	3.968031000	6.019342000	-0.331451000
C	2.817413000	7.675828000	-1.008643000
C	2.021537000	6.550450000	-1.209110000
C	2.258197000	8.911863000	-1.386134000
C	0.367987000	7.753064000	-2.039914000
O	1.481361000	2.472213000	-2.344180000
O	3.991476000	1.685666000	-2.969284000
O	3.179716000	3.345318000	0.077889000
H	1.317223000	4.062297000	-0.449121000
H	1.876328000	1.755962000	-2.868557000
H	2.404637000	4.215835000	-2.972709000
H	4.301430000	1.981257000	-3.833673000
H	4.653288000	3.543076000	-2.303394000
H	3.385395000	1.391001000	-0.574145000
H	5.861742000	3.140402000	-0.125509000
H	5.861885000	1.435198000	-0.607594000
H	3.821322000	10.104097000	-0.818520000
H	2.457431000	10.939678000	-1.486692000
H	4.736069000	5.389610000	0.083290000
H	-0.628710000	7.821983000	-2.462733000

10B-RC-complex

C	-0.475599000	4.815675000	-0.961953000
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C	0.029801000	5.677082000	0.224687000
O	1.273337000	5.838256000	0.356441000
C	-1.338780000	3.642428000	-0.437080000
C	-0.614022000	2.649110000	0.421368000
C	-0.457726000	2.707853000	1.781744000
C	0.058151000	1.450173000	-0.003487000
N	0.263572000	1.620631000	2.227674000
C	0.596108000	0.831094000	1.157244000
C	0.261013000	0.837709000	-1.248288000
C	1.323907000	-0.357065000	1.098792000
C	0.981385000	-0.343931000	-1.310465000
C	1.510125000	-0.935190000	-0.147239000
O	-0.853743000	6.159339000	0.975813000
H	-1.774408000	3.122704000	-1.296057000
H	-2.165629000	4.070980000	0.130275000
H	-0.807374000	3.455793000	2.473749000
H	-0.134044000	1.288063000	-2.150107000
H	1.145556000	-0.822707000	-2.267921000
H	1.731944000	-0.807605000	1.995007000
H	2.072606000	-1.856954000	-0.227697000
H	-1.160065000	5.465332000	-1.519777000
H	0.524046000	1.450475000	3.183338000
C	0.626650000	4.354098000	-1.909444000
H	1.351437000	3.723981000	-1.394512000
H	0.204478000	3.778592000	-2.737780000
H	1.165948000	5.203457000	-2.327255000
N	4.988839000	6.074983000	-1.281996000
N	3.531086000	7.038297000	-2.687327000
N	6.660723000	7.697859000	-4.559133000
N	7.058824000	6.502879000	-2.512212000
N	4.549077000	8.339558000	-5.278494000
C	5.502351000	5.365524000	-0.127483000
C	5.259300000	6.075238000	1.216695000
C	4.125401000	5.246468000	1.842323000
C	4.413942000	3.834164000	1.301191000
C	3.247635000	2.935469000	1.279907000
C	3.674134000	6.390194000	-1.556520000
C	4.813719000	7.159685000	-3.187911000
C	5.735572000	6.565204000	-2.329135000
C	5.332157000	7.748113000	-4.355447000
C	7.429353000	7.090209000	-3.647693000
O	6.442120000	5.973833000	1.994779000
O	4.177900000	5.243251000	3.262861000
O	4.869806000	4.092384000	-0.052562000
H	6.575214000	5.256051000	-0.290356000
H	6.153496000	5.883662000	2.916211000

H	4.983801000	7.122927000	1.069029000
H	3.600777000	5.938441000	3.598755000
H	3.153954000	5.582893000	1.476953000
H	5.236127000	3.403321000	1.883022000
H	2.373994000	3.214800000	0.707589000
H	3.214819000	2.048284000	1.892467000
H	3.571947000	8.482724000	-5.091722000
H	4.974224000	8.838611000	-6.041184000
H	2.863972000	6.103870000	-0.893620000
H	8.492090000	7.079227000	-3.866270000

10B-PC-complex

C	2.255294000	2.930684000	0.502685000
C	1.718607000	3.716065000	1.729532000
O	1.165634000	3.081918000	2.657647000
C	1.355367000	3.243112000	-0.747923000
C	-0.088811000	2.885891000	-0.608722000
C	-1.104607000	3.741851000	-0.272166000
C	-0.695555000	1.591221000	-0.766189000
N	-2.302010000	3.061320000	-0.204560000
C	-2.085094000	1.740178000	-0.506561000
C	-0.206694000	0.323665000	-1.112485000
C	-2.975299000	0.668641000	-0.579225000
C	-1.087956000	-0.743076000	-1.186918000
C	-2.459610000	-0.572294000	-0.920788000
O	1.886046000	4.966347000	1.684786000
H	1.786936000	2.718644000	-1.605498000
H	1.444706000	4.311230000	-0.947456000
H	-1.063719000	4.799252000	-0.067575000
H	0.847664000	0.183121000	-1.312776000
H	-0.719559000	-1.726258000	-1.452597000
H	-4.030516000	0.802675000	-0.376184000
H	-3.124116000	-1.424885000	-0.985195000
H	3.224932000	3.373311000	0.251022000
H	-3.193497000	3.474980000	0.006254000
C	2.440623000	1.480439000	0.736391000
H	1.875535000	0.967661000	1.500028000
H	3.047268000	0.895909000	0.055273000
H	5.127306000	2.880212000	2.159251000
N	4.691313000	6.188480000	-1.304994000
N	2.576730000	6.907650000	-1.494947000
N	3.924161000	8.216461000	-4.688490000
N	5.590978000	7.052692000	-3.405854000
N	1.721179000	8.467093000	-4.002147000
C	5.905062000	5.611309000	-0.740440000
C	6.682382000	6.590669000	0.155575000

C	6.267845000	6.135604000	1.565074000
C	6.116271000	4.627473000	1.382389000
C	5.224951000	3.941853000	2.388697000
C	3.435313000	6.261408000	-0.740920000
C	3.300726000	7.288333000	-2.607147000
C	4.619680000	6.851390000	-2.507505000
C	2.963935000	8.003659000	-3.770883000
C	5.153100000	7.738584000	-4.459277000
O	8.069421000	6.376972000	-0.048535000
O	7.252530000	6.411373000	2.548602000
O	5.553160000	4.498607000	0.059535000
H	6.529869000	5.309560000	-1.582458000
H	8.501607000	6.519363000	0.807229000
H	6.412208000	7.627833000	-0.058365000
H	7.111561000	7.298854000	2.899343000
H	5.304538000	6.577241000	1.833706000
H	7.117309000	4.181080000	1.387141000
H	4.232303000	4.392030000	2.388679000
H	5.665685000	4.039681000	3.382376000
H	1.013726000	8.393578000	-3.292252000
H	1.547282000	9.046573000	-4.805323000
H	3.185690000	5.787315000	0.201053000
H	5.884331000	7.941134000	-5.234877000

11A-RC-complex

C	-2.960889000	-1.127473000	-0.265306000
C	-3.003469000	-0.690918000	-1.713828000
O	-2.713126000	0.588528000	-1.879600000
C	-1.485853000	-1.031085000	0.236979000
C	-0.468986000	-1.625951000	-0.691619000
C	-0.176196000	-2.952887000	-0.876861000
C	0.361609000	-0.899972000	-1.618512000
N	0.771856000	-3.095455000	-1.865668000
C	1.125032000	-1.855925000	-2.338493000
C	0.544316000	0.461042000	-1.902189000
C	2.039240000	-1.488307000	-3.326291000
C	1.458383000	0.829531000	-2.873274000
C	2.195035000	-0.136289000	-3.583383000
O	-3.233875000	-1.448866000	-2.642781000
H	-1.447437000	-1.515790000	1.214859000
H	-1.244726000	0.020169000	0.396183000
H	-0.570413000	-3.820203000	-0.373593000
H	-0.038118000	1.211083000	-1.383966000
H	1.596792000	1.877428000	-3.107804000
H	2.600359000	-2.234154000	-3.875009000
H	2.885747000	0.183144000	-4.353078000

H	-3.540521000	-0.399154000	0.308380000
H	1.159646000	-3.970637000	-2.172562000
C	-3.556131000	-2.517376000	-0.076388000
H	-2.987258000	-3.263975000	-0.630413000
H	-3.544491000	-2.786855000	0.980717000
H	-4.586997000	-2.554883000	-0.430045000
H	-2.500987000	0.789141000	-2.850843000
N	-0.382771000	2.676043000	-5.321924000
N	-1.782585000	1.265096000	-4.307730000
N	-0.049522000	-1.130105000	-6.550370000
N	0.750068000	1.118748000	-6.810107000
N	-1.716085000	-1.746768000	-5.064965000
C	0.322625000	3.908722000	-5.683125000
C	-0.202419000	4.516730000	-6.987180000
C	-1.240952000	5.525468000	-6.468835000
C	-0.570490000	6.029819000	-5.170750000
C	-1.482067000	6.567251000	-4.148520000
C	-1.369693000	2.508676000	-4.392393000
C	-1.022650000	0.567126000	-5.229164000
C	-0.144755000	1.435957000	-5.870142000
C	-0.942766000	-0.792124000	-5.599316000
C	0.725456000	-0.184071000	-7.085707000
O	0.872015000	5.184368000	-7.622079000
O	-1.448092000	6.611485000	-7.350359000
O	0.121471000	4.861457000	-4.663554000
H	1.380031000	3.658185000	-5.775138000
H	0.494227000	5.940015000	-8.096440000
H	-0.638014000	3.756090000	-7.640079000
H	-2.145555000	6.384404000	-7.976852000
H	-2.177608000	5.014123000	-6.235389000
H	0.169844000	6.782524000	-5.464024000
H	-2.020219000	5.893013000	-3.496730000
H	-1.712544000	7.621829000	-4.128813000
H	-2.301204000	-1.560134000	-4.255453000
H	-1.527360000	-2.703289000	-5.314640000
H	-1.725409000	3.325756000	-3.790018000
H	1.425578000	-0.524902000	-7.841291000

11A-PC-complex

C	-2.854471000	-1.186055000	-0.491948000
C	-3.521363000	-1.098678000	-1.856481000
O	-3.888273000	0.143991000	-2.172157000
C	-1.535368000	-0.453930000	-0.611893000
C	-0.557636000	-0.704204000	-1.583064000
C	-0.479063000	-1.742703000	-2.524987000
C	0.603935000	0.139906000	-1.854774000

N	0.628840000	-1.575779000	-3.312869000
C	1.304820000	-0.434059000	-2.939080000
C	1.071425000	1.332375000	-1.300572000
C	2.452314000	0.144496000	-3.474056000
C	2.215422000	1.917396000	-1.826490000
C	2.898970000	1.327069000	-2.901247000
O	-3.631029000	-2.033594000	-2.627556000
H	-1.405895000	0.420056000	0.012065000
H	-1.470313000	6.018232000	-2.988091000
H	-1.153296000	-2.561421000	-2.699127000
H	0.547013000	1.801246000	-0.477334000
H	2.584226000	2.845216000	-1.408430000
H	2.965762000	-0.304188000	-4.313919000
H	3.784424000	1.807576000	-3.297530000
H	-3.479802000	-0.614106000	0.196884000
H	0.873981000	-2.169101000	-4.087401000
C	-2.741957000	-2.627680000	0.013067000
H	-2.118381000	-3.230564000	-0.645037000
H	-2.295774000	-2.634214000	1.007699000
H	-3.726303000	-3.095327000	0.070992000
H	-3.740604000	0.278923000	-3.154186000
N	-0.823152000	1.854222000	-5.009040000
N	-2.647422000	0.669726000	-4.494932000
N	-0.865048000	-1.856300000	-6.540716000
N	0.335462000	0.217623000	-6.393230000
N	-2.882992000	-2.263691000	-5.462075000
C	0.180295000	2.929994000	-4.996266000
C	0.290411000	3.625849000	-6.355297000
C	-0.680344000	4.806418000	-6.178894000
C	-0.491817000	5.166506000	-4.706135000
C	-1.673708000	5.832623000	-4.042995000
C	-2.016650000	1.812674000	-4.345361000
C	-1.816216000	-0.095467000	-5.291909000
C	-0.677773000	0.634571000	-5.628809000
C	-1.870743000	-1.423209000	-5.758966000
C	0.151140000	-1.030608000	-6.815548000
O	1.621531000	4.088969000	-6.502338000
O	-0.350846000	5.921758000	-6.990751000
O	-0.213349000	3.902433000	-4.058160000
H	1.129431000	2.479971000	-4.704493000
H	1.575332000	4.921390000	-6.996095000
H	0.013262000	2.960024000	-7.175466000
H	-0.769658000	5.821637000	-7.853928000
H	-1.705910000	4.474603000	-6.361540000
H	0.397855000	5.798722000	-4.621349000
H	-2.566951000	5.211303000	-4.126012000

H	-1.869196000	6.790288000	-4.528304000
H	-3.414470000	-2.089108000	-4.615870000
H	-2.747746000	-3.231185000	-5.711378000
H	-2.359452000	2.642307000	-3.752664000
H	0.927124000	-1.439626000	-7.453650000

11B-RC-complex

C	-2.613372000	0.686777000	-0.313728000
C	-3.619366000	0.587210000	-1.494110000
O	-3.802384000	1.648929000	-2.150517000
C	-1.212388000	1.101436000	-0.801861000
C	-0.490039000	0.156264000	-1.716431000
C	-0.967776000	-0.936061000	-2.389899000
C	0.870423000	0.327814000	-2.153077000
N	0.011332000	-1.453050000	-3.215868000
C	1.146615000	-0.691736000	-3.102751000
C	1.866595000	1.268712000	-1.862451000
C	2.371324000	-0.781141000	-3.761800000
C	3.086450000	1.183714000	-2.515098000
C	3.335317000	0.168676000	-3.457997000
O	-4.177980000	-0.515713000	-1.713447000
H	-0.583312000	1.292215000	0.075829000
H	-1.302334000	2.057288000	-1.324312000
H	-1.953562000	-1.367380000	-2.370474000
H	1.676388000	2.064606000	-1.153277000
H	3.860284000	1.911837000	-2.305471000
H	2.555148000	-1.553110000	-4.498178000
H	4.294082000	0.132735000	-3.960042000
H	-2.972556000	1.530999000	0.285145000
H	-0.118474000	-2.218051000	-3.854163000
C	-2.586016000	-0.546910000	0.586369000
H	-2.242296000	-1.429296000	0.048237000
H	-1.915273000	-0.384835000	1.435242000
H	-3.580969000	-0.766817000	0.975535000
N	-0.701118000	1.289031000	-5.187441000
N	-2.443339000	-0.107108000	-5.394058000
N	-0.160976000	-1.648276000	-7.872727000
N	0.801913000	0.292533000	-6.832495000
N	-2.270659000	-2.470109000	-7.355522000
C	0.139341000	2.402519000	-4.729188000
C	0.204037000	3.515017000	-5.777035000
C	-0.993027000	4.389016000	-5.368716000
C	-0.945679000	4.286248000	-3.826927000
C	-2.224693000	4.475101000	-3.120514000
C	-1.968089000	0.946992000	-4.771851000
C	-1.434558000	-0.487596000	-6.256665000

C	-0.341894000	0.370606000	-6.142648000
C	-1.305408000	-1.545176000	-7.173471000
C	0.804087000	-0.743434000	-7.667939000
O	1.422695000	4.216613000	-5.601869000
O	-0.856137000	5.743564000	-5.759064000
O	-0.422053000	2.966446000	-3.570686000
H	1.127501000	2.000096000	-4.507502000
H	1.251802000	5.140784000	-5.836304000
H	0.117978000	3.122356000	-6.793069000
H	-1.207603000	5.853804000	-6.650511000
H	-1.920158000	3.956302000	-5.750655000
H	-0.206409000	5.028140000	-3.493694000
H	-2.780212000	3.616881000	-2.763585000
H	-2.616026000	5.476082000	-3.004749000
H	-3.176053000	-2.333999000	-6.940497000
H	-2.182876000	-3.129236000	-8.110288000
H	-2.472863000	1.481409000	-3.981089000
H	1.701742000	-0.875973000	-8.262897000

11B-PC-complex

C	-2.716190000	0.144120000	-0.330988000
C	-3.316251000	0.000340000	-1.772216000
O	-3.759186000	1.060761000	-2.287632000
C	-1.401704000	0.874130000	-0.364223000
C	-0.275455000	0.479882000	-1.095060000
C	-0.123315000	-0.627653000	-1.941393000
C	0.983861000	1.210107000	-1.195239000
N	1.116061000	-0.594976000	-2.534499000
C	1.809537000	0.515175000	-2.109728000
C	1.450479000	2.396781000	-0.630367000
C	3.073114000	0.976316000	-2.468382000
C	2.708911000	2.868271000	-0.984249000
C	3.510726000	2.163580000	-1.895723000
O	-3.306891000	-1.134701000	-2.305730000
H	-1.326480000	1.799141000	0.194936000
H	-0.971501000	3.404239000	-1.966398000
H	-0.845917000	-1.382958000	-2.194516000
H	0.835541000	2.953782000	0.065855000
H	3.076128000	3.792720000	-0.557105000
H	3.685857000	0.436108000	-3.178718000
H	4.485561000	2.553335000	-2.160390000
H	-3.421591000	0.781617000	0.208175000
H	1.455105000	-1.271880000	-3.195638000
C	-2.626187000	-1.197616000	0.412520000
H	-1.924510000	-1.870033000	-0.078146000
H	-2.290936000	-1.042418000	1.440774000

H	-3.599779000	-1.690962000	0.437897000
N	-1.295199000	0.764106000	-5.891896000
N	-3.430701000	0.127172000	-6.145323000
N	-2.050131000	-1.190386000	-9.320389000
N	-0.372569000	-0.115102000	-7.976004000
N	-4.284089000	-1.341813000	-8.707521000
C	-0.075448000	1.303204000	-5.281040000
C	0.532791000	2.463491000	-6.086203000
C	0.038185000	3.692135000	-5.300943000
C	-0.004179000	3.171698000	-3.867174000
C	-0.966569000	3.881099000	-2.945555000
C	-2.565342000	0.724718000	-5.358825000
C	-2.694621000	-0.257454000	-7.247514000
C	-1.360750000	0.119962000	-7.103241000
C	-3.027084000	-0.942824000	-8.429987000
C	-0.807681000	-0.773282000	-9.047758000
O	1.945909000	2.361464000	-6.017528000
O	0.924396000	4.798415000	-5.390455000
O	-0.405888000	1.797224000	-4.009550000
H	0.646699000	0.487457000	-5.201346000
H	2.285493000	3.266752000	-5.951102000
H	0.195723000	2.455722000	-7.124208000
H	0.702154000	5.321330000	-6.169667000
H	-0.967139000	3.964325000	-5.632879000
H	1.008743000	3.200199000	-3.451665000
H	-1.977861000	3.855527000	-3.354654000
H	-0.658600000	4.921601000	-2.826803000
H	-4.999899000	-1.268948000	-8.005504000
H	-4.450863000	-1.927599000	-9.508041000
H	-2.787685000	1.111865000	-4.375054000
H	-0.062259000	-1.005046000	-9.801261000

12A-RC-complex

N	-2.946364000	0.930253000	1.118563000
N	-3.031175000	-0.832104000	2.504177000
N	-5.274255000	-2.083542000	-0.165622000
N	-4.436006000	0.118699000	-0.639451000
N	-4.745804000	-3.269781000	1.756288000
C	-2.614706000	2.239834000	0.584441000
C	-3.364925000	3.401561000	1.253847000
C	-2.315230000	3.964813000	2.227966000
C	-1.001793000	3.746824000	1.446935000
C	0.219545000	3.684831000	2.265494000
C	-2.524665000	0.357871000	2.300694000
C	-3.835722000	-1.062100000	1.404620000
C	-3.794699000	0.019627000	0.529095000

C	-4.622859000	-2.160368000	1.008640000
C	-5.146666000	-0.975684000	-0.904467000
O	-3.676242000	4.354027000	0.253298000
O	-2.491408000	5.342314000	2.492924000
O	-1.225650000	2.474908000	0.783700000
H	-2.851986000	2.211035000	-0.478917000
H	-3.654760000	5.224995000	0.677869000
H	-4.268103000	3.052711000	1.761272000
H	-3.069777000	5.449305000	3.257358000
H	-2.300082000	3.378530000	3.149302000
H	-0.932939000	4.536738000	0.691959000
H	0.426286000	2.798061000	2.850062000
H	0.840007000	4.561287000	2.374890000
H	-4.230947000	-3.367553000	2.613620000
H	-5.280338000	-4.049147000	1.412779000
H	-1.798542000	0.839508000	2.935421000
H	-5.694186000	-0.973633000	-1.840978000
O	2.702515000	-1.874632000	-0.674352000
H	2.701168000	1.892908000	0.127827000
N	0.457284000	-2.028410000	-0.656154000
C	1.487895000	0.153836000	-0.151603000
C	2.406490000	-0.875492000	2.589869000
H	3.710519000	-0.217519000	-2.176358000
C	1.202253000	0.011081000	2.387208000
N	0.831447000	0.377670000	1.135289000
H	3.240262000	-0.242508000	2.901514000
C	1.604486000	-1.341912000	-0.514081000
H	0.073215000	1.051839000	1.108892000
H	0.817765000	0.603917000	-0.885752000
H	0.585593000	-3.009341000	-0.856775000
H	2.187984000	-1.561795000	3.405813000
H	3.591157000	0.383463000	0.347753000
O	0.561308000	0.418989000	3.358708000
H	2.713050000	-1.435485000	1.711474000
C	2.832132000	0.879940000	-0.250778000
C	-0.908591000	-1.556634000	-0.478820000
H	-1.167609000	-1.463397000	0.575158000
H	-1.061207000	-0.595116000	-0.966870000
H	-1.579813000	-2.275096000	-0.943187000
S	3.450869000	1.081402000	-1.958346000

12A-PC-complex

N	-2.966656000	0.848746000	1.081634000
N	-3.038465000	-0.840721000	2.555174000
N	-5.530327000	-2.089879000	0.114278000
N	-4.617302000	0.039388000	-0.526213000

N	-4.923006000	-3.215444000	2.049175000
C	-2.607012000	2.112927000	0.458488000
C	-3.340065000	3.326256000	1.051553000
C	-2.283038000	3.915384000	2.002451000
C	-0.981709000	3.627819000	1.258175000
C	0.259014000	3.576058000	2.115292000
C	-2.490677000	0.311818000	2.259096000
C	-3.929217000	-1.078792000	1.526376000
C	-3.898531000	-0.041204000	0.598340000
C	-4.799341000	-2.148859000	1.241888000
C	-5.400118000	-1.025706000	-0.686021000
O	-3.619568000	4.229765000	-0.003555000
O	-2.428353000	5.311926000	2.194003000
O	-1.216373000	2.333881000	0.650730000
H	-2.842962000	2.018504000	-0.601598000
H	-3.552427000	5.122779000	0.367071000
H	-4.257119000	3.024881000	1.563788000
H	-3.034523000	5.472204000	2.926988000
H	-2.296784000	3.380999000	2.956257000
H	-0.871025000	4.371703000	0.462713000
H	0.180302000	2.786593000	2.863505000
H	0.384004000	4.537171000	2.616479000
H	-4.370022000	-3.291975000	2.884539000
H	-5.538842000	-3.968759000	1.795789000
H	-1.698531000	0.784314000	2.817393000
H	-6.013874000	-1.036748000	-1.580502000
O	2.527441000	-2.240332000	-0.715734000
H	1.144839000	3.389968000	1.508640000
N	0.287296000	-2.066349000	-0.775636000
C	1.599069000	-0.046654000	-0.228996000
C	2.483379000	-0.941664000	2.503860000
H	4.650070000	2.073931000	-0.273616000
C	1.258809000	-0.083620000	2.301697000
N	0.902860000	0.255210000	1.037339000
H	3.373894000	-0.319121000	2.394330000
C	1.517552000	-1.551416000	-0.592503000
H	0.126337000	0.904462000	0.970793000
H	1.002703000	0.485969000	-0.977906000
H	0.284127000	-3.058158000	-0.964228000
H	2.457723000	-1.346834000	3.512067000
H	3.827806000	-0.262158000	-0.326924000
O	0.598989000	0.322524000	3.260283000
H	2.561917000	-1.750187000	1.779487000
C	3.007718000	0.435120000	-0.301159000
C	-1.006685000	-1.417316000	-0.631789000
H	-1.313334000	-1.364544000	0.412324000

H	-0.992021000	-0.412022000	-1.048888000
H	-1.743238000	-1.994808000	-1.185830000
S	3.313908000	2.127553000	-0.155609000

12B-RC-complex

O	-1.462403000	-2.810302000	-0.300855000
H	-4.503645000	-0.192153000	-0.253657000
N	-1.156635000	-2.104806000	1.815294000
C	-2.483744000	-0.704369000	0.270455000
C	-2.743831000	-1.217113000	-2.791703000
H	-5.248538000	-1.909344000	1.336484000
C	-1.927601000	-0.107454000	-2.176468000
N	-1.912223000	0.060726000	-0.830221000
H	-3.802113000	-0.949155000	-2.772650000
C	-1.654627000	-1.967765000	0.574183000
H	-1.329777000	0.835055000	-0.529135000
H	-2.439645000	-0.024181000	1.118030000
H	-0.602797000	-2.937927000	1.952947000
H	-2.436614000	-1.328478000	-3.828393000
H	-4.095424000	-1.891594000	-0.582320000
O	-1.292131000	0.676422000	-2.887963000
H	-2.607568000	-2.153596000	-2.257387000
O	-4.410786000	-1.441341000	1.420670000
C	-3.961816000	-1.067715000	0.118433000
C	-1.337662000	-1.220564000	2.960753000
H	-0.859532000	-0.253810000	2.799028000
H	-2.394172000	-1.079218000	3.184441000
H	-0.861814000	-1.687245000	3.819553000
N	1.448703000	0.563521000	0.034833000
N	1.607513000	-1.189586000	-1.358323000
N	2.210797000	-2.941932000	1.849022000
N	1.885444000	-0.580760000	2.149362000
N	2.187255000	-3.985657000	-0.223989000
C	1.205156000	1.905574000	0.513042000
C	2.050461000	2.996634000	-0.164851000
C	1.041872000	3.683614000	-1.103437000
C	-0.277284000	3.558775000	-0.315693000
C	-1.499910000	3.646031000	-1.131808000
C	1.383288000	0.093567000	-1.262049000
C	1.828094000	-1.603615000	-0.057978000
C	1.734969000	-0.530704000	0.823580000
C	2.074326000	-2.865052000	0.512690000
C	2.119780000	-1.820033000	2.573260000
O	2.487669000	3.896566000	0.838250000
O	1.343531000	5.046493000	-1.331284000
O	-0.167848000	2.240925000	0.283494000

H	1.413078000	1.890951000	1.582340000
H	2.535327000	4.772533000	0.425758000
H	2.900867000	2.568677000	-0.701889000
H	1.904566000	5.123458000	-2.111984000
H	0.958506000	3.130678000	-2.041599000
H	-0.270210000	4.316235000	0.474507000
H	-1.713941000	2.858795000	-1.842708000
H	-2.115886000	4.531846000	-1.101795000
H	1.945176000	-3.967563000	-1.199663000
H	2.233049000	-4.876112000	0.242070000
H	1.117388000	0.738492000	-2.083322000
H	2.244400000	-1.943804000	3.643646000

12B-PC-complex

O	0.133700000	-1.093201000	-2.980483000
H	-0.287241000	2.963729000	1.734146000
N	2.231245000	-0.274733000	-3.090617000
C	0.926417000	0.117874000	-1.043036000
C	-1.506672000	-1.570265000	-0.245121000
H	1.973540000	-1.033616000	1.789088000
C	-1.570641000	-0.080028000	-0.478762000
N	-0.434224000	0.591995000	-0.772822000
H	-1.035245000	-1.767848000	0.719752000
C	1.055858000	-0.469751000	-2.464583000
H	-0.546244000	1.595931000	-0.853598000
H	1.520640000	1.033975000	-0.989655000
H	2.269212000	-0.632491000	-4.033790000
H	-2.522088000	-1.958526000	-0.225596000
H	1.462638000	-1.911335000	-0.189410000
O	-2.634173000	0.537120000	-0.364064000
H	-0.930812000	-2.071432000	-1.018870000
O	1.684000000	-0.334600000	1.189376000
C	1.503726000	-0.838683000	-0.063302000
C	3.379443000	0.478439000	-2.604942000
H	3.174645000	1.550602000	-2.577831000
H	3.677769000	0.139198000	-1.613032000
H	4.208976000	0.306604000	-3.286333000
N	-0.712891000	3.176971000	-3.132646000
N	-1.869396000	1.586958000	-4.217876000
N	1.366791000	1.259135000	-5.990447000
N	1.420914000	2.972845000	-4.307755000
N	-0.513693000	-0.016397000	-6.461293000
C	-0.373046000	4.187530000	-2.157835000
C	-1.437601000	5.281648000	-1.955431000
C	-2.033088000	4.932806000	-0.575894000
C	-0.843407000	4.309663000	0.149492000

C	-1.189793000	3.393663000	1.298672000
C	-1.900823000	2.486779000	-3.272358000
C	-0.588995000	1.668289000	-4.732846000
C	0.147668000	2.645553000	-4.070878000
C	0.082401000	0.949363000	-5.738555000
C	1.947332000	2.233597000	-5.281235000
O	-0.775073000	6.533736000	-1.907548000
O	-2.491162000	6.074511000	0.127917000
O	-0.179935000	3.557090000	-0.886566000
H	0.558900000	4.639789000	-2.495245000
H	-1.260513000	7.079471000	-1.269757000
H	-2.183310000	5.272130000	-2.754135000
H	-3.416709000	6.235053000	-0.090593000
H	-2.828625000	4.190868000	-0.683872000
H	-0.183343000	5.117813000	0.484438000
H	-1.840564000	2.584673000	0.962494000
H	-1.703674000	3.966889000	2.071695000
H	-1.417554000	-0.358930000	-6.184422000
H	0.047088000	-0.587219000	-7.071257000
H	-2.745051000	2.683935000	-2.632040000
H	2.984100000	2.436243000	-5.527288000

13A-RC-complex

H	-1.508027000	-2.804380000	1.550686000
H	4.232373000	-4.426823000	-0.618765000
H	4.176444000	-3.128803000	-1.753362000
C	-4.421418000	-2.120961000	-1.135081000
O	-2.535636000	1.167228000	2.073581000
O	-0.372285000	-0.711834000	2.471705000
C	-3.498311000	-1.872156000	0.051134000
O	0.140288000	-0.901033000	-1.361869000
H	0.099357000	-4.116136000	1.601871000
H	2.330365000	-4.923006000	0.880821000
C	0.692124000	-1.868641000	-0.845106000
N	0.045176000	-2.562581000	0.223225000
O	-5.444873000	-1.499194000	-1.321202000
O	-4.015584000	-3.113526000	-1.923773000
C	-1.245472000	-2.120904000	0.735588000
O	-4.861164000	-0.085588000	1.004050000
C	-1.185861000	-0.701671000	1.313198000
C	-2.580123000	-0.194848000	1.674339000
C	2.486129000	-3.353686000	-0.655815000
C	-3.565362000	-0.405771000	0.526229000
O	-2.186610000	-2.247611000	-0.316056000
N	3.694415000	-3.732578000	-1.107342000
N	1.908272000	-2.316915000	-1.241592000

C	0.647070000	-3.637877000	0.802770000
C	1.861458000	-4.074319000	0.407865000
H	-3.877801000	-2.510038000	0.865972000
H	-3.278977000	0.245190000	-0.310322000
H	-2.950233000	-0.758927000	2.537611000
H	-0.769453000	-0.050361000	0.549123000
H	-5.475966000	-0.249119000	0.273304000
H	0.458532000	-0.235729000	2.258896000
H	-1.848311000	1.613565000	1.549996000
H	-4.669202000	-3.228962000	-2.634638000
N	1.785209000	2.160012000	-0.007248000
N	3.493332000	1.660332000	-1.384782000
N	3.995155000	-1.020067000	1.118061000
N	2.080493000	0.340503000	1.611653000
N	5.315688000	-0.721442000	-0.762199000
C	0.659476000	2.861273000	0.603000000
C	0.510257000	4.310552000	0.143442000
C	-0.408148000	4.177510000	-1.091502000
C	-1.317068000	2.978225000	-0.718569000
C	-1.698707000	2.081937000	-1.825763000
C	2.495015000	2.468379000	-1.153906000
C	3.455864000	0.757576000	-0.341310000
C	2.398089000	1.040664000	0.515855000
C	4.277389000	-0.333672000	-0.003934000
C	2.932587000	-0.663864000	1.835832000
O	-0.155421000	5.007452000	1.178511000
O	-1.212108000	5.323429000	-1.297456000
O	-0.576108000	2.239224000	0.284805000
H	0.796184000	2.797539000	1.680406000
H	-0.727720000	5.663507000	0.752130000
H	1.467749000	4.782946000	-0.089014000
H	-0.739816000	5.946858000	-1.862434000
H	0.174933000	3.950738000	-1.984647000
H	-2.205548000	3.400169000	-0.235211000
H	-1.117496000	1.189508000	-2.011280000
H	-2.509218000	2.359532000	-2.483840000
H	5.604331000	-0.164472000	-1.547930000
H	5.936150000	-1.436340000	-0.421174000
H	2.238188000	3.310342000	-1.773396000
H	2.725075000	-1.272493000	2.708785000

13A-PC-complex

H	-2.004393000	2.035075000	-1.907866000
H	-0.695053000	6.263165000	2.633387000
H	-0.289140000	4.984179000	3.726598000
C	-4.439679000	-1.047583000	-1.052210000

O	0.202817000	-1.426768000	-2.398571000
O	0.490517000	1.492067000	-1.786184000
C	-3.297636000	-0.195895000	-1.593602000
O	-0.954562000	0.901375000	1.619871000
H	-1.984619000	4.001658000	-1.285728000
H	-1.496945000	5.807952000	0.339019000
C	-1.058631000	2.093721000	1.337337000
N	-1.489267000	2.471035000	0.031090000
O	-4.885353000	-1.983266000	-1.685112000
O	-4.902625000	-0.666888000	0.128761000
C	-1.739100000	1.476860000	-1.002970000
O	-2.530005000	-2.021299000	-3.052599000
C	-0.520188000	0.612926000	-1.313220000
C	-0.845668000	-0.458871000	-2.359073000
C	-0.916204000	4.358844000	1.893189000
C	-2.191202000	-1.068659000	-2.144020000
O	-2.833895000	0.680355000	-0.589305000
N	-0.612504000	5.279627000	2.820717000
N	-0.776983000	3.081792000	2.219892000
C	-1.641474000	3.788241000	-0.283734000
C	-1.374021000	4.769129000	0.602577000
H	-3.752514000	0.386809000	-2.420143000
H	-2.231295000	-2.801972000	0.057558000
H	-0.820978000	0.021263000	-3.348319000
H	-0.214616000	0.114071000	-0.395546000
H	-3.447906000	-2.301281000	-2.870528000
H	1.308895000	0.988899000	-1.877581000
H	0.226955000	-1.871407000	-1.531961000
H	-5.632173000	-1.258237000	0.383540000
N	2.330051000	-0.974705000	0.564730000
N	2.777809000	1.225415000	0.542308000
N	4.907807000	0.169363000	-2.302460000
N	3.736654000	-1.678101000	-1.305782000
N	4.726721000	2.356118000	-1.548772000
C	1.740611000	-2.243096000	0.927287000
C	1.577337000	-2.460185000	2.441345000
C	0.060539000	-2.288311000	2.647208000
C	-0.505669000	-2.831946000	1.339091000
C	-1.903557000	-2.376286000	1.005872000
C	2.103354000	0.269216000	1.122274000
C	3.485138000	0.592543000	-0.465257000
C	3.220376000	-0.774791000	-0.468894000
C	4.381743000	1.062409000	-1.444905000
C	4.565818000	-1.118349000	-2.184748000
O	1.972679000	-3.788833000	2.740017000
O	-0.429516000	-3.044337000	3.743160000

O	0.429962000	-2.339641000	0.353411000
H	2.384722000	-3.015076000	0.507961000
H	1.400523000	-4.089685000	3.462789000
H	2.169899000	-1.747039000	3.018970000
H	-0.396215000	-2.504002000	4.541170000
H	-0.195894000	-1.230665000	2.742001000
H	-0.451105000	-3.926069000	1.366392000
H	-1.947039000	-1.289361000	0.948313000
H	-2.583158000	-2.719927000	1.787727000
H	4.313307000	3.045293000	-0.945554000
H	5.337586000	2.654448000	-2.289701000
H	1.398793000	0.406833000	1.925830000
H	5.024900000	-1.790320000	-2.902024000

13B-RC-complex

H	2.447480000	0.749368000	-1.535076000
H	6.364075000	4.247111000	2.405684000
H	6.502234000	4.894408000	0.806243000
C	1.990357000	-2.222627000	1.333252000
O	3.164462000	-3.330068000	-1.590018000
O	4.722507000	-0.700440000	-2.010942000
C	1.337389000	-1.309238000	0.297661000
O	4.283644000	2.066650000	-2.157020000
H	3.647484000	0.429163000	1.815375000
H	5.126263000	2.159801000	2.859507000
C	4.436739000	2.191960000	-0.931057000
N	3.820182000	1.252042000	-0.078811000
O	1.265707000	-3.341315000	1.481937000
O	2.987355000	-1.973612000	1.961763000
C	2.908062000	0.264274000	-0.673928000
O	0.480452000	-1.121220000	-1.956107000
C	3.658038000	-0.992588000	-1.120844000
C	2.682401000	-1.997978000	-1.745709000
C	5.404717000	3.183595000	0.933756000
C	1.286479000	-1.927414000	-1.113035000
O	1.921508000	-0.019238000	0.300289000
N	6.142884000	4.189268000	1.427488000
N	5.173469000	3.173648000	-0.375789000
C	4.103090000	1.228841000	1.250728000
C	4.902026000	2.168873000	1.804101000
H	0.315306000	-1.169777000	0.653108000
H	0.893424000	-2.944192000	-1.037541000
H	2.570998000	-1.748080000	-2.804833000
H	4.093567000	-1.451353000	-0.229034000
H	-0.434660000	-1.158948000	-1.624007000
H	4.585538000	0.191003000	-2.383298000

H	4.054778000	-3.372987000	-1.961553000
H	1.681260000	-3.905533000	2.155012000
N	-3.613144000	0.248798000	-0.350425000
N	-5.419544000	0.625767000	-1.626231000
N	-5.512412000	3.694134000	0.449556000
N	-3.664780000	2.266132000	1.019060000
N	-7.058145000	3.196196000	-1.206017000
C	-2.423890000	-0.387055000	0.209087000
C	-2.683988000	-1.026741000	1.572290000
C	-3.089772000	-2.457251000	1.181009000
C	-2.154405000	-2.740704000	-0.014749000
C	-2.625670000	-3.732518000	-0.991519000
C	-4.433639000	-0.194482000	-1.363698000
C	-5.245263000	1.670916000	-0.740383000
C	-4.125969000	1.456794000	0.059564000
C	-5.958710000	2.863340000	-0.509889000
C	-4.417907000	3.357646000	1.141154000
O	-1.456935000	-1.031728000	2.279476000
O	-2.835138000	-3.402136000	2.200042000
O	-2.005634000	-1.432162000	-0.651769000
H	-1.644700000	0.372295000	0.281213000
H	-1.455544000	-1.816098000	2.848544000
H	-3.462041000	-0.498084000	2.127157000
H	-3.606340000	-3.466586000	2.775900000
H	-4.134182000	-2.478122000	0.863009000
H	-1.187291000	-3.037386000	0.401136000
H	-3.394352000	-3.470144000	-1.704536000
H	-2.280591000	-4.753654000	-0.935604000
H	-7.407801000	2.594158000	-1.930363000
H	-7.534256000	4.060079000	-1.011142000
H	-4.235985000	-1.120990000	-1.874148000
H	-4.108166000	4.068942000	1.899466000

13B-PC-complex

H	1.893820000	-0.583458000	0.806036000
H	7.435552000	0.003122000	-2.646230000
H	7.658558000	-1.244501000	-1.467708000
C	0.194247000	2.768175000	-1.006675000
O	0.474825000	2.693000000	2.780134000
O	3.067296000	1.271883000	2.407321000
C	0.050478000	1.330663000	-0.485902000
O	3.987603000	-1.301518000	1.393549000
H	3.158985000	1.728687000	-1.611384000
H	5.407563000	1.417634000	-2.670388000
C	4.340601000	-0.730834000	0.348439000
N	3.466787000	0.212202000	-0.233117000

O	-1.016189000	3.312132000	-1.202944000
O	1.237367000	3.348386000	-1.180402000
C	2.129447000	0.369778000	0.340094000
O	-1.625429000	1.287793000	1.336440000
C	2.080158000	1.463258000	1.407519000
C	0.678709000	1.487933000	2.022982000
C	5.898446000	-0.234688000	-1.303689000
C	-0.336201000	1.350187000	0.956609000
O	1.252644000	0.616194000	-0.743338000
N	7.087767000	-0.513474000	-1.857878000
N	5.524720000	-0.957780000	-0.251718000
C	3.869578000	0.988020000	-1.274374000
C	5.084315000	0.810034000	-1.839516000
H	-0.738525000	0.851652000	-1.071345000
H	-3.861762000	3.110562000	-0.526937000
H	0.593071000	0.627182000	2.704081000
H	2.275964000	2.429817000	0.938334000
H	-2.221379000	1.049469000	0.590892000
H	3.282947000	0.324998000	2.459684000
H	1.117891000	2.685806000	3.502286000
H	-0.908897000	4.240509000	-1.468262000
N	-2.537045000	-1.601073000	0.041679000
N	-1.452070000	-2.268633000	1.891756000
N	1.263162000	-2.747209000	-0.582825000
N	-0.759514000	-1.942007000	-1.595790000
N	1.500137000	-3.137030000	1.695420000
C	-3.502299000	-0.943315000	-0.798440000
C	-4.981679000	-1.258913000	-0.507423000
C	-5.528906000	0.080657000	0.035189000
C	-4.645995000	1.112518000	-0.661290000
C	-4.565700000	2.466159000	-0.000276000
C	-2.565670000	-1.788240000	1.411699000
C	-0.623737000	-2.400396000	0.790394000
C	-1.276266000	-1.987369000	-0.367458000
C	0.724466000	-2.775197000	0.648825000
C	0.510209000	-2.345125000	-1.611055000
O	-5.606102000	-1.594410000	-1.733517000
O	-6.888048000	0.289928000	-0.301765000
O	-3.344933000	0.482426000	-0.640851000
H	-3.267280000	-1.218809000	-1.825434000
H	-6.511542000	-1.249986000	-1.686204000
H	-5.088134000	-2.075635000	0.210157000
H	-7.449429000	-0.043055000	0.408217000
H	-5.374895000	0.137705000	1.115519000
H	-4.975488000	1.209950000	-1.701207000
H	-4.248752000	2.372586000	1.039682000

H	-5.550148000	2.934502000	-0.023742000
H	1.136636000	-2.964428000	2.619363000
H	2.497098000	-3.004539000	1.583413000
H	-3.439535000	-1.545111000	1.994528000
H	1.002608000	-2.335976000	-2.576983000

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H	-3.331217	-2.134831	1.165676
H	-7.512529	2.558270	1.869017
H	-6.632023	3.539995	0.747890
C	0.531821	-1.353974	2.017460
O	-1.433017	-3.200167	-2.178379
O	-3.961304	-2.180338	-1.323764
C	-0.737152	-1.873512	1.294488
O	-2.852747	1.233387	-0.655732
H	-4.968044	-1.387396	2.130687
H	-6.738617	0.303961	2.513732
C	-3.809076	1.029998	0.086496
N	-3.920008	-0.215163	0.772589
O	1.502508	-2.168513	1.985968
O	0.510956	-0.236956	2.557643
C	-2.926569	-1.273644	0.620290
O	0.492006	-3.495544	-0.064455
C	-2.705906	-1.727782	-0.825182
C	-1.672505	-2.842812	-0.816615
C	-5.796755	1.717157	1.111380
C	-0.402632	-2.392596	-0.116930
O	-1.724842	-0.846760	1.221135
N	-6.725126	2.677150	1.256789
N	-4.786309	1.951365	0.288400
C	-4.957664	-0.430680	1.628418
C	-5.920500	0.491672	1.835980
H	-1.123067	-2.716821	1.887017
H	0.030608	-1.567477	-0.690181
H	-2.083843	-3.706657	-0.276199
H	-2.330405	-0.892485	-1.415708
H	1.119337	-3.245010	0.656729
H	-3.794066	-2.616614	-2.168707
H	-0.759920	-3.892238	-2.183011
N	2.727499	0.360333	-0.404188
N	4.149837	-1.279789	-0.974503
N	6.008184	0.135166	1.900867
N	3.946115	1.299823	1.489480
N	6.756047	-1.647671	0.616866
C	1.512519	1.179173	-0.357484
C	1.749100	2.626130	-0.804983

C	1.299958	2.590357	-2.276594
C	0.136035	1.576871	-2.229267
C	-0.169807	0.893952	-3.496540
C	3.009070	-0.692114	-1.242799
C	4.648761	-0.581436	0.107280
C	3.775139	0.438922	0.479239
C	5.818649	-0.715900	0.877335
C	5.083173	1.072383	2.142094
O	0.897882	3.466184	-0.044301
O	0.828979	3.841702	-2.742864
O	0.574383	0.614520	-1.246844
H	1.138918	1.143221	0.667032
H	0.636162	4.196970	-0.624291
H	2.795312	2.919116	-0.688792
H	1.568831	4.347361	-3.099334
H	2.106297	2.206152	-2.905329
H	-0.749246	2.096110	-1.847452
H	0.426704	0.047801	-3.808629
H	-0.914383	1.297337	-4.166285
H	6.575967	-2.364007	-0.064910
H	7.514547	-1.777968	1.264570
H	2.323174	-0.976470	-2.021492
H	5.292591	1.728912	2.980165

¹³C-PC-complex

H	3.517675	-2.026243	-1.118751
H	7.140073	3.056296	-2.175339
H	6.233385	3.967496	-1.016264
C	-0.472375	-1.657706	-1.660216
O	1.940221	-3.141143	2.403031
O	4.333771	-1.881922	1.338166
C	0.922746	-2.035853	-1.086962
O	2.807862	1.315283	0.661469
H	5.015823	-1.139474	-2.199970
H	6.572780	0.717207	-2.725353
C	3.736112	1.195107	-0.133425
N	3.936405	-0.047375	-0.800860
O	-1.371520	-2.528816	-1.434522
O	-0.599136	-0.613593	-2.310495
C	3.069228	-1.195651	-0.559054
O	-0.107205	-3.601515	0.488455
C	3.000782	-1.624510	0.909005
C	2.126420	-2.868391	1.009435
C	5.575247	2.058745	-1.291460
C	0.848567	-2.659862	0.277050

O	1.791151	-0.902398	-1.076464
N	6.388992	3.105010	-1.510190
N	4.597611	2.207461	-0.410640
C	4.936187	-0.176509	-1.716262
C	5.782327	0.835538	-2.000837
H	1.331459	-2.773971	-1.809782
H	0.442623	-1.201783	3.075631
H	2.686918	-3.713565	0.563099
H	2.548729	-0.827624	1.496235
H	-0.806076	-3.379869	-0.211025
H	4.287093	-2.234430	2.235423
H	1.250562	-3.812276	2.479807
N	-3.022131	0.366586	0.233433
N	-4.823959	-0.918641	0.605388
N	-6.092228	1.058118	-2.260204
N	-3.850771	1.676730	-1.650234
N	-7.322267	-0.570318	-1.155432
C	-1.662641	0.902478	0.339412
C	-1.607698	2.255040	1.064211
C	-1.185913	1.842516	2.486600
C	-0.287621	0.634812	2.225692
C	-0.181598	-0.354878	3.361534
C	-3.600453	-0.630451	0.979805
C	-5.067174	-0.064360	-0.452204
C	-3.956509	0.741566	-0.698360
C	-6.178637	0.127208	-1.293604
C	-4.959819	1.762120	-2.380536
O	-0.602477	3.048775	0.455133
O	-0.452427	2.854482	3.161304
O	-0.892283	-0.009220	1.086348
H	-1.277859	0.988779	-0.676247
H	-0.159029	3.530968	1.169376
H	-2.573427	2.765717	1.035391
H	-1.068072	3.448234	3.606798
H	-2.064444	1.543933	3.064628
H	0.705033	0.996106	1.939935
H	-1.169765	-0.723308	3.645028
H	0.269590	0.133317	4.227472
H	-7.368881	-1.339370	-0.510151
H	-8.049850	-0.469228	-1.842345
H	-3.054963	-1.113907	1.771502
H	-4.951933	2.498966	-3.176917

13D-RC-complex

H	-1.939468000	-0.555854000	0.842655000
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H	-8.393902000	-0.037659000	0.033593000
H	-7.963727000	-1.704518000	-0.147358000
C	-1.734448000	3.646204000	0.104249000
O	0.769818000	0.996226000	-1.677887000
O	-1.617737000	-0.530378000	-1.807924000
C	-1.188281000	2.472338000	0.981858000
O	-3.328259000	-2.065380000	-0.308484000
H	-4.189538000	2.139003000	0.323964000
H	-6.674430000	1.734057000	0.180415000
C	-4.182589000	-1.180079000	-0.108856000
N	-3.742494000	0.132919000	0.139477000
O	-0.932344000	4.599372000	-0.012899000
O	-2.892416000	3.560095000	-0.361970000
C	-2.292242000	0.365854000	0.371911000
O	0.925937000	1.522315000	1.591080000
C	-1.507272000	0.576691000	-0.923467000
C	-0.046978000	0.773937000	-0.530795000
C	-6.377837000	-0.431153000	-0.016553000
C	0.146535000	1.930053000	0.464438000
O	-2.139645000	1.427900000	1.275735000
N	-7.683838000	-0.744151000	-0.041207000
N	-5.504821000	-1.429444000	-0.131988000
C	-4.631242000	1.156381000	0.214652000
C	-5.963083000	0.924257000	0.124147000
H	-0.991744000	2.915370000	1.957972000
H	0.643042000	2.750408000	-0.055411000
H	0.270384000	-0.144183000	-0.028488000
H	-1.885467000	1.465541000	-1.433805000
H	1.805783000	1.244269000	1.281646000
H	-2.083007000	-1.256436000	-1.344453000
H	0.712540000	0.199529000	-2.222919000
N	3.065260000	-1.458659000	-0.023628000
N	1.775231000	-2.246850000	-1.686574000
N	-0.287919000	-3.305526000	1.200028000
N	1.727724000	-2.190657000	1.882042000
N	-0.861018000	-3.691291000	-1.019082000
C	4.031877000	-0.643741000	0.686010000
C	5.410315000	-0.567866000	0.027459000
C	5.343384000	0.755111000	-0.759415000
C	4.455377000	1.641301000	0.142301000
C	3.684320000	2.676653000	-0.566435000
C	2.857979000	-1.582528000	-1.382327000
C	1.216080000	-2.578517000	-0.464555000
C	1.999332000	-2.094503000	0.579522000
C	0.006200000	-3.199998000	-0.107158000
C	0.570785000	-2.814016000	2.099469000

O	6.372467000	-0.478743000	1.062252000
O	6.609872000	1.362823000	-0.919581000
O	3.552019000	0.699499000	0.775864000
H	4.108352000	-1.059595000	1.688723000
H	7.101322000	0.061545000	0.721160000
H	5.606316000	-1.430593000	-0.614509000
H	7.014694000	1.048865000	-1.737011000
H	4.856685000	0.600912000	-1.724316000
H	5.102399000	2.079791000	0.908499000
H	2.812751000	2.381738000	-1.135500000
H	4.044017000	3.693623000	-0.608377000
H	-0.719651000	-3.423921000	-1.980240000
H	-1.822869000	-3.778898000	-0.724020000
H	3.541878000	-1.163925000	-2.101647000
H	0.279819000	-2.931556000	3.137751000

13D-PC-complex

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symmetry c1

H	-3.871476000	-2.408610000	-0.150688000
H	-8.814517000	1.886996000	-0.278246000
H	-9.089341000	0.715461000	-1.521927000
C	-1.859118000	0.379588000	2.506744000
O	-0.097976000	-1.133610000	-1.030410000
O	-2.731965000	-0.965452000	-2.080382000
C	-2.123439000	-1.095966000	2.051147000
O	-5.300886000	-1.954503000	-1.953405000
H	-4.503718000	0.763499000	1.340945000
H	-6.683246000	1.967363000	0.976894000
C	-5.722394000	-1.056074000	-1.201738000
N	-4.900601000	-0.624732000	-0.143910000
O	-0.746167000	0.507014000	3.096241000
O	-2.694233000	1.264564000	2.262400000
C	-3.657538000	-1.378268000	0.143642000
O	0.243101000	-1.454274000	1.646836000
C	-2.484783000	-0.864264000	-0.687192000
C	-1.224399000	-1.654760000	-0.323322000
C	-7.275851000	0.563872000	-0.605336000
C	-1.017804000	-1.562547000	1.151074000
O	-3.434801000	-1.325339000	1.528704000
N	-8.489419000	1.100793000	-0.812264000
N	-6.925122000	-0.471861000	-1.363754000
C	-5.234333000	0.463374000	0.598086000
C	-6.409906000	1.103004000	0.391305000
H	-2.088638000	-1.682608000	2.976295000
H	-0.319431000	2.197989000	1.122738000

H	-1.384261000	-2.697337000	-0.648138000
H	-2.310877000	0.188693000	-0.442695000
H	0.175391000	-0.768513000	2.367791000
H	-3.554787000	-1.476993000	-2.221745000
H	-0.322500000	-1.171263000	-1.970047000
N	3.909811000	0.242927000	0.190439000
N	3.583656000	-1.919686000	-0.304005000
N	7.288926000	-1.873430000	-0.293944000
N	6.350764000	0.283946000	0.198951000
N	6.010613000	-3.766504000	-0.705561000
C	3.641976000	1.654542000	0.464088000
C	3.730655000	2.523561000	-0.798537000
C	2.253763000	2.624856000	-1.214428000
C	1.539363000	2.657534000	0.134748000
C	0.104359000	2.192336000	0.119543000
C	3.006821000	-0.769338000	-0.046363000
C	4.937184000	-1.653604000	-0.239909000
C	5.160148000	-0.312859000	0.066366000
C	6.081310000	-2.451697000	-0.422893000
C	7.352979000	-0.570281000	0.004272000
O	4.233799000	3.796368000	-0.428455000
O	1.963064000	3.806190000	-1.945024000
O	2.331171000	1.780850000	0.970314000
H	4.378705000	1.984224000	1.198456000
H	3.791522000	4.446269000	-0.995157000
H	4.362104000	2.060241000	-1.560725000
H	2.127716000	3.648622000	-2.882264000
H	1.960156000	1.731997000	-1.772925000
H	1.610699000	3.675927000	0.532537000
H	0.034525000	1.179944000	-0.279294000
H	-0.483326000	2.862761000	-0.510748000
H	5.122254000	-4.192854000	-0.903216000
H	6.851516000	-4.273047000	-0.923958000
H	1.942470000	-0.610010000	0.006355000
H	8.353858000	-0.161464000	0.095771000

14A-RC-complex

O	3.791582000	1.245220000	-2.102128000
H	1.015964000	-0.298535000	0.905761000
C	2.643583000	0.675852000	-0.077190000
N	1.709503000	1.756227000	-0.360197000
C	3.684281000	0.446759000	-1.194870000
H	2.246366000	2.570582000	-0.633529000
H	3.242684000	0.988448000	0.785233000
H	1.521303000	-1.154435000	-0.539184000
C	1.890389000	-0.606385000	0.325415000

C	2.625256000	-1.592132000	1.195302000
O	2.508674000	-2.792217000	1.112279000
O	3.399424000	-1.002763000	2.124774000
H	3.803147000	-1.695691000	2.672624000
C	4.590529000	-0.751811000	-1.084778000
H	5.013878000	-0.824107000	-0.081199000
H	4.019003000	-1.666661000	-1.261213000
H	5.387854000	-0.683229000	-1.821310000
C	0.713685000	1.479229000	-1.397115000
H	0.164208000	2.397535000	-1.602490000
H	1.140132000	1.114264000	-2.339570000
H	-0.005349000	0.741829000	-1.038838000
N	-3.141681000	0.888706000	1.600237000
N	-4.731577000	-0.304558000	2.642362000
N	-6.494002000	0.354652000	-0.549315000
N	-4.298612000	1.332550000	-0.504347000
N	-7.401243000	-0.843708000	1.217268000
C	-1.891895000	1.594192000	1.371917000
C	-1.816007000	2.979006000	2.044433000
C	-0.885665000	2.723008000	3.245472000
C	0.047712000	1.620726000	2.702773000
C	0.707301000	0.785757000	3.718506000
C	-3.527322000	0.200935000	2.728629000
C	-5.173654000	0.072496000	1.388871000
C	-4.199645000	0.815025000	0.724790000
C	-6.374929000	-0.153643000	0.690241000
C	-5.473336000	1.050746000	-1.063273000
O	-1.222753000	3.887782000	1.134953000
O	-0.126995000	3.862311000	3.606690000
O	-0.840589000	0.806338000	1.904564000
H	-1.792237000	1.712154000	0.292436000
H	-0.671527000	4.487980000	1.660190000
H	-2.807260000	3.325962000	2.348113000
H	-0.610138000	4.372255000	4.267680000
H	-1.459456000	2.341613000	4.092670000
H	0.782930000	2.095920000	2.043306000
H	0.158439000	-0.016920000	4.191701000
H	1.703170000	1.024620000	4.058522000
H	-7.312967000	-1.281575000	2.117299000
H	-8.218477000	-1.027247000	0.660846000
H	-2.862785000	0.093782000	3.569879000
H	-5.628734000	1.434090000	-2.066208000

14A-PC-complex

O	0.475617000	-1.644426000	-1.953828000
H	1.858294000	3.801821000	1.791471000

C	1.596510000	-0.465161000	-0.172451000
N	1.842816000	0.595693000	-1.137778000
C	0.726592000	-1.647047000	-0.773699000
H	2.183892000	0.158505000	-1.985976000
H	2.548715000	-0.967901000	0.037907000
H	0.367400000	0.887376000	1.086722000
C	1.037661000	0.042303000	1.099654000
C	1.311440000	-0.482508000	2.410839000
O	0.783729000	-0.059732000	3.431799000
O	2.222273000	-1.485453000	2.438428000
H	2.333917000	-1.765320000	3.360411000
C	0.312189000	-2.752330000	0.149809000
H	1.152003000	-3.069449000	0.767891000
H	-0.459604000	-2.373175000	0.825764000
H	-0.082911000	-3.588438000	-0.422834000
C	0.686950000	1.433503000	-1.478698000
H	0.946800000	2.033638000	-2.350330000
H	-0.217979000	0.863277000	-1.716681000
H	0.454735000	2.118962000	-0.663939000
N	-2.335352000	1.363204000	1.349502000
N	-2.383724000	-0.881394000	1.372031000
N	-3.270928000	-0.318710000	-2.181350000
N	-2.931108000	1.740452000	-0.989494000
N	-3.100714000	-2.412266000	-1.197622000
C	-2.061643000	2.728651000	1.747234000
C	-2.332953000	3.033744000	3.229780000
C	-0.911488000	3.115235000	3.820951000
C	-0.110511000	3.678700000	2.650158000
C	1.377629000	3.430015000	2.696827000
C	-2.158953000	0.200313000	2.070409000
C	-2.711363000	-0.419488000	0.109642000
C	-2.682698000	0.971482000	0.073448000
C	-3.027374000	-1.074205000	-1.095838000
C	-3.214106000	1.012940000	-2.068295000
O	-2.975821000	4.295791000	3.305641000
O	-0.832941000	3.987364000	4.936962000
O	-0.680289000	3.009826000	1.509498000
H	-2.682365000	3.365304000	1.117281000
H	-2.659832000	4.716697000	4.119957000
H	-2.948892000	2.265928000	3.703377000
H	-1.006987000	3.488055000	5.743371000
H	-0.543808000	2.115421000	4.065435000
H	-0.314629000	4.753799000	2.579010000
H	1.585232000	2.365731000	2.800394000
H	1.804464000	3.955698000	3.552312000
H	-2.853377000	-2.996751000	-0.418675000

H	-3.23920000	-2.836256000	-2.099000000
H	-1.835082000	0.214731000	3.097513000
H	-3.422306000	1.567727000	-2.976856000

14B-RC-complex

O	0.413791000	-1.705076000	-1.874700000
H	1.996486000	1.220685000	0.961197000
C	1.795806000	-0.393031000	-0.416882000
N	1.845558000	0.624885000	-1.466460000
C	0.851447000	-1.560257000	-0.747850000
H	2.010636000	0.153204000	-2.348769000
H	2.783724000	-0.868780000	-0.366316000
H	0.494746000	0.370324000	1.165795000
C	1.553301000	0.221602000	0.966171000
C	2.187967000	-0.507467000	2.173384000
O	1.674682000	-0.245683000	3.291700000
O	3.175595000	-1.253535000	1.964031000
C	0.536994000	-2.543880000	0.346458000
H	1.446286000	-2.813510000	0.884697000
H	-0.133441000	-2.071717000	1.069534000
H	0.053276000	-3.424986000	-0.070830000
C	0.621566000	1.421077000	-1.597840000
H	0.718961000	2.078203000	-2.463263000
H	-0.284817000	0.819347000	-1.728368000
H	0.484167000	2.048517000	-0.716683000
N	-2.149355000	1.615763000	1.329658000
N	-2.242337000	-0.612163000	1.600970000
N	-3.291232000	-0.419231000	-1.945726000
N	-2.863977000	1.749954000	-1.003289000
N	-3.100934000	-2.397827000	-0.746764000
C	-1.824818000	3.009734000	1.577304000
C	-2.418800000	3.581088000	2.871403000
C	-1.226361000	3.533916000	3.843699000
C	-0.024124000	3.785453000	2.906399000
C	1.256768000	3.227988000	3.375761000
C	-1.967012000	0.534495000	2.165064000
C	-2.619052000	-0.281751000	0.312491000
C	-2.568424000	1.096906000	0.123476000
C	-3.000205000	-1.056423000	-0.798316000
C	-3.212459000	0.916000000	-1.980513000
O	-2.797135000	4.923404000	2.618741000
O	-1.283000000	4.543356000	4.834659000
O	-0.413387000	3.154917000	1.666067000
H	-2.205961000	3.560702000	0.718189000
H	-2.643296000	5.415330000	3.439743000

H	-3.272663000	2.994191000	3.220097000
H	-1.763065000	4.209866000	5.602111000
H	-1.144344000	2.544745000	4.298079000
H	0.046606000	4.869110000	2.756554000
H	1.431758000	2.160976000	3.300738000
H	1.956552000	3.858136000	3.905173000
H	-2.753859000	-2.893220000	0.056358000
H	-3.235139000	-2.910944000	-1.601776000
H	-1.609619000	0.652388000	3.174281000
H	-3.462004000	1.373475000	-2.931922000

14B-PC-complex

O	0.623958000	-1.744982000	-1.693429000
H	1.597323000	4.305114000	1.155534000
C	1.671006000	-0.280826000	-0.088885000
N	1.753891000	0.714049000	-1.158106000
C	0.925423000	-1.579577000	-0.529562000
H	2.090339000	0.236821000	-1.986929000
H	2.683998000	-0.650858000	0.121627000
H	0.368058000	1.022473000	1.135231000
C	1.144691000	0.276000000	1.185150000
C	1.608449000	-0.136144000	2.528487000
O	0.961792000	0.340379000	3.511325000
O	2.598595000	-0.917655000	2.604809000
C	0.652189000	-2.611130000	0.524977000
H	1.479389000	-2.665573000	1.232646000
H	-0.228112000	-2.286322000	1.087950000
H	0.451245000	-3.577061000	0.064582000
C	0.489090000	1.376924000	-1.498123000
H	0.628667000	1.929204000	-2.428113000
H	-0.350184000	0.684252000	-1.636950000
H	0.211984000	2.093150000	-0.725391000
N	-2.318583000	1.419737000	1.440198000
N	-2.196466000	-0.822042000	1.458742000
N	-3.556945000	-0.347784000	-1.953118000
N	-3.236048000	1.737675000	-0.802086000
N	-3.097036000	-2.418544000	-1.007320000
C	-2.130578000	2.808703000	1.811816000
C	-2.143236000	3.071655000	3.325551000
C	-0.650257000	3.282418000	3.638114000
C	-0.150702000	3.952056000	2.361145000
C	1.335369000	3.851826000	2.112356000
C	-1.958482000	0.276963000	2.125930000
C	-2.717932000	-0.392795000	0.252410000
C	-2.798072000	0.996392000	0.219204000
C	-3.120395000	-1.074479000	-0.909546000

C	-3.594157000	0.985130000	-1.840459000
O	-2.875528000	4.266198000	3.557528000
O	-0.446001000	4.138928000	4.754859000
O	-0.866968000	3.259375000	1.321373000
H	-2.931293000	3.369101000	1.329177000
H	-2.445706000	4.705560000	4.307542000
H	-2.584964000	2.245258000	3.886627000
H	-0.386872000	3.603506000	5.554333000
H	-0.147119000	2.319926000	3.764036000
H	-0.462709000	5.003747000	2.375756000
H	1.654014000	2.809999000	2.112016000
H	1.868852000	4.384866000	2.901215000
H	-2.634247000	-2.959688000	-0.297342000
H	-3.249155000	-2.844714000	-1.906002000
H	-1.466713000	0.321591000	3.084026000
H	-3.958592000	1.517218000	-2.712789000

15-RC-complex

P	-4.725904	1.729353	0.058796
O	-6.187001	1.663895	0.614154
O	-4.738103	2.421994	-1.364151
O	-4.057640	0.422146	0.135504
O	-4.027073	2.873596	0.929245
P	-2.641581	3.681832	0.741137
O	-2.882482	4.658925	-0.461955
O	-2.232796	4.340622	1.972222
O	-1.660543	2.588518	0.141544
P	-0.750396	1.383521	0.778252
O	-1.782911	0.469429	1.513239
O	0.341024	1.855441	1.623713
O	-0.266951	0.696978	-0.544219
C	-1.124253	0.253543	-1.622737
C	-0.258701	-0.397453	-2.680499
O	0.693713	0.554544	-3.205606
C	0.572385	-1.593704	-2.221934
O	0.772699	-2.451939	-3.337014
C	1.878435	-0.941204	-1.775309
O	2.962184	-1.837562	-1.887544
C	1.982396	0.279080	-2.719665
N	2.504891	1.453793	-2.014373
C	1.936176	2.702033	-1.876751
N	2.657173	3.507375	-1.139991
C	3.755267	2.757087	-0.767928
C	4.874164	3.077775	0.057032
O	5.148674	4.123658	0.632833
N	5.742234	1.963900	0.176537

C	5.570926	0.733625	-0.397838
N	6.527052	-0.193587	-0.182188
N	4.534469	0.446737	-1.158670
C	3.672173	1.479283	-1.306752
H	-1.629284	1.120739	-2.047102
H	-1.862552	-0.453813	-1.244461
H	-0.912862	-0.697054	-3.500722
H	0.094734	-2.131115	-1.402876
H	1.624960	-2.891517	-3.207997
H	1.760112	-0.593843	-0.749514
H	3.759216	-1.317638	-1.662323
H	2.654529	0.059465	-3.553016
H	0.992414	2.934093	-2.338150
H	7.198432	-0.079863	0.557995
H	6.340215	-1.134461	-0.485581
H	6.563186	2.132197	0.742594
H	-2.617049	0.250525	1.015848
H	-3.245524	4.257946	-1.267866
H	-4.817485	1.821102	-2.119929
H	-6.726434	2.462386	0.514626
N	-0.406100	-3.274060	1.039933
N	-0.155105	-4.932139	-0.454093
N	-3.478057	-3.682561	-1.522092
N	-2.598041	-2.452276	0.343974
N	-2.376579	-5.467761	-2.512088
C	-0.061838	-2.269687	2.021361
C	0.527211	-2.804459	3.339561
C	2.003607	-2.366672	3.264023
C	1.925292	-1.078661	2.417982
C	3.174431	-0.706903	1.733508
C	0.390092	-4.283365	0.541620
C	-1.378095	-4.313594	-0.641469
C	-1.550524	-3.277719	0.272274
C	-2.413621	-4.503514	-1.577163
C	-3.509566	-2.725731	-0.586989
O	-0.132562	-2.153720	4.411996
O	2.560544	-2.088481	4.535044
O	0.913934	-1.403886	1.445012
H	-0.977460	-1.718679	2.229251
H	0.528973	-2.030618	5.110097
H	0.417687	-3.888950	3.422108
H	2.971952	-2.887149	4.885665
H	2.590569	-3.115923	2.728315
H	1.573301	-0.264920	3.060888
H	3.513019	-1.296822	0.893670
H	3.794616	0.094255	2.105280

H	-1.559885	-6.043828	-2.617209
H	-3.103857	-5.519305	-3.204776
H	1.365288	-4.486043	0.954524
H	-4.379577	-2.079531	-0.596867

15-PC-complex

P	5.012249	-0.992684	0.069595
O	6.445394	-0.744474	0.647157
O	5.135387	-1.550228	-1.407450
O	4.142780	0.178700	0.245525
O	4.507649	-2.305347	0.830969
P	3.291477	-3.324012	0.529724
O	3.738679	-4.154633	-0.723745
O	2.965271	-4.132265	1.694832
O	2.153899	-2.375200	-0.037820
P	1.024644	-1.399846	0.642482
O	1.854849	-0.400539	1.513307
O	0.000080	-2.125395	1.385552
O	0.490876	-0.680738	-0.642760
C	1.305455	-0.136905	-1.709219
C	0.375353	0.500052	-2.723535
O	-0.541444	-0.521981	-3.227676
C	-0.510143	1.584463	-2.204387
O	-0.547939	2.726607	-2.939936
C	-1.793011	0.935186	-1.777970
O	-2.894556	1.802970	-1.902722
C	-1.845909	-0.280636	-2.754729
N	-2.353167	-1.485109	-2.099610
C	-1.760931	-2.725960	-1.991501
N	-2.489991	-3.576509	-1.316575
C	-3.618904	-2.866653	-0.957040
C	-4.756222	-3.244807	-0.183510
O	-5.023774	-4.318320	0.342638
N	-5.653473	-2.156485	-0.049311
C	-5.487813	-0.898301	-0.561197
N	-6.468700	0.000427	-0.336640
N	-4.431714	-0.556416	-1.271171
C	-3.545347	-1.565239	-1.437976
H	1.860275	-0.951874	-2.173714
H	1.997442	0.605174	-1.310573
H	0.980254	0.858483	-3.558583
H	-2.661242	-1.331577	1.400831
H	-1.284954	3.271563	-2.620818
H	-1.694132	0.557993	-0.757244
H	-3.674722	1.271268	-1.651894

H	-2.511633	-0.040490	-3.588524
H	-0.795689	-2.917029	-2.426200
H	-7.163167	-0.159034	0.373094
H	-6.290177	0.957350	-0.590776
H	-6.486164	-2.364834	0.485531
H	2.633640	0.028967	1.071195
H	4.063318	-3.638795	-1.479229
H	5.096786	-0.881356	-2.106937
H	7.104522	-1.438455	0.494873
N	-0.223962	2.958624	1.114892
N	-0.764622	4.556669	-0.365804
N	2.803296	4.117735	-1.261867
N	2.129351	2.667930	0.530581
N	1.383335	5.651343	-2.271753
C	-0.369114	1.931757	2.118026
C	-1.070548	2.367683	3.425253
C	-2.342902	1.488886	3.442838
C	-1.928743	0.280905	2.605981
C	-3.057216	-0.507104	1.991876
C	-1.200941	3.771414	0.585739
C	0.577357	4.242056	-0.484403
C	0.928454	3.240197	0.414511
C	1.586956	4.683031	-1.357921
C	3.001636	3.163593	-0.344024
O	-0.225470	2.055683	4.519884
O	-2.712483	1.086732	4.752859
O	-1.143410	0.873160	1.564037
H	0.637235	1.585712	2.352243
H	-0.802287	1.716540	5.222417
H	-1.301443	3.435712	3.420442
H	-3.340787	1.720916	5.117272
H	-3.163630	2.011380	2.945528
H	-1.295729	-0.373096	3.217578
H	-3.659055	0.136570	1.349182
H	-3.693463	-0.915428	2.778210
H	0.448617	5.973253	-2.455168
H	2.092491	5.826404	-2.963683
H	-2.218207	3.729802	0.940572
H	3.992747	2.725965	-0.319907

16-RC-complex

C	-2.433618000	1.318335000	0.638423000
C	-3.825050000	1.880796000	0.324278000
C	-4.814591000	0.730998000	0.132746000
C	-4.303017000	-0.219591000	-0.931439000
C	-2.899639000	-0.716655000	-0.577903000

O	-2.024652000	0.396354000	-0.366039000
N	-4.360033000	2.807978000	1.314433000
O	-6.084356000	1.224663000	-0.279532000
O	-5.146544000	-1.367805000	-1.063688000
C	-2.270060000	-1.544696000	-1.695474000
O	-2.882165000	-2.822017000	-1.831196000
O	-2.479609000	0.732396000	1.909847000
C	-1.205966000	0.518613000	2.513444000
H	-1.675362000	2.107221000	0.604198000
H	-3.746357000	2.411755000	-0.627143000
H	-4.916212000	0.178504000	1.075702000
H	-4.255763000	0.320617000	-1.885413000
H	-2.961263000	-1.328196000	0.328980000
H	-3.899225000	3.708240000	1.260688000
H	-4.207029000	2.442154000	2.248481000
H	-6.246858000	2.010795000	0.264517000
H	-6.030964000	-1.064056000	-1.302853000
H	-2.320573000	-0.976340000	-2.632979000
H	-1.219589000	-1.715757000	-1.461470000
H	-3.840571000	-2.679281000	-1.841746000
H	-1.389083000	0.081447000	3.492556000
H	-0.594258000	-0.166748000	1.923965000
H	-0.667273000	1.463972000	2.628982000
N	2.360319000	0.035355000	-0.543381000
N	1.310508000	1.993715000	-0.233210000
N	4.795034000	3.231138000	-0.467522000
N	4.659262000	0.843952000	-0.714582000
N	2.950958000	4.590520000	-0.102664000
C	2.576489000	-1.399315000	-0.754541000
C	3.381377000	-2.037582000	0.382943000
C	2.269252000	-2.599897000	1.282241000
C	1.221889000	-3.053032000	0.244395000
C	-0.159336000	-3.150112000	0.740881000
C	1.167818000	0.696160000	-0.359531000
C	2.670113000	2.205174000	-0.347607000
C	3.340137000	1.000385000	-0.550268000
C	3.466539000	3.365192000	-0.305231000
C	5.302693000	2.008039000	-0.660041000
O	4.159364000	-3.085778000	-0.167326000
O	2.687818000	-3.708731000	2.054853000
O	1.321542000	-2.046101000	-0.797000000
H	3.098993000	-1.523373000	-1.704703000
H	4.242064000	-3.764961000	0.518558000
H	4.011006000	-1.306653000	0.894136000
H	3.058911000	-3.393955000	2.887731000
H	1.856575000	-1.806364000	1.909155000

H	1.556423000	-4.014358000	-0.159161000
H	-0.727392000	-2.251959000	0.932245000
H	-0.575844000	-4.105790000	1.019977000
H	1.957478000	4.719798000	-0.026940000
H	3.550760000	5.397057000	-0.127660000
H	0.228418000	0.172118000	-0.347089000
H	6.379279000	1.964796000	-0.787465000

16-PC-complex

C	-2.563498000	1.406065000	0.715586000
C	-3.988080000	1.863712000	0.378266000
C	-4.863261000	0.648536000	0.064514000
C	-4.229298000	-0.176959000	-1.036541000
C	-2.791364000	-0.559596000	-0.656507000
O	-2.029931000	0.607037000	-0.333674000
N	-4.643662000	2.666540000	1.403790000
O	-6.155377000	1.057989000	-0.367444000
O	-4.937197000	-1.405142000	-1.251268000
C	-2.061638000	-1.255102000	-1.760685000
O	-2.598996000	-2.404224000	-2.265585000
O	-2.603740000	0.726494000	1.939292000
C	-1.331335000	0.531157000	2.551739000
H	-1.883238000	2.262042000	0.773145000
H	-3.920841000	2.466552000	-0.530178000
H	-4.948775000	0.023426000	0.962564000
H	-4.211137000	0.412466000	-1.959996000
H	-2.854970000	-1.213457000	0.229455000
H	-4.265667000	3.605754000	1.431167000
H	-4.494763000	2.250605000	2.317307000
H	-6.406166000	1.787693000	0.220155000
H	-5.827539000	-1.195936000	-1.559584000
H	-0.979934000	-1.242630000	-1.762985000
H	-0.970270000	-3.419435000	-0.272595000
H	-3.561749000	-2.384425000	-2.106845000
H	-1.511050000	0.037675000	3.504304000
H	-0.686521000	-0.099260000	1.936750000
H	-0.831259000	1.489380000	2.723739000
N	2.380074000	0.042195000	-0.496414000
N	1.420970000	2.041675000	-0.158317000
N	4.947628000	3.131287000	-0.481623000
N	4.705353000	0.751496000	-0.718319000
N	3.172591000	4.568729000	-0.075473000
C	2.546137000	-1.400202000	-0.684565000
C	3.255475000	-2.069393000	0.502852000
C	2.071926000	-2.657447000	1.290562000
C	1.105537000	-3.043603000	0.174456000

C	-0.343144000	-3.161934000	0.580052000
C	1.221602000	0.750776000	-0.277476000
C	2.784595000	2.196895000	-0.308927000
C	3.398254000	0.965064000	-0.526086000
C	3.630180000	3.322130000	-0.288981000
C	5.398715000	1.887314000	-0.681355000
O	4.082153000	-3.104139000	-0.002274000
O	2.424583000	-3.805919000	2.044383000
O	1.267679000	-1.989476000	-0.801501000
H	3.126752000	-1.549355000	-1.596921000
H	4.069285000	-3.816977000	0.654087000
H	3.839562000	-1.349033000	1.079369000
H	2.741483000	-3.531673000	2.913079000
H	1.626323000	-1.887713000	1.926160000
H	1.452335000	-3.985259000	-0.265094000
H	-0.703432000	-2.226923000	1.009541000
H	-0.439083000	-3.948321000	1.330352000
H	2.186381000	4.741479000	0.008905000
H	3.804045000	5.349342000	-0.129629000
H	0.261854000	0.266871000	-0.236669000
H	6.469483000	1.798244000	-0.831939000

17A-RC-complex

O	4.849630000	1.332550000	-0.499032000
O	3.067869000	-0.145500000	0.317900000
H	-0.420468000	-2.018588000	-1.061116000
O	4.995387000	0.276209000	1.887237000
C	1.402861000	-2.448684000	-0.018224000
O	-1.149403000	0.284404000	-0.147486000
H	-1.629536000	-1.704811000	1.128646000
H	1.835653000	-2.249687000	0.966621000
C	1.108488000	0.238636000	-1.025514000
H	1.625128000	2.026339000	-1.649862000
H	-1.146697000	-3.225935000	0.830975000
C	1.382918000	-3.939540000	-0.280163000
H	5.535310000	-1.846537000	0.247514000
O	5.379475000	-1.060771000	-0.294214000
H	-1.166872000	1.169638000	0.252119000
C	2.443470000	-0.506533000	-0.944609000
H	5.774159000	1.599277000	-0.594342000
P	4.616350000	0.104766000	0.480404000
O	1.265175000	1.636652000	-0.845008000
O	2.274116000	-1.877953000	-1.025137000
H	0.934763000	-4.151333000	-1.253045000
C	0.014948000	-1.797772000	-0.074840000
H	0.685878000	0.020800000	-2.011747000

H	3.103749000	-0.218431000	-1.762767000
H	0.811565000	-4.455651000	0.491114000
C	0.140264000	-0.279577000	0.031000000
N	-0.808013000	-2.291798000	1.028928000
H	0.528254000	-0.023462000	1.023580000
H	2.399016000	-4.334646000	-0.269854000
N	-3.519148000	1.346783000	1.596843000
N	-3.706251000	-0.845982000	2.043318000
N	-5.347274000	-0.791853000	-1.276191000
N	-4.608244000	1.389520000	-0.588972000
N	-5.066235000	-2.702806000	0.010598000
C	-3.039367000	2.708333000	1.657346000
C	-3.092896000	3.351108000	3.051094000
C	-1.625847000	3.290938000	3.520271000
C	-0.858277000	3.446560000	2.201398000
C	0.525757000	2.939907000	2.202504000
C	-3.253437000	0.305547000	2.461649000
C	-4.290533000	-0.565656000	0.821739000
C	-4.177987000	0.787253000	0.521570000
C	-4.904483000	-1.377402000	-0.149259000
C	-5.180479000	0.526684000	-1.426757000
O	-3.505303000	4.696648000	2.888460000
O	-1.285034000	4.344216000	4.401122000
O	-1.666121000	2.738094000	1.238678000
H	-3.645071000	3.281818000	0.957641000
H	-3.065001000	5.210165000	3.582828000
H	-3.772422000	2.815770000	3.718478000
H	-1.432501000	4.060455000	5.311027000
H	-1.405489000	2.318462000	3.965213000
H	-0.876712000	4.519640000	1.947078000
H	1.160639000	3.180006000	3.043792000
H	0.953537000	2.520495000	1.303767000
H	-4.659853000	-3.170936000	0.801718000
H	-5.426096000	-3.254811000	-0.749218000
H	-2.721601000	0.459126000	3.386318000
H	-5.557957000	0.941962000	-2.355157000

17A-PC-complex

O	4.082666000	0.903210000	2.814043000
O	2.129334000	0.428149000	1.399959000
H	1.116370000	-1.888504000	-2.054928000
O	1.705242000	1.725624000	3.506179000
C	0.572447000	-1.514178000	-0.016398000
O	1.667749000	0.770257000	-2.733151000
H	-0.526649000	-0.128137000	-2.841537000
H	0.077930000	-0.725836000	0.555948000

C	2.939083000	-0.034833000	-0.827109000
H	4.539345000	1.102646000	-0.815495000
H	-1.174639000	-1.481654000	-2.217740000
C	-0.177490000	-2.817066000	0.145996000
H	1.575243000	-0.958145000	4.002181000
O	2.454930000	-0.734397000	3.667117000
H	2.378340000	1.428556000	-2.685863000
C	2.713714000	-0.616745000	0.575268000
H	4.537282000	0.981966000	3.664132000
P	2.523316000	0.656141000	2.905933000
O	3.584189000	1.234103000	-0.810434000
O	1.891465000	-1.728504000	0.544452000
H	0.289688000	-3.606840000	-0.445473000
C	0.687288000	-1.046058000	-1.477242000
H	3.579023000	-0.764109000	-1.351857000
H	3.657891000	-0.930181000	1.019038000
H	-1.214907000	-2.697120000	-0.164627000
C	1.641365000	0.097943000	-1.545369000
N	-0.632828000	-0.657712000	-1.983989000
H	-1.058216000	3.541059000	-1.972642000
H	-0.176266000	-3.116434000	1.194416000
N	-3.452356000	0.874534000	1.208547000
N	-3.481370000	-1.262377000	0.528873000
N	-6.047475000	-1.463771000	3.193157000
N	-5.138118000	0.750431000	2.971412000
N	-5.366901000	-3.266651000	1.899464000
C	-3.065833000	2.277779000	1.326648000
C	-1.917166000	2.506511000	2.321300000
C	-0.694635000	2.645824000	1.393456000
C	-1.302214000	3.300246000	0.154317000
C	-0.557645000	3.053476000	-1.135071000
C	-2.943060000	-0.078352000	0.355725000
C	-4.388389000	-1.085933000	1.554730000
C	-4.384253000	0.237300000	1.992099000
C	-5.276562000	-1.959369000	2.208910000
C	-5.937013000	-0.168012000	3.509931000
O	-2.147812000	3.724285000	3.010303000
O	0.312936000	3.467605000	1.942046000
O	-2.627351000	2.731610000	0.062227000
H	-3.953470000	2.821123000	1.654715000
H	-1.279065000	4.149836000	3.093711000
H	-1.827695000	1.674396000	3.024243000
H	0.871005000	2.909819000	2.525729000
H	-0.300042000	1.657082000	1.141778000
H	-1.392747000	4.375017000	0.348084000
H	-0.484485000	1.985014000	-1.336855000

H	0.451713000	3.460607000	-1.054464000
H	-4.873944000	-3.631637000	1.103316000
H	-6.081856000	-3.829575000	2.327756000
H	-2.186079000	0.150397000	-0.380159000
H	-6.584519000	0.172804000	4.311046000

17B-RC-complex

O	5.537279000	1.003465000	0.751739000
O	3.038042000	0.475724000	0.634181000
H	0.830501000	-1.808552000	-2.074800000
O	3.922060000	1.357004000	2.778625000
C	2.110930000	-2.022493000	-0.369098000
O	-0.591329000	0.320609000	-1.503932000
H	-1.205081000	-1.837881000	-0.671191000
H	2.060198000	-1.827576000	0.706633000
C	1.820805000	0.654170000	-1.406701000
H	2.320621000	2.526738000	-1.685463000
H	-0.378506000	-3.232788000	-0.598118000
C	2.441201000	-3.481810000	-0.607745000
H	4.014640000	-1.252387000	2.681111000
O	4.643511000	-0.965658000	2.007745000
H	-0.936051000	1.071482000	-0.998352000
C	3.095052000	0.129666000	-0.730252000
P	4.370111000	0.588184000	1.580735000
O	1.633320000	2.049212000	-1.206932000
O	3.197742000	-1.263004000	-0.928944000
H	2.474658000	-3.697886000	-1.677772000
C	0.780936000	-1.584827000	-0.998144000
H	1.903257000	0.429404000	-2.476234000
H	3.990735000	0.558179000	-1.184387000
H	1.698014000	-4.129182000	-0.141451000
C	0.609099000	-0.076717000	-0.846212000
N	-0.342385000	-2.254312000	-0.337016000
H	0.531081000	0.159283000	0.219015000
H	3.413294000	-3.718318000	-0.174062000
N	-3.507127000	0.934079000	1.070905000
N	-3.828681000	-1.261688000	1.405861000
N	-7.364896000	-0.179625000	1.176347000
N	-5.833775000	1.653856000	0.907408000
N	-6.694556000	-2.367006000	1.559855000
C	-2.824084000	2.208195000	0.813649000
C	-2.999313000	3.203058000	1.958895000
C	-1.797137000	2.865197000	2.855571000
C	-0.694443000	2.495721000	1.849306000
C	0.277270000	1.501602000	2.340483000
C	-2.942737000	-0.306806000	1.264750000

C	-5.047173000	-0.621999000	1.291597000
C	-4.868341000	0.742775000	1.075837000
C	-6.378162000	-1.078432000	1.342758000
C	-7.044188000	1.103216000	0.971548000
O	-2.875586000	4.507298000	1.422245000
O	-1.366815000	3.967032000	3.635852000
O	-1.442400000	1.972075000	0.686963000
H	-3.216248000	2.615851000	-0.118861000
H	-2.452575000	5.051973000	2.102827000
H	-3.957271000	3.072890000	2.467262000
H	-1.862410000	3.982401000	4.463259000
H	-2.036932000	2.005482000	3.485437000
H	-0.197220000	3.408323000	1.518441000
H	-0.087903000	0.587647000	2.791916000
H	1.342195000	1.620912000	2.204869000
H	-5.974077000	-3.064573000	1.623214000
H	-7.656407000	-2.658203000	1.525455000
H	-1.874584000	-0.439551000	1.275435000
H	-7.883276000	1.778578000	0.841533000

17B-PC-complex

O	5.230981000	-0.289955000	0.898020000
O	2.949620000	0.424234000	-0.009852000
H	-0.243835000	-1.984918000	-1.576659000
O	4.235960000	2.088769000	1.330843000
C	0.668563000	-1.296718000	0.236637000
O	0.142148000	0.305536000	-3.087958000
H	-1.315161000	0.429336000	-0.306078000
H	0.714346000	-0.365450000	0.808359000
C	2.206959000	-0.501837000	-2.095862000
H	3.618245000	0.179746000	-3.280597000
H	-1.912745000	-0.290400000	-1.639295000
C	0.029180000	-2.380512000	1.077878000
H	2.737841000	0.675187000	2.875196000
O	3.322487000	0.012375000	2.488980000
H	0.820487000	0.727237000	-3.638211000
C	2.819662000	-0.785427000	-0.716363000
P	4.077943000	0.614855000	1.169978000
O	2.861722000	0.548799000	-2.810859000
O	2.015082000	-1.727443000	-0.040540000
H	0.010584000	-3.325898000	0.531122000
C	-0.086848000	-1.014955000	-1.074237000
H	2.303417000	-1.439156000	-2.670886000
H	3.797283000	-1.257574000	-0.818600000
H	-0.991946000	-2.103278000	1.334127000
C	0.764536000	-0.157962000	-1.959292000

N	-1.410865000	-0.466476000	-0.776778000
H	1.144190000	2.151364000	1.160249000
H	0.597512000	-2.521768000	1.998042000
N	-3.372930000	0.783748000	1.727188000
N	-3.520573000	-1.286653000	2.585947000
N	-5.687846000	-1.735490000	-0.383974000
N	-4.804546000	0.494165000	-0.229507000
N	-5.250509000	-3.397832000	1.175105000
C	-2.899498000	2.134532000	1.496873000
C	-2.979289000	3.061679000	2.718482000
C	-1.525769000	3.078749000	3.229222000
C	-0.714232000	2.924499000	1.943359000
C	0.641669000	2.283126000	2.117440000
C	-2.989362000	-0.099544000	2.713693000
C	-4.292330000	-1.197282000	1.442614000
C	-4.206124000	0.076719000	0.888934000
C	-5.078848000	-2.133233000	0.747284000
C	-5.520360000	-0.473991000	-0.797007000
O	-3.356305000	4.349998000	2.261956000
O	-1.182230000	4.294152000	3.873963000
O	-1.531171000	2.090444000	1.100808000
H	-3.510886000	2.532889000	0.688202000
H	-2.884463000	4.990069000	2.816618000
H	-3.688979000	2.690877000	3.462196000
H	-1.396078000	4.228377000	4.812173000
H	-1.347486000	2.226788000	3.889773000
H	-0.615577000	3.912656000	1.480794000
H	0.528671000	1.305083000	2.590198000
H	1.267860000	2.914001000	2.750209000
H	-4.721742000	-3.742150000	1.957430000
H	-5.736072000	-4.056633000	0.590489000
H	-2.313046000	0.192135000	3.500512000
H	-6.035146000	-0.211494000	-1.715258000

17C-RC-complex

O	5.467433	1.271335	-0.750364
O	3.148381	0.222699	-0.474486
H	2.088010	-3.795340	0.076548
O	3.357857	2.717290	-0.506711
C	2.739351	-2.068540	1.168406
O	0.445226	-2.837645	-1.689338
H	-0.301393	-3.314461	0.552506
H	2.326022	-1.100409	1.461556
C	2.635561	-1.770971	-1.682174
H	3.022418	-0.991422	-3.443115
H	0.557529	-3.647078	1.888719

C	3.209329	-2.820503	2.397841
O	4.262780	1.427574	1.504981
H	0.320247	-2.372752	-2.525987
C	3.642204	-1.021559	-0.793752
P	4.158095	1.521840	-0.011736
O	2.262501	-1.040926	-2.852431
O	3.896300	-1.850198	0.350129
H	3.607751	-3.800137	2.122998
C	1.666276	-2.821164	0.368181
H	3.092086	-2.725347	-1.969194
H	4.613747	-0.942140	-1.289965
H	2.392872	-2.960799	3.107353
C	1.359117	-2.051674	-0.908720
N	0.434414	-2.960079	1.154087
H	0.894351	-1.097247	-0.649425
H	3.995998	-2.254473	2.898365
N	-2.544561	0.248832	-0.234264
N	-3.282106	-1.581245	0.835177
N	-6.459926	-0.502042	-0.734024
N	-4.633000	0.960995	-1.281896
N	-6.252234	-2.354361	0.648518
C	-1.611669	1.253826	-0.773594
C	-1.907136	2.653346	-0.234811
C	-1.044344	2.680411	1.036465
C	0.195986	1.862881	0.644476
C	0.828292	1.129058	1.755609
C	-2.242683	-0.825158	0.571025
C	-4.326358	-0.980564	0.160709
C	-3.885608	0.155050	-0.517262
C	-5.690898	-1.298511	0.029298
C	-5.899691	0.555955	-1.332777
O	-1.436995	3.596369	-1.182791
O	-0.647633	3.993899	1.402930
O	-0.308302	0.929140	-0.382668
H	-1.692751	1.229194	-1.861694
H	-1.078938	4.342108	-0.678131
H	-2.970583	2.798761	-0.032503
H	-1.340727	4.394540	1.941066
H	-1.580612	2.190893	1.853326
H	0.929901	2.504637	0.155629
H	0.218511	0.500024	2.392490
H	1.903526	1.141179	1.872755
H	-5.675840	-3.017385	1.136671
H	-7.205759	-2.599574	0.443125
H	-1.236037	-1.008513	0.910337
H	-6.569686	1.158102	-1.937593

17C-PC-complex

O	4.624461000	2.194219000	-0.877848000
O	2.427278000	1.056817000	-0.195756000
H	0.823324000	-2.746421000	-1.384925000
O	3.025638000	3.272243000	0.817680000
C	1.990942000	-1.751994000	0.112077000
O	-1.039111000	-0.732357000	-1.792459000
H	-1.295715000	-2.365307000	-0.050395000
H	1.811710000	-1.064841000	0.943111000
C	1.253960000	0.036566000	-2.029011000
H	1.145064000	1.624485000	-3.181341000
H	-0.235227000	-3.424197000	0.573861000
C	2.624134000	-3.028922000	0.626984000
O	4.387772000	1.207463000	1.471710000
H	-1.146044000	0.092175000	-2.291657000
C	2.566589000	0.161540000	-1.229665000
P	3.745712000	2.016229000	0.352911000
O	0.680965000	1.294888000	-2.403584000
O	2.926346000	-1.159937000	-0.797433000
H	2.801864000	-3.728477000	-0.193075000
C	0.643744000	-1.987675000	-0.595991000
H	1.501304000	-0.524199000	-2.947977000
H	3.381143000	0.462628000	-1.892185000
H	1.982632000	-3.510949000	1.365800000
C	0.226563000	-0.722585000	-1.264309000
N	-0.372501000	-2.442522000	0.363024000
H	1.330704000	1.075725000	2.057413000
H	3.578688000	-2.803321000	1.103834000
N	-3.166487000	1.111227000	1.067661000
N	-3.636331000	-1.062904000	0.778689000
N	-6.999032000	0.354963000	0.135099000
N	-5.377296000	2.055062000	0.642543000
N	-6.501079000	-1.909888000	0.043271000
C	-2.410546000	2.336777000	1.353151000
C	-2.709867000	2.879191000	2.753893000
C	-1.608297000	2.202186000	3.586717000
C	-0.427811000	2.172764000	2.616022000
C	0.566302000	1.056716000	2.832099000
C	-2.705922000	-0.183842000	1.062806000
C	-4.776138000	-0.307785000	0.582626000
C	-4.503200000	1.048103000	0.756315000
C	-6.103232000	-0.641249000	0.254785000
C	-6.594299000	1.615786000	0.329322000
O	-2.528707000	4.284451000	2.732020000

O	-1.255786000	2.941954000	4.745593000
O	-1.035314000	2.047677000	1.305903000
H	-2.675065000	3.069572000	0.589793000
H	-2.156559000	4.531227000	3.592069000
H	-3.719248000	2.618562000	3.081281000
H	-1.840024000	2.692595000	5.471398000
H	-1.912659000	1.185010000	3.847166000
H	0.077993000	3.142250000	2.662853000
H	0.070484000	0.084523000	2.819519000
H	1.048060000	1.186707000	3.803164000
H	-5.871309000	-2.672961000	0.219538000
H	-7.477077000	-2.107417000	-0.097455000
H	-1.670157000	-0.414092000	1.242938000
H	-7.361970000	2.374364000	0.217783000

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H	3.978761000	1.747926000	-1.506103000
C	-3.358441000	2.549210000	-0.529176000
C	0.064983000	2.133281000	-1.227315000
C	3.907726000	1.110108000	-0.616165000
C	1.256673000	2.427131000	1.004731000
N	0.091747000	2.388131000	0.122739000
N	-1.141774000	2.150162000	-1.737768000
O	3.376681000	1.873038000	3.030572000
N	-1.695591000	2.821878000	1.727446000
C	-1.214231000	2.566893000	0.505951000
C	3.524670000	1.980827000	0.575404000
C	-1.966134000	2.415970000	-0.661176000
O	6.667706000	-1.452085000	0.006283000
O	5.147257000	0.494427000	-0.347417000
O	4.995929000	-1.507429000	-1.939373000
C	-3.022179000	2.931100000	1.723376000
H	3.122123000	0.371669000	-0.801618000
H	-3.864597000	1.966253000	-2.398166000
H	1.085991000	0.909009000	2.577954000
N	-3.861274000	2.812728000	0.688167000
H	3.589410000	0.188659000	1.796064000
C	1.605923000	1.079845000	1.637870000
O	2.382970000	2.807854000	0.238919000
H	4.357572000	2.646707000	0.814216000
O	4.155528000	-1.718522000	0.467434000
H	1.037381000	3.183443000	1.762123000
H	1.360380000	0.284205000	0.938450000
C	3.112556000	1.169884000	1.806500000
H	-3.488000000	3.136673000	2.681312000
H	0.975112000	1.949615000	-1.771260000

N	-4.206889000	2.449787000	-1.582525000
H	-5.177727000	2.283987000	-1.361411000
P	5.245565000	-1.197585000	-0.466974000
H	4.332640000	1.937259000	3.140277000
N	-2.006949000	-1.183573000	-0.363522000
N	-3.666336000	-0.814387000	-1.828769000
N	-5.547759000	-0.312170000	1.321286000
N	-3.242861000	-0.862332000	1.717630000
N	-6.455291000	-0.033730000	-0.798896000
C	-0.676300000	-1.470362000	0.158109000
C	-0.351679000	-2.969140000	0.256477000
C	0.502605000	-3.205005000	-1.001357000
C	1.268532000	-1.876203000	-1.130792000
C	1.755732000	-1.541679000	-2.478359000
C	-2.397857000	-1.103917000	-1.679387000
C	-4.145711000	-0.694837000	-0.538064000
C	-3.127278000	-0.917733000	0.387533000
C	-5.404438000	-0.358288000	-0.012875000
C	-4.482944000	-0.556725000	2.093345000
O	0.418566000	-3.178744000	1.427869000
O	1.418680000	-4.276530000	-0.849282000
O	0.275432000	-0.891778000	-0.707915000
H	-0.634249000	-1.021620000	1.152266000
H	1.076738000	-3.856329000	1.209836000
H	-1.261020000	-3.575980000	0.274281000
H	0.983581000	-5.102049000	-1.093434000
H	-0.143159000	-3.357539000	-1.869905000
H	2.106213000	-1.879417000	-0.424447000
H	1.043591000	-1.298608000	-3.257367000
H	2.822420000	-1.531934000	-2.662853000
H	-6.415345000	-0.245786000	-1.781696000
H	-7.364859000	0.044887000	-0.374455000
H	-1.690396000	-1.243704000	-2.478751000
H	-4.656699000	-0.496278000	3.162366000

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H	1.909841000	1.728331000	-2.057598000
C	-4.768062000	1.312747000	2.009455000
C	-2.002274000	1.290447000	-0.165552000
C	2.038933000	1.624928000	-0.975054000
C	-0.740784000	3.487450000	0.295166000
N	-1.846715000	2.502770000	0.459430000
N	-3.063702000	0.630455000	0.233725000
O	2.441974000	3.006056000	1.999495000
N	-3.161525000	3.618809000	2.190325000
C	-2.890866000	2.617492000	1.343635000

C	1.444251000	2.841352000	-0.282417000
C	-3.633898000	1.446777000	1.189913000
O	5.520632000	0.571560000	0.231096000
O	3.424476000	1.543753000	-0.684878000
O	3.535238000	-0.986958000	-0.296561000
C	-4.256469000	3.377659000	2.906626000
H	1.507845000	0.722699000	-0.658437000
H	-5.276094000	-0.580243000	1.453645000
H	-0.253438000	3.829239000	2.482653000
N	-5.057492000	2.306025000	2.865854000
H	1.016427000	1.654222000	1.412999000
C	0.112808000	3.545857000	1.509144000
O	0.090289000	3.044280000	-0.759841000
H	2.046308000	3.727097000	-0.511938000
O	3.419072000	0.603592000	1.685618000
H	-1.214487000	4.437938000	0.034803000
H	-0.343180000	-1.536045000	-0.626202000
C	1.297359000	2.703192000	1.243482000
H	-4.535508000	4.140919000	3.624894000
H	-1.294408000	0.956632000	-0.903332000
N	-5.587347000	0.240330000	1.945643000
H	-6.264566000	0.114090000	2.679630000
P	4.033384000	0.319556000	0.283528000
H	2.970022000	2.156312000	1.964827000
N	-0.880613000	0.102093000	3.878394000
N	-2.977409000	-0.214267000	4.620601000
N	-2.373609000	3.161566000	6.018252000
N	-0.474472000	2.326381000	4.806197000
N	-4.346664000	1.966653000	6.298216000
C	0.343088000	-0.104862000	3.117842000
C	1.227804000	-1.280634000	3.586317000
C	0.906555000	-2.370635000	2.542927000
C	0.661224000	-1.542696000	1.279685000
C	-0.195114000	-2.201027000	0.225618000
C	-1.984643000	-0.718453000	3.933130000
C	-2.513111000	1.017684000	5.040771000
C	-1.212717000	1.234088000	4.587116000
C	-3.098896000	2.054584000	5.787240000
C	-1.131139000	3.232490000	5.525820000
O	2.601500000	-0.967031000	3.574302000
O	1.938139000	-3.326917000	2.414349000
O	-0.017661000	-0.360992000	1.771948000
H	0.903582000	0.825679000	3.211544000
H	2.869924000	-0.394037000	2.780896000
H	0.969426000	-1.587267000	4.600133000
H	2.759126000	-2.846104000	2.608510000

H	-0.004296000	-2.907436000	2.822654000
H	1.627239000	-1.254415000	0.855315000
H	-1.172855000	-2.473293000	0.628291000
H	0.302456000	-3.104930000	-0.130738000
H	-4.965717000	1.268141000	5.920936000
H	-4.771297000	2.812492000	6.642684000
H	-1.999337000	-1.671129000	3.430001000
H	-0.595334000	4.151118000	5.740144000

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H	-1.073375000	-2.214566000	-1.252256000
C	-3.864944000	-3.371993000	0.196118000
H	-4.631981000	-2.704389000	-0.200524000
H	-4.237916000	-4.391951000	0.163417000
H	-3.651289000	-3.095804000	1.224991000
C	-2.627037000	-3.289535000	-0.659614000
H	-3.116956000	0.656936000	0.885385000
H	-1.226659000	-0.276768000	-0.261725000
H	-0.514203000	-0.576653000	3.252344000
H	-3.966467000	-0.874872000	0.914971000
O	-2.299866000	-4.219127000	-1.396387000
C	-1.350408000	-1.317763000	1.619107000
C	-1.905159000	-0.982883000	0.215025000
N	-1.888331000	-2.144635000	-0.660782000
S	-3.967744000	0.103473000	-1.291177000
C	-3.260596000	-0.277464000	0.346397000
O	-1.442988000	-2.453205000	2.076874000
N	-0.753264000	-0.322958000	2.303935000
C	-5.285477000	1.236082000	-0.758593000
H	-5.967392000	0.727347000	-0.078380000
H	-4.863970000	2.119922000	-0.279537000
H	-5.824899000	1.537801000	-1.655443000
C	-0.699970000	1.097142000	1.995085000
H	-1.605179000	1.612981000	2.322463000
H	0.153641000	1.530564000	2.512315000
H	-0.561978000	1.264143000	0.929294000
N	-5.328717000	-1.275779000	3.319574000
N	-5.386842000	-3.491053000	3.678846000
N	-7.656130000	-3.314943000	0.755812000
N	-6.840775000	-1.150994000	1.406796000
N	-7.094077000	-5.278744000	1.853679000
C	-4.968478000	0.127006000	3.462731000
C	-5.616043000	0.827233000	4.665499000
C	-4.488377000	0.806474000	5.712124000
C	-3.228572000	0.953066000	4.828669000
C	-1.986673000	0.423641000	5.416109000

C	-4.883322000	-2.346561000	4.063813000
C	-6.213310000	-3.166495000	2.620241000
C	-6.189555000	-1.795500000	2.379509000
C	-6.993351000	-3.943904000	1.743182000
C	-7.544116000	-1.986988000	0.645474000
O	-5.913303000	2.157982000	4.282612000
O	-4.561557000	1.882741000	6.626162000
O	-3.564025000	0.216887000	3.631839000
H	-5.282228000	0.618499000	2.541817000
H	-5.808937000	2.708428000	5.073395000
H	-6.514525000	0.302433000	5.000453000
H	-5.100088000	1.623029000	7.383292000
H	-4.471288000	-0.154435000	6.231013000
H	-3.123344000	2.016342000	4.585481000
H	-1.823397000	-0.645325000	5.441892000
H	-1.311148000	1.077610000	5.946388000
H	-6.558961000	-5.775232000	2.544295000
H	-7.609013000	-5.800181000	1.165043000
H	-4.172608000	-2.216813000	4.862521000
H	-8.094888000	-1.536634000	-0.173284000

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H	-0.810629000	-1.545129000	-0.650327000
C	-0.007545000	-1.080184000	2.573891000
H	-0.915913000	-0.650564000	3.000309000
H	0.368228000	-1.838571000	3.255261000
H	0.733711000	-0.294710000	2.452482000
C	-0.334078000	-1.748773000	1.261996000
H	-1.267673000	2.355642000	0.560127000
H	-0.990830000	0.588803000	-1.038203000
H	2.195733000	2.285491000	-0.882196000
H	-0.723272000	1.358054000	1.901603000
O	-0.399718000	-2.974317000	1.175556000
C	0.969673000	0.888061000	-0.196091000
C	-0.506516000	0.439964000	-0.073690000
N	-0.617877000	-0.988050000	0.168676000
S	-2.942743000	0.760415000	1.207549000
C	-1.231675000	1.337007000	0.941049000
O	1.866765000	0.238337000	0.331412000
N	1.222435000	2.014894000	-0.890257000
C	-3.490718000	1.888434000	2.363209000
H	-2.558911000	-2.855950000	2.790592000
H	-2.940064000	2.794768000	2.566665000
H	-4.437780000	1.684455000	2.840017000
C	0.302954000	2.914791000	-1.571786000
H	-0.016722000	3.734558000	-0.924817000

H	0.807877000	3.336027000	-2.439143000
H	-0.576885000	2.384021000	-1.926979000
N	-7.260097000	-2.301902000	2.756834000
N	-8.163840000	-4.342446000	2.519800000
N	-11.242475000	-2.299755000	2.240433000
N	-9.282892000	-0.949155000	2.578579000
N	-11.201277000	-4.615834000	2.120451000
C	-6.269203000	-1.248092000	2.977587000
C	-6.200479000	-0.800577000	4.444805000
C	-5.008656000	-1.619935000	4.972443000
C	-4.091324000	-1.686084000	3.753286000
C	-3.147175000	-2.863052000	3.707944000
C	-7.059646000	-3.661628000	2.704975000
C	-9.152472000	-3.380782000	2.449781000
C	-8.610034000	-2.105602000	2.594918000
C	-10.546398000	-3.450487000	2.263765000
C	-10.586984000	-1.143356000	2.394912000
O	-5.909032000	0.585916000	4.474861000
O	-4.333277000	-0.984299000	6.045923000
O	-4.997299000	-1.747045000	2.629300000
H	-6.547354000	-0.406980000	2.340819000
H	-5.319116000	0.732289000	5.230058000
H	-7.133596000	-1.012820000	4.972194000
H	-4.757320000	-1.228082000	6.877275000
H	-5.341466000	-2.622348000	5.254296000
H	-3.530417000	-0.748269000	3.696644000
H	-3.696267000	-3.804501000	3.766916000
H	-2.459228000	-2.807740000	4.553258000
H	-10.696064000	-5.483427000	2.080334000
H	-12.190263000	-4.615296000	1.938943000
H	-6.071587000	-4.079984000	2.791696000
H	-11.203287000	-0.250887000	2.366597000

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N	-0.829246000	1.326277000	-2.990257000
H	-4.466139000	3.312515000	-4.200173000
H	3.227339000	-1.932918000	-0.974081000
O	-3.559362000	-0.882085000	-1.825919000
H	-5.016707000	0.400591000	-0.880242000
C	-2.713862000	0.257321000	-1.764502000
C	4.284473000	0.202287000	-1.473256000
H	4.348712000	-0.074548000	-0.421030000
C	-4.008337000	1.759134000	-3.126264000
N	2.899883000	0.494639000	-1.851583000
H	-1.526179000	3.270151000	-3.569335000
O	3.447520000	2.722147000	-2.154071000

N	0.522038000	3.113213000	-3.000531000
O	-4.725157000	1.320868000	-0.799044000
H	-1.996039000	0.184988000	-0.947588000
C	1.971884000	-0.525684000	-1.860653000
H	-3.064935000	-1.664801000	-1.559278000
H	-3.052031000	2.339608000	-1.302901000
C	1.224139000	1.993641000	-2.588339000
C	0.398351000	0.880532000	-2.576281000
C	-2.029319000	0.495036000	-3.119292000
C	2.586339000	1.848445000	-2.202572000
N	2.389719000	-1.764883000	-1.516397000
H	-1.730905000	-0.444758000	-3.582909000
C	-0.690301000	2.681850000	-3.228326000
O	-4.046063000	3.137049000	-3.348926000
H	-4.959219000	1.292138000	-3.393008000
O	-2.985291000	1.137597000	-3.927465000
H	4.679034000	-0.607511000	-2.084993000
H	1.659813000	-2.451972000	-1.431259000
C	-3.626087000	1.484071000	-1.661845000
N	0.709185000	-0.374441000	-2.218390000
H	4.869161000	1.098564000	-1.638623000
N	6.061586000	-4.397019000	-0.504652000
N	8.282973000	-4.257988000	-0.791778000
N	7.593789000	-7.186763000	-2.956319000
N	5.599336000	-6.326379000	-1.926739000
N	9.703899000	-6.287113000	-2.617695000
C	4.720900000	-4.127466000	-0.004868000
C	4.415708000	-4.813225000	1.331232000
C	4.745087000	-3.707695000	2.348678000
C	4.275994000	-2.439518000	1.601779000
C	4.915787000	-1.179094000	2.008838000
C	7.235132000	-3.743034000	-0.200722000
C	7.780946000	-5.315373000	-1.526055000
C	6.401811000	-5.418532000	-1.361650000
C	8.382850000	-6.265335000	-2.374480000
C	6.279671000	-7.164102000	-2.706849000
O	3.033283000	-5.115956000	1.356004000
O	4.025926000	-3.833976000	3.558197000
O	4.585797000	-2.729551000	0.211346000
H	4.022747000	-4.467812000	-0.769789000
H	2.747334000	-5.060065000	2.280076000
H	5.023219000	-5.711456000	1.469108000
H	4.530143000	-4.379367000	4.173608000
H	5.822613000	-3.665950000	2.524424000
H	3.188621000	-2.379960000	1.717529000
H	5.904601000	-0.933764000	1.647011000

H	4.457397000	-0.558693000	2.764418000
H	10.312555000	-5.601496000	-2.206581000
H	10.088332000	-6.976544000	-3.240555000
H	7.243262000	-2.882274000	0.446603000
H	5.696839000	-7.931025000	-3.206210000

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N	-0.712393000	1.382453000	-2.994129000
H	-4.108660000	3.803959000	-4.069380000
H	2.885183000	-2.363209000	-1.011172000
O	-3.652547000	-0.571258000	-1.889552000
H	-4.957465000	0.818179000	-0.875856000
C	-2.690032000	0.467913000	-1.791501000
C	4.215155000	-0.298487000	-1.640271000
H	3.659051000	-0.683717000	1.349345000
C	-3.823824000	2.161954000	-3.070246000
N	2.925750000	0.096662000	-1.926602000
H	-1.202683000	3.410420000	-3.486469000
O	3.693456000	2.278156000	-2.136034000
N	0.818340000	3.017011000	-2.937707000
O	-4.567933000	1.696979000	-0.756875000
H	-1.977181000	0.283905000	-0.988076000
C	1.865511000	-0.816857000	-1.948741000
H	-3.239915000	-1.414915000	-1.673666000
H	-2.797769000	2.550918000	-1.233796000
C	1.400158000	1.813793000	-2.575925000
C	0.461385000	0.794095000	-2.605641000
C	-1.995751000	0.690198000	-3.143752000
C	2.737695000	1.518988000	-2.214240000
N	2.134173000	-2.108061000	-1.643070000
H	-1.803308000	-0.254798000	-3.650421000
C	-0.432313000	2.724106000	-3.176435000
O	-3.707206000	3.543859000	-3.230984000
H	-4.823549000	1.817750000	-3.345046000
O	-2.883234000	1.465974000	-3.911026000
H	4.454082000	-1.338550000	-1.539001000
H	1.314989000	-2.692401000	-1.588456000
C	-3.463899000	1.780034000	-1.624253000
N	0.636111000	-0.497418000	-2.291636000
H	4.959280000	0.474412000	-1.605591000
N	5.939916000	-4.382545000	-0.569935000
N	7.990014000	-3.682284000	-1.154123000
N	8.024622000	-7.016720000	-2.769794000
N	5.954338000	-6.580179000	-1.629161000
N	9.789895000	-5.514419000	-2.847171000
C	4.616417000	-4.411554000	0.041519000

C	4.596691000	-5.081725000	1.421168000
C	4.693141000	-3.874040000	2.371218000
C	3.896627000	-2.806394000	1.624520000
C	4.251347000	-1.375731000	1.947857000
C	6.887603000	-3.384994000	-0.513627000
C	7.765210000	-4.947829000	-1.659667000
C	6.495846000	-5.400354000	-1.307886000
C	8.549847000	-5.824856000	-2.433379000
C	6.787194000	-7.318245000	-2.360233000
O	3.348600000	-5.734007000	1.570971000
O	4.098012000	-4.115979000	3.634026000
O	4.181871000	-3.075057000	0.227719000
H	3.954741000	-4.942029000	-0.643667000
H	3.110066000	-5.672617000	2.508312000
H	5.426058000	-5.783862000	1.535823000
H	4.753151000	-4.504611000	4.225790000
H	5.735898000	-3.564429000	2.478611000
H	2.831773000	-2.987102000	1.799445000
H	5.308515000	-1.184099000	1.758795000
H	4.043736000	-1.184780000	3.001766000
H	10.216039000	-4.644890000	-2.579222000
H	10.327416000	-6.185052000	-3.369019000
H	6.690944000	-2.458116000	-0.002439000
H	6.419710000	-8.292640000	-2.664400000

21A-RC-complex

N	0.401141000	-0.888357000	-1.413481000
N	-1.048448000	0.791008000	-1.747595000
N	-3.328459000	-1.625898000	-0.109018000
N	-1.096731000	-2.489675000	-0.335317000
N	-3.965103000	0.484876000	-0.831534000
C	1.624534000	-1.668731000	-1.443811000
C	1.936618000	-2.307658000	-2.809093000
C	3.054461000	-1.403582000	-3.361735000
C	3.789674000	-0.997277000	-2.065011000
C	4.593633000	0.231408000	-2.158673000
C	0.185109000	0.382258000	-1.903432000
C	-1.690051000	-0.265016000	-1.130060000
C	-0.806561000	-1.318909000	-0.911920000
C	-3.014809000	-0.455905000	-0.693718000
C	-2.374091000	-2.552549000	0.034674000
O	2.424946000	-3.616502000	-2.578461000
O	3.937867000	-2.084037000	-4.229266000
O	2.714019000	-0.812198000	-1.123694000
H	1.510991000	-2.453122000	-0.694845000
H	3.057023000	-3.810281000	-3.287154000

H	1.053565000	-2.324483000	-3.452929000
H	3.630665000	-1.989182000	-5.138585000
H	2.626033000	-0.518200000	-3.836346000
H	4.409115000	-1.848516000	-1.759873000
H	4.100502000	1.194364000	-2.190530000
H	5.636028000	0.168357000	-2.434969000
H	-3.766671000	1.342558000	-1.315947000
H	-4.911240000	0.284952000	-0.556015000
H	0.984051000	0.976803000	-2.314325000
H	-2.687116000	-3.474071000	0.514110000
H	0.122107000	2.840621000	-0.059483000
C	2.022260000	2.121032000	0.638927000
P	3.770701000	2.549507000	0.657311000
O	1.508556000	3.306364000	-1.456729000
O	4.598902000	1.204346000	0.902306000
H	1.682427000	1.977064000	1.666088000
H	2.459888000	3.503701000	-1.488183000
O	4.201880000	3.298307000	-0.550201000
H	1.947525000	1.161770000	0.125181000
O	3.953275000	3.313518000	2.042487000
H	1.221978000	4.133001000	0.434354000
C	1.161173000	3.167859000	-0.081969000
H	4.797590000	3.779114000	2.128488000
H	4.758750000	0.718257000	0.072085000

21A-PC-complex

N	-0.030291000	-1.140235000	-1.444150000
N	-1.190696000	0.752550000	-1.769142000
N	-3.967384000	-1.458739000	-0.707232000
N	-1.855955000	-2.606655000	-0.749686000
N	-4.227503000	0.771524000	-1.290809000
C	1.081224000	-2.080550000	-1.419314000
C	1.405087000	-2.689382000	-2.795440000
C	2.637812000	-1.876465000	-3.230252000
C	3.333096000	-1.614014000	-1.896450000
C	4.268639000	-0.429790000	-1.871067000
C	-0.010220000	0.186400000	-1.812243000
C	-2.042346000	-0.254271000	-1.357776000
C	-1.340004000	-1.439562000	-1.150559000
C	-3.428366000	-0.296232000	-1.115681000
C	-3.169308000	-2.521398000	-0.550745000
O	1.748987000	-4.051779000	-2.607506000
O	3.499522000	-2.597759000	-4.095382000
O	2.240832000	-1.394255000	-0.980327000
H	0.802964000	-2.873705000	-0.724024000
H	2.436239000	-4.258108000	-3.259145000

H	0.561897000	-2.590983000	-3.483756000
H	3.217213000	-2.467069000	-5.008346000
H	2.324359000	-0.931707000	-3.682548000
H	3.866073000	-2.526677000	-1.606048000
H	3.741564000	0.487441000	-2.134858000
H	5.076495000	-0.595235000	-2.585666000
H	-3.834554000	1.667828000	-1.518825000
H	-5.198223000	0.715061000	-1.034395000
H	0.908614000	0.686476000	-2.068814000
H	-3.661760000	-3.429470000	-0.219060000
H	4.708661000	-0.308368000	-0.880836000
C	3.766075000	2.385388000	0.733541000
P	3.957594000	4.178431000	0.773157000
O	2.289928000	2.434317000	-1.241730000
O	5.416157000	4.512190000	1.331968000
H	3.781791000	1.992074000	1.750034000
H	2.708859000	3.313758000	-1.334965000
O	3.661068000	4.793584000	-0.545325000
H	4.666878000	2.008931000	0.222312000
O	3.024599000	4.620089000	1.981445000
H	2.098085000	0.993322000	0.200329000
C	2.514308000	1.975214000	0.025718000
H	2.866243000	5.573274000	2.039461000
H	6.085379000	4.594355000	0.637913000

21B-RC-complex

N	0.315222	-0.950672	-1.347023
N	-1.080388	0.798555	-1.496469
N	-3.495741	-1.780132	-0.381606
N	-1.271226	-2.659162	-0.619724
N	-4.057814	0.426877	-0.826378
C	1.522865	-1.759168	-1.435568
C	1.763125	-2.355416	-2.832356
C	2.823774	-1.407794	-3.419347
C	3.642459	-1.043920	-2.160526
C	4.413330	0.205244	-2.249013
C	0.154358	0.385158	-1.643959
C	-1.776995	-0.321710	-1.087916
C	-0.926750	-1.420414	-0.988545
C	-3.127724	-0.543074	-0.760152
C	-2.568651	-2.743963	-0.333895
O	2.295081	-3.657707	-2.668927
O	3.658267	-2.033543	-4.373960
O	2.638685	-0.940953	-1.129497
H	1.416505	-2.564345	-0.707452
H	2.890867	-3.813942	-3.417108

H	0.842748	-2.376431	-3.421775
H	3.279702	-1.918671	-5.253508
H	2.348564	-0.512291	-3.825851
H	4.301463	-1.894565	-1.948850
H	3.925134	1.160698	-2.111351
H	5.417336	0.180214	-2.647347
H	-3.787809	1.374864	-1.022247
H	-4.992452	0.242973	-0.503991
H	0.985350	1.014300	-1.920886
H	-2.925870	-3.719602	-0.021416
H	0.412783	2.754097	0.055452
C	2.392322	2.160688	0.697991
P	4.136941	2.723080	0.629064
O	1.734750	3.218154	-1.415875
O	4.987764	1.330296	0.802810
H	2.098070	2.050347	1.744081
H	2.711055	3.327855	-1.456444
O	4.371473	3.252911	-0.771294
H	2.330041	1.177008	0.228007
O	4.478873	3.576200	1.809026
H	1.472342	4.111406	0.448181
C	1.438510	3.118860	-0.021268
H	4.974106	0.819685	-0.022139

21B-PC-complex

N	0.114404	-1.146339	-1.615855
N	-1.061211	0.694715	-1.099418
N	-3.365574	-1.866200	0.265639
N	-1.397769	-2.840863	-0.711750
N	-3.772688	0.417323	0.319910
C	1.209384	-1.972894	-2.070961
C	1.727759	-1.633722	-3.483874
C	3.101088	-0.994219	-3.197347
C	3.531877	-1.711008	-1.920279
C	4.573069	-0.996638	-1.094277
C	0.032685	0.229034	-1.644172
C	-1.744039	-0.431438	-0.677716
C	-1.028152	-1.585996	-0.984401
C	-2.974967	-0.611117	-0.019451
C	-2.573439	-2.884518	-0.088799
O	1.882332	-2.845569	-4.204484
O	4.040409	-1.224173	-4.236134
O	2.307622	-1.813984	-1.173486
H	0.846044	-3.000912	-2.054813
H	2.670295	-2.736016	-4.759116

H	1.048274	-0.960178	-4.011899
H	3.994279	-0.501300	-4.872629
H	2.983253	0.073776	-2.998585
H	3.880924	-2.715567	-2.191171
H	4.262819	0.025966	-0.876569
H	5.510452	-0.955104	-1.651609
H	-3.463544	1.364481	0.188755
H	-4.604857	0.245786	0.857842
H	0.815506	0.828981	-2.080593
H	-2.940966	-3.872505	0.168000
H	4.754860	-1.530566	-0.160660
C	2.120537	2.895814	-0.080872
P	3.924037	3.151673	0.180634
O	2.403287	2.570268	-2.495821
O	4.253127	2.259231	1.514589
H	1.552180	3.508966	0.618994
H	3.324268	2.420144	-2.143106
O	4.598118	2.496739	-1.010679
H	1.912270	1.840720	0.165191
O	4.234297	4.568754	0.532040
H	0.693879	3.430336	-1.740347
C	1.720942	3.198002	-1.487240
H	4.320598	1.320011	1.301789

21C-RC-complex

N	1.143251000	0.081786000	-0.025200000
N	0.408787000	2.127091000	-0.576908000
N	-2.262438000	1.151448000	1.809828000
N	-0.611386000	-0.571766000	1.532632000
N	-2.196346000	3.204773000	0.736795000
C	1.943165000	-1.135705000	-0.024345000
C	1.564035000	-2.108032000	-1.149105000
C	2.593622000	-1.762025000	-2.237258000
C	3.843923000	-1.431940000	-1.390098000
C	4.840005000	-0.561172000	-2.034564000
C	1.335649000	1.224742000	-0.768139000
C	-0.454332000	1.557186000	0.341445000
C	-0.015547000	0.279717000	0.688884000
C	-1.645403000	2.007931000	0.959214000
C	-1.727328000	-0.048651000	2.039180000
O	1.764005000	-3.428077000	-0.675683000
O	2.874700000	-2.845061000	-3.102606000
O	3.303605000	-0.788939000	-0.215269000
H	1.796044000	-1.610188000	0.946196000
H	2.029835000	-3.963630000	-1.438166000

H	0.532177000	-1.958194000	-1.477756000
H	2.258775000	-2.828118000	-3.844780000
H	2.272318000	-0.878887000	-2.794102000
H	4.295395000	-2.390336000	-1.105638000
H	5.619345000	-0.992148000	-2.645118000
H	4.719446000	0.512746000	-2.002016000
H	-1.686956000	4.023506000	0.320502000
H	-2.998488000	3.424300000	1.307115000
H	2.191060000	1.334351000	-1.413277000
H	-2.275218000	-0.679717000	2.732334000
H	2.655743000	4.559912000	1.836681000
C	0.627585000	5.334204000	1.959100000
P	-0.593366000	6.380772000	1.026817000
O	2.587323000	6.382096000	0.919048000
O	-1.698345000	6.745702000	2.010778000
H	0.171959000	4.360917000	2.164649000
H	1.829333000	6.986289000	0.690556000
O	0.243877000	7.586784000	0.546327000
H	0.821559000	5.815781000	2.923285000
O	-1.083211000	5.514004000	-0.151181000
H	1.780844000	4.558652000	0.305992000
C	1.953819000	5.136020000	1.223922000

21C-PC-complex

N	1.153609000	0.278180000	-0.019669000
N	0.365730000	2.264854000	-0.698817000
N	-2.327186000	1.329642000	1.678144000
N	-0.617970000	-0.351765000	1.528050000
N	-2.280742000	3.342010000	0.523412000
C	2.001206000	-0.904114000	0.079238000
C	1.634557000	-2.000050000	-0.932958000
C	2.656264000	-1.754983000	-2.057157000
C	3.884630000	-1.287171000	-1.278837000
C	4.861373000	-0.435882000	-2.054407000
C	1.325105000	1.384000000	-0.820994000
C	-0.497664000	1.717668000	0.232886000
C	-0.026838000	0.474815000	0.656775000
C	-1.710205000	2.163762000	0.807907000
C	-1.764355000	0.157242000	1.977199000
O	1.859930000	-3.259530000	-0.322312000
O	2.967730000	-2.929176000	-2.789559000
O	3.338691000	-0.523295000	-0.183160000
H	1.894259000	-1.286632000	1.095096000
H	2.170676000	-3.856414000	-1.019717000
H	0.598040000	-1.906094000	-1.266406000
H	2.340182000	-3.027458000	-3.515298000

H	2.301550000	-0.960361000	-2.718927000
H	4.388969000	-2.172946000	-0.877093000
H	5.265902000	-1.014344000	-2.886508000
H	5.690315000	-0.123254000	-1.418936000
H	-1.733911000	4.161217000	0.168417000
H	-3.089398000	3.569072000	1.082303000
H	2.190910000	1.484164000	-1.453321000
H	-2.313463000	-0.458408000	2.682989000
H	4.370156000	0.453407000	-2.453246000
C	0.344603000	5.256541000	2.181902000
P	-0.600849000	6.450028000	1.087316000
O	2.456138000	5.891502000	1.099289000
O	-1.769047000	6.978251000	1.905964000
H	-0.249443000	4.355713000	2.348043000
H	1.819358000	6.671842000	0.951814000
O	0.476776000	7.517498000	0.769528000
H	0.427533000	5.774670000	3.148796000
O	-1.023948000	5.663390000	-0.165252000
H	1.896523000	3.902446000	1.265333000
C	1.689911000	4.896212000	1.651097000

22A-RC-complex

N	0.373334000	-1.438036000	-1.881094000
N	-0.381523000	0.062897000	-3.374575000
N	-1.475769000	1.751164000	-0.259835000
N	-0.330915000	-0.310240000	0.173395000
N	-1.857938000	2.571059000	-2.392646000
C	1.043101000	-2.584177000	-1.289151000
C	1.244787000	-3.766760000	-2.235554000
C	2.672760000	-3.532426000	-2.766133000
C	3.391819000	-2.936246000	-1.535378000
C	4.518931000	-2.036374000	-1.832028000
C	0.251961000	-1.066067000	-3.207431000
C	-0.691374000	0.480490000	-2.094466000
C	-0.225787000	-0.431665000	-1.155723000
C	-1.353539000	1.619979000	-1.595546000
C	-0.965998000	0.809190000	0.532413000
O	1.196743000	-4.943119000	-1.450251000
O	3.317119000	-4.729440000	-3.151096000
O	2.346022000	-2.206822000	-0.840195000
H	0.450836000	-2.883403000	-0.425752000
H	1.786918000	-5.586418000	-1.871159000
H	0.496632000	-3.801374000	-3.030916000
H	3.133833000	-4.907072000	-4.081350000
H	2.661926000	-2.807415000	-3.582745000
H	3.710998000	-3.773453000	-0.907706000

H	4.319518000	-1.037383000	-2.194692000
H	5.535496000	-2.396967000	-1.791604000
H	-1.763361000	2.507345000	-3.391217000
H	-2.304167000	3.378088000	-1.991057000
H	0.641855000	-1.674084000	-4.006481000
H	-1.044806000	0.979056000	1.599145000
H	2.904960000	0.204038000	-0.345801000
H	1.912180000	-1.381274000	2.622590000
H	1.050811000	-0.756353000	1.341179000
C	2.795817000	0.324543000	1.795878000
N	2.009485000	-0.952617000	1.705175000
C	2.813088000	0.991807000	0.405205000
C	2.156747000	1.225957000	2.885940000
O	0.989455000	0.922423000	3.230549000
H	1.851704000	1.477362000	0.232600000
H	3.807207000	0.051321000	2.091863000
O	2.868311000	2.167602000	3.287024000
C	3.933900000	1.979813000	0.214573000
C	3.696122000	3.350329000	0.156234000
C	5.251344000	1.536772000	0.074242000
C	4.733562000	4.258075000	-0.029844000
H	2.684186000	3.721694000	0.262498000
C	6.299135000	2.427526000	-0.108412000
H	5.463312000	0.473882000	0.103103000
C	6.040930000	3.796311000	-0.159709000
H	4.527595000	5.321452000	-0.072930000
H	7.317137000	2.076686000	-0.218579000
O	7.107208000	4.633444000	-0.344137000
H	6.808425000	5.551081000	-0.363391000
H	2.434401000	-1.613835000	1.045421000

22A-PC-complex

N	0.390417000	-1.436444000	-1.749860000
N	-1.409099000	-1.951341000	-2.992045000
N	-3.138058000	-0.743955000	0.058114000
N	-0.750752000	-0.593569000	0.243636000
N	-4.222635000	-1.553092000	-1.822372000
C	1.764786000	-1.254356000	-1.340184000
C	2.768802000	-2.275618000	-1.912085000
C	3.602072000	-1.426696000	-2.898691000
C	3.549953000	-0.035180000	-2.276688000
C	3.789223000	1.119406000	-3.215879000
C	-0.104909000	-1.911145000	-2.949153000
C	-1.812235000	-1.465517000	-1.762562000
C	-0.711669000	-1.127495000	-0.984438000
C	-3.081224000	-1.260169000	-1.185562000

C	-2.002331000	-0.439113000	0.683603000
O	3.572710000	-2.752050000	-0.849745000
O	4.948777000	-1.858725000	-2.986201000
O	2.206077000	0.043797000	-1.754758000
H	1.776295000	-1.320979000	-0.252048000
H	4.485958000	-2.773656000	-1.176028000
H	2.265644000	-3.112316000	-2.400696000
H	5.025538000	-2.536580000	-3.668336000
H	3.123290000	-1.416177000	-3.881093000
H	4.262094000	-0.005859000	-1.447751000
H	3.061466000	1.111740000	-4.028797000
H	4.792373000	1.039931000	-3.636720000
H	-4.207987000	-1.943488000	-2.748324000
H	-5.106376000	-1.391551000	-1.369963000
H	0.549979000	-2.213526000	-3.750132000
H	-2.106367000	-0.003786000	1.671259000
H	3.716723000	2.067525000	-2.682195000
H	1.597070000	1.400847000	-0.465753000
H	0.438451000	0.869661000	0.583940000
C	2.056444000	1.894089000	1.558525000
N	1.107068000	1.643887000	0.402980000
C	3.401429000	2.270061000	1.045667000
C	1.438851000	3.056038000	2.405602000
O	0.558285000	3.736347000	1.823170000
H	3.512458000	3.291317000	0.698595000
H	2.078608000	0.991327000	2.162582000
O	1.907238000	3.193711000	3.548288000
C	4.491671000	1.395782000	0.879948000
C	5.683362000	1.868486000	0.261756000
C	4.473792000	0.025154000	1.258717000
C	6.755671000	1.038439000	0.019442000
H	5.737065000	2.906366000	-0.042751000
C	5.547868000	-0.803648000	1.020928000
H	3.593451000	-0.395702000	1.723887000
C	6.695140000	-0.309990000	0.393374000
H	7.645351000	1.422875000	-0.465734000
H	5.509762000	-1.848920000	1.296476000
O	7.712746000	-1.184137000	0.167445000
H	8.442298000	-0.742265000	-0.285404000
H	0.577999000	2.527241000	0.318601000

22B-RC-complex

H	-1.697705000	-2.669302000	-1.534431000
H	-2.283837000	-1.336098000	-0.838106000
C	-0.476188000	-1.037960000	-1.692168000
N	-1.807120000	-1.668997000	-1.673516000

C	-0.660929000	0.445626000	-2.069058000
C	0.290622000	-1.174830000	-0.349066000
O	-0.368372000	-0.929366000	0.696006000
H	-1.342844000	0.895367000	-1.345738000
H	0.119392000	-1.526060000	-2.466728000
H	-1.161815000	0.474819000	-3.040259000
O	1.499397000	-1.508815000	-0.407987000
C	0.610616000	1.250811000	-2.123858000
C	1.054388000	1.973092000	-1.015770000
C	1.396258000	1.285542000	-3.278077000
C	2.236147000	2.705667000	-1.052362000
H	0.477530000	1.958576000	-0.100108000
C	2.580153000	2.010448000	-3.332438000
H	1.075071000	0.737331000	-4.156708000
C	3.003478000	2.725216000	-2.214398000
H	2.559363000	3.262542000	-0.179800000
H	3.179669000	2.034263000	-4.233637000
O	4.174728000	3.429871000	-2.317308000
H	4.358604000	3.884424000	-1.485983000
N	-2.854493000	4.723310000	0.604610000
N	-4.734131000	5.949168000	0.568873000
N	-2.244760000	8.685613000	0.359092000
N	-1.207750000	6.519936000	0.472295000
N	-4.540681000	9.013015000	0.392011000
C	-1.966855000	3.566697000	0.691243000
C	-1.604323000	3.196691000	2.136760000
C	-2.611439000	2.076047000	2.446026000
C	-2.720887000	1.364390000	1.080225000
C	-3.958861000	0.605423000	0.847809000
C	-4.229615000	4.741946000	0.632223000
C	-3.631795000	6.778679000	0.501287000
C	-2.453657000	6.035098000	0.522595000
C	-3.488646000	8.176722000	0.414460000
C	-1.201191000	7.848444000	0.389365000
O	-0.279451000	2.696962000	2.150177000
O	-2.141004000	1.163769000	3.421147000
O	-2.620541000	2.451487000	0.124196000
H	-1.065896000	3.818387000	0.130737000
H	-0.257107000	1.972802000	2.794115000
H	-1.704819000	4.054658000	2.806815000
H	-2.371101000	1.490369000	4.299194000
H	-3.574383000	2.504719000	2.733263000
H	-1.849381000	0.705909000	0.978493000
H	-4.844089000	1.103091000	0.476438000
H	-4.019369000	-0.428644000	1.153626000
H	-5.479224000	8.654593000	0.398935000

H	-4.392876000	10.003067000	0.298209000
H	-4.797100000	3.827905000	0.678982000
H	-0.224743000	8.318887000	0.340696000

22B-PC-complex

H	-1.624926000	-1.211929000	-0.839922000
H	-2.193240000	0.235751000	-1.336181000
C	-1.301378000	-0.904841000	-2.808802000
N	-2.122874000	-0.742480000	-1.591661000
C	-0.623094000	0.350487000	-3.272915000
C	-0.253677000	-2.071658000	-2.627201000
O	-0.015381000	-2.449698000	-1.455282000
H	-2.750177000	-0.224776000	1.226948000
H	-1.943114000	-1.240975000	-3.627374000
H	-0.773711000	0.636594000	-4.307584000
O	0.250236000	-2.511035000	-3.685090000
C	0.165974000	1.210179000	-2.478360000
C	0.572723000	0.892707000	-1.152815000
C	0.568883000	2.481020000	-2.976184000
C	1.254323000	1.803213000	-0.373198000
H	0.347365000	-0.084135000	-0.751000000
C	1.235577000	3.396608000	-2.187509000
H	0.304890000	2.750647000	-3.992219000
C	1.549602000	3.080181000	-0.862115000
H	1.539260000	1.549760000	0.639463000
H	1.487403000	4.378780000	-2.567115000
O	2.119777000	4.039249000	-0.072505000
H	1.830701000	3.886959000	0.847068000
N	-2.454418000	4.597454000	0.766650000
N	-4.439919000	5.637281000	0.880233000
N	-2.573910000	8.154884000	-1.097264000
N	-1.215978000	6.254089000	-0.531555000
N	-4.791893000	8.382191000	-0.457714000
C	-1.417209000	3.603402000	0.980688000
C	-0.778418000	3.659035000	2.385590000
C	-1.370057000	2.412172000	3.074245000
C	-1.588894000	1.455703000	1.903120000
C	-2.635086000	0.389477000	2.120033000
C	-3.754633000	4.574731000	1.218669000
C	-3.544366000	6.412209000	0.168381000
C	-2.304314000	5.783062000	0.086085000
C	-3.655747000	7.664194000	-0.466307000
C	-1.443817000	7.438248000	-1.094817000
O	0.635203000	3.534219000	2.277254000
O	-0.481051000	1.835172000	4.016556000
O	-1.999756000	2.319778000	0.830503000

H	-0.658196000	3.783574000	0.220956000
H	0.922369000	2.959674000	3.005436000
H	-1.030003000	4.589386000	2.897403000
H	-0.639422000	2.221522000	4.886137000
H	-2.327409000	2.664320000	3.536040000
H	-0.627786000	0.995989000	1.649113000
H	-3.599286000	0.838495000	2.363988000
H	-2.329388000	-0.256825000	2.944041000
H	-5.622933000	8.018815000	-0.025624000
H	-4.837620000	9.255074000	-0.954633000
H	-4.137831000	3.734087000	1.772956000
H	-0.606839000	7.885117000	-1.620988000

22C-RC-complex

N	0.526411000	-1.365868000	-1.824030000
N	-1.261998000	-1.808805000	-3.109230000
N	-2.870545000	0.486556000	-0.691019000
N	-0.535850000	0.173720000	-0.231042000
N	-3.967731000	-0.543468000	-2.451298000
C	1.904416000	-1.301817000	-1.373040000
C	2.699865000	-2.601333000	-1.539000000
C	3.503076000	-2.348055000	-2.829219000
C	3.763203000	-0.825563000	-2.767654000
C	3.939163000	-0.161927000	-4.069795000
C	0.009877000	-2.028996000	-2.920473000
C	-1.616863000	-0.942031000	-2.095541000
C	-0.519546000	-0.648017000	-1.292502000
C	-2.842583000	-0.336101000	-1.758309000
C	-1.749683000	0.690039000	-0.008346000
O	3.570340000	-2.704931000	-0.426247000
O	4.737658000	-3.036922000	-2.848289000
O	2.598608000	-0.293386000	-2.093378000
H	1.862840000	-1.040214000	-0.316898000
H	4.382913000	-3.129266000	-0.742515000
H	2.051893000	-3.478421000	-1.606016000
H	4.615976000	-3.903396000	-3.254719000
H	2.902103000	-2.592394000	-3.707219000
H	4.644224000	-0.674650000	-2.135760000
H	3.069684000	0.085322000	-4.663214000
H	4.927109000	-0.030020000	-4.484843000
H	-3.973229000	-1.153849000	-3.250005000
H	-4.820631000	-0.087814000	-2.174015000
H	0.623399000	-2.664908000	-3.536907000
H	-1.831907000	1.362939000	0.838346000
H	2.609633000	1.262684000	-0.293959000
H	0.567530000	0.889521000	2.647559000

H	0.724445000	2.288712000	1.799580000
C	2.486643000	1.168250000	1.846812000
N	0.994294000	1.303799000	1.817678000
C	3.084141000	1.758212000	0.554977000
C	3.069365000	1.860472000	3.071993000
O	2.441120000	3.016615000	3.321585000
H	2.820503000	2.815937000	0.500884000
H	2.712403000	0.108294000	1.931954000
O	4.005447000	1.435669000	3.692535000
C	4.580515000	1.586302000	0.477809000
C	5.434518000	2.684050000	0.540048000
C	5.144724000	0.314789000	0.348420000
C	6.814850000	2.527979000	0.470086000
H	5.022769000	3.680827000	0.642399000
C	6.517795000	0.142917000	0.278998000
H	4.509308000	-0.560899000	0.295733000
C	7.359870000	1.253145000	0.340193000
H	7.464544000	3.394096000	0.515098000
H	6.949412000	-0.843838000	0.173027000
O	8.703809000	1.027366000	0.266139000
H	9.186245000	1.861654000	0.323990000
H	0.556064000	0.821247000	0.970054000
H	2.850061000	3.455867000	4.086030000

22C-PC-complex

N	0.443937000	-1.574518000	-1.491739000
N	-1.358365000	-2.322159000	-2.603425000
N	-3.047092000	0.016599000	-0.272774000
N	-0.668026000	0.001197000	0.017012000
N	-4.147933000	-1.284275000	-1.841253000
C	1.810933000	-1.362545000	-1.066050000
C	2.786042000	-2.507477000	-1.358033000
C	3.536279000	-2.005542000	-2.607512000
C	3.592560000	-0.496644000	-2.382826000
C	3.710619000	0.346656000	-3.627830000
C	-0.060219000	-2.389391000	-2.488216000
C	-1.746816000	-1.405456000	-1.645316000
C	-0.642872000	-0.922342000	-0.955128000
C	-3.004901000	-0.898127000	-1.262794000
C	-1.909942000	0.411467000	0.292390000
O	3.668280000	-2.595186000	-0.252787000
O	4.851759000	-2.521167000	-2.696180000
O	2.338629000	-0.200574000	-1.718207000
H	1.771896000	-1.191701000	0.009400000
H	4.530168000	-2.865774000	-0.604674000
H	2.276851000	-3.460000000	-1.517835000

H	4.837196000	-3.357680000	-3.176367000
H	2.959785000	-2.232020000	-3.508447000
H	4.412698000	-0.282642000	-1.691794000
H	2.877488000	0.151055000	-4.304514000
H	4.645053000	0.107234000	-4.137639000
H	-4.144775000	-1.965031000	-2.580874000
H	-5.023127000	-0.893646000	-1.535663000
H	0.581793000	-3.013152000	-3.088087000
H	-1.997583000	1.164336000	1.067559000
H	3.721034000	1.407145000	-3.374935000
H	0.673582000	1.170696000	0.263059000
H	1.287376000	2.701728000	-0.114249000
C	2.484391000	1.709071000	1.308639000
N	1.549935000	1.745346000	0.121638000
C	3.776033000	2.380075000	0.991008000
C	1.843573000	2.375482000	2.521408000
O	1.074715000	3.413294000	2.168574000
H	3.738698000	3.458412000	0.893736000
H	2.619803000	0.663306000	1.566194000
O	2.056152000	2.026508000	3.651942000
C	5.003611000	1.727746000	0.785312000
C	6.150577000	2.505563000	0.456389000
C	5.189706000	0.318955000	0.867040000
C	7.376517000	1.927401000	0.220624000
H	6.049421000	3.581364000	0.386965000
C	6.415774000	-0.258448000	0.629183000
H	4.362242000	-0.336035000	1.099727000
C	7.521302000	0.536046000	0.303709000
H	8.231909000	2.543317000	-0.030109000
H	6.542154000	-1.331324000	0.687464000
O	8.700369000	-0.094668000	0.078963000
H	9.390758000	0.543889000	-0.143361000
H	2.014885000	1.309910000	-0.693166000
H	0.717732000	3.842933000	2.964061000

22D-RC-complex

H	-2.638494000	-1.994588000	0.743298000
H	-3.388031000	-0.755503000	1.495179000
C	-1.666523000	-0.196254000	0.534545000
N	-2.873418000	-1.011607000	0.658747000
C	-2.059709000	1.280838000	0.333896000
C	-0.708581000	-0.346983000	1.712275000
O	-1.303003000	-0.068924000	2.889499000
H	-2.690932000	1.591474000	1.167270000
H	-1.108070000	-0.536730000	-0.338005000
H	-2.676410000	1.316393000	-0.565810000

O	0.449358000	-0.681134000	1.628910000
C	-0.886612000	2.219224000	0.206445000
C	-0.346901000	2.851855000	1.326597000
C	-0.291011000	2.464773000	-1.032701000
C	0.744881000	3.705856000	1.220399000
H	-0.779621000	2.683736000	2.304222000
C	0.801047000	3.312836000	-1.156338000
H	-0.691326000	1.989260000	-1.920735000
C	1.322921000	3.937830000	-0.025425000
H	1.141565000	4.193861000	2.103346000
H	1.253476000	3.502479000	-2.121182000
O	2.395823000	4.767685000	-0.200433000
H	2.669620000	5.138306000	0.647815000
H	-0.653186000	-0.179007000	3.602499000
N	-3.828157000	5.650367000	3.134178000
N	-5.681929000	6.915124000	3.154248000
N	-3.153482000	9.586575000	2.707183000
N	-2.155671000	7.404071000	2.844714000
N	-5.436773000	9.966319000	2.857156000
C	-2.957625000	4.481862000	3.210461000
C	-2.531648000	4.140933000	4.644175000
C	-3.558583000	3.066822000	5.040162000
C	-3.752842000	2.315677000	3.704652000
C	-5.019717000	1.584601000	3.550178000
C	-5.199515000	5.700358000	3.235089000
C	-4.568583000	7.717377000	2.996345000
C	-3.406298000	6.949570000	2.981121000
C	-4.402428000	9.107929000	2.849694000
C	-2.126894000	8.728342000	2.711675000
O	-1.228257000	3.588102000	4.593887000
O	-3.073063000	2.170546000	6.020880000
O	-3.653953000	3.359232000	2.706095000
H	-2.082782000	4.701002000	2.598477000
H	-1.172817000	2.928405000	5.301582000
H	-2.562327000	5.019585000	5.293573000
H	-3.266375000	2.522090000	6.898101000
H	-4.494078000	3.535415000	5.353785000
H	-2.903593000	1.632815000	3.598006000
H	-5.908356000	2.103244000	3.218515000
H	-5.091715000	0.556930000	3.873497000
H	-6.381150000	9.627129000	2.909022000
H	-5.275407000	10.946257000	2.699948000
H	-5.783073000	4.802111000	3.345540000
H	-1.145375000	9.174795000	2.591783000

22D-PC-complex

H	-3.973672000	0.064100000	-1.214228000
H	-4.145171000	1.221872000	-0.084107000
C	-2.263825000	0.421340000	-0.146260000
N	-3.506308000	0.853186000	-0.780839000
C	-1.594475000	1.578982000	0.534171000
C	-2.413028000	-0.697114000	0.895548000
O	-3.533431000	-0.574408000	1.631382000
H	-3.695765000	1.250675000	3.389980000
H	-1.613110000	0.003628000	-0.916965000
H	-2.253385000	2.353894000	0.907868000
O	-1.602654000	-1.576818000	1.072044000
C	-0.214919000	1.703985000	0.773756000
C	0.743598000	0.720999000	0.403667000
C	0.284349000	2.869127000	1.423786000
C	2.089586000	0.895935000	0.658360000
H	0.418241000	-0.195077000	-0.068582000
C	1.625572000	3.040874000	1.678221000
H	-0.407214000	3.642044000	1.730702000
C	2.543579000	2.055456000	1.295004000
H	2.800200000	0.130072000	0.369226000
H	1.985458000	3.933163000	2.174351000
O	3.859120000	2.279336000	1.570854000
H	4.397653000	1.539814000	1.261054000
H	-3.542909000	-1.280284000	2.298454000
N	-4.139782000	5.864372000	2.922917000
N	-6.330078000	6.256880000	3.214684000
N	-5.185003000	9.728750000	2.611189000
N	-3.377197000	8.146903000	2.522857000
N	-7.386679000	9.141161000	3.044124000
C	-2.864864000	5.150650000	2.806178000
C	-1.973402000	5.345042000	4.037946000
C	-2.327298000	4.107896000	4.882579000
C	-2.585737000	3.040133000	3.820497000
C	-3.539157000	1.939374000	4.219383000
C	-5.388059000	5.346567000	3.178164000
C	-5.669692000	7.444547000	2.969370000
C	-4.307335000	7.220592000	2.782380000
C	-6.102645000	8.780989000	2.873710000
C	-3.906441000	9.366492000	2.453839000
O	-0.622308000	5.295244000	3.615069000
O	-1.263699000	3.691034000	5.723989000
O	-3.123377000	3.770653000	2.691446000
H	-2.363913000	5.522534000	1.911247000
H	-0.126072000	4.832824000	4.307393000
H	-2.188956000	6.287426000	4.546389000
H	-1.312352000	4.168878000	6.560601000

H	-3.234785000	4.299721000	5.460688000
H	-1.623102000	2.612779000	3.524030000
H	-4.502063000	2.348917000	4.529297000
H	-3.114678000	1.380327000	5.055142000
H	-8.097506000	8.444676000	3.182724000
H	-7.659085000	10.099996000	2.911732000
H	-5.531091000	4.288306000	3.312240000
H	-3.215201000	10.175766000	2.243211000

23A-RC-complex

C	-0.551080000	-2.232007000	-0.244226000
N	-0.409233000	-2.041675000	-1.677993000
C	-2.005102000	-2.600513000	0.113158000
C	-2.955747000	-1.446599000	-0.169396000
C	-4.402111000	-1.786915000	0.045020000
O	-5.194915000	-0.708043000	-0.130661000
H	-0.311635000	-1.286380000	0.250300000
H	-2.079612000	-2.877584000	1.165180000
H	-2.297557000	-3.480092000	-0.465746000
O	-4.846531000	-2.874262000	0.333003000
C	0.403354000	-3.287895000	0.332603000
O	1.044165000	-4.016449000	-0.398784000
H	-2.843837000	-1.099872000	-1.199308000
H	-2.713668000	-0.583147000	0.453269000
H	-6.116620000	-0.980742000	0.008089000
C	0.764995000	-1.259911000	-2.062676000
H	0.636684000	-0.232737000	-1.720973000
H	1.709483000	-1.644123000	-1.655668000
H	0.845247000	-1.245042000	-3.150161000
H	-0.360021000	-2.954934000	-2.117435000
C	0.488771000	-3.409609000	1.833656000
H	-0.317347000	-4.060822000	2.181692000
H	1.436937000	-3.865755000	2.111936000
H	0.374488000	-2.441958000	2.320897000
N	1.371879000	1.636872000	0.218692000
N	3.090742000	1.758871000	-1.223222000
N	4.214038000	-1.154475000	0.770376000
N	2.105529000	-0.288015000	1.531371000
N	5.399446000	-0.256698000	-1.008972000
C	0.054684000	1.832654000	0.792649000
C	-0.371040000	3.298901000	0.938748000
C	-1.308619000	3.505549000	-0.266304000
C	-1.961137000	2.112896000	-0.416541000
C	-2.448036000	1.785982000	-1.767257000
C	1.941182000	2.268473000	-0.867870000
C	3.297181000	0.719837000	-0.335228000

C	2.238814000	0.622056000	0.562540000
C	4.325344000	-0.232961000	-0.203285000
C	3.137329000	-1.129008000	1.562877000
O	-1.093192000	3.417817000	2.151895000
O	-2.306590000	4.478924000	-0.026744000
O	-0.914562000	1.198255000	-0.037117000
H	0.075115000	1.349993000	1.768904000
H	-1.770304000	4.096476000	2.008212000
H	0.485827000	3.977442000	0.928445000
H	-1.983295000	5.344692000	-0.303062000
H	-0.732110000	3.744180000	-1.162205000
H	-2.778291000	2.061503000	0.313588000
H	-1.750005000	1.425991000	-2.510033000
H	-3.470778000	1.991615000	-2.044603000
H	5.494560000	0.408272000	-1.756136000
H	6.098183000	-0.970478000	-0.893628000
H	1.460304000	3.101933000	-1.353091000
H	3.101750000	-1.898120000	2.326230000

23A-PC-complex

C	0.419475000	2.270969000	0.298876000
N	-0.484665000	2.499369000	1.406117000
C	-0.179828000	2.840917000	-1.024514000
C	-1.348716000	2.054724000	-1.465466000
C	-2.701215000	2.512853000	-1.290983000
O	-3.618119000	1.581864000	-1.669539000
H	0.548754000	1.194242000	0.176129000
H	0.588566000	2.811310000	-1.802442000
H	-0.453949000	3.882904000	-0.854073000
O	-3.034372000	3.607547000	-0.861018000
C	1.805578000	2.910383000	0.486586000
O	1.932522000	3.912140000	1.160436000
H	-3.428288000	0.922413000	1.365747000
H	-1.201528000	1.064893000	-1.871311000
H	-4.500476000	1.958274000	-1.526467000
C	-0.164759000	1.704180000	2.589613000
H	-0.308905000	0.649232000	2.354913000
H	0.862677000	1.840716000	2.956299000
H	-0.850723000	1.967650000	3.395081000
H	-0.463538000	3.486522000	1.640458000
C	2.969519000	2.241395000	-0.188264000
H	2.694695000	1.827563000	-1.158415000
H	3.808259000	2.927191000	-0.287761000
H	3.272871000	1.399189000	0.440337000
N	0.546756000	-1.665896000	0.102303000
N	2.221200000	-1.852885000	1.586227000

N	4.201463000	-0.953123000	-1.413993000
N	1.845214000	-1.055280000	-1.875685000
N	5.114594000	-1.352369000	0.679746000
C	-0.797742000	-1.606727000	-0.428879000
C	-1.638112000	-2.889144000	-0.245260000
C	-2.706119000	-2.452935000	0.780656000
C	-2.839056000	-0.957183000	0.503778000
C	-3.391319000	-0.131288000	1.639091000
C	0.929394000	-1.929561000	1.399950000
C	2.729655000	-1.515698000	0.345528000
C	1.705031000	-1.388255000	-0.589199000
C	4.037605000	-1.279819000	-0.119577000
C	3.122212000	-0.858920000	-2.198192000
O	-2.240165000	-3.209035000	-1.487942000
O	-3.951021000	-3.104737000	0.587537000
O	-1.487169000	-0.555198000	0.233514000
H	-0.693851000	-1.400818000	-1.495542000
H	-3.129154000	-3.540221000	-1.286124000
H	-1.025709000	-3.721972000	0.109013000
H	-3.973402000	-3.913793000	1.111947000
H	-2.334736000	-2.607212000	1.796917000
H	-3.447952000	-0.819773000	-0.397174000
H	-2.769232000	-0.240185000	2.528614000
H	-4.403676000	-0.465492000	1.871023000
H	5.020684000	-1.626781000	1.641768000
H	6.032952000	-1.202894000	0.298472000
H	0.203984000	-2.163462000	2.162586000
H	3.316727000	-0.584210000	-3.229365000

23B-RC-complex

C	-2.071517000	1.342859000	0.603173000
N	-3.445174000	0.950766000	0.311620000
C	-1.559756000	2.299517000	-0.486459000
C	-0.125695000	2.804257000	-0.275433000
C	0.439102000	3.394659000	-1.578706000
O	0.125716000	4.578912000	-1.857098000
H	-1.458448000	0.439885000	0.585536000
H	-2.244428000	3.149867000	-0.551805000
H	-1.624032000	1.751726000	-1.427642000
O	1.154274000	2.628861000	-2.282671000
C	-1.916808000	1.995851000	1.986345000
O	-2.718418000	2.831012000	2.359495000
H	0.512914000	1.983854000	0.045398000
H	-0.111051000	3.568742000	0.505551000
C	-3.956902000	-0.111127000	1.176614000
H	-3.363091000	-1.014650000	1.029042000

H	-3.942025000	0.133095000	2.248564000
H	-4.985956000	-0.339094000	0.897083000
H	-4.036589000	1.771250000	0.397149000
C	-0.769860000	1.540839000	2.843264000
H	-0.649946000	2.186415000	3.711195000
H	-0.983216000	0.519195000	3.174953000
H	0.155345000	1.488184000	2.266892000
N	0.591443000	-1.170940000	-0.174006000
N	-0.661898000	-0.790914000	-1.994445000
N	-2.729364000	-3.421995000	-0.407158000
N	-0.754672000	-2.923357000	0.868927000
N	-3.260823000	-2.376010000	-2.409810000
C	1.674993000	-1.077214000	0.798462000
C	2.931058000	-1.850550000	0.380245000
C	3.785878000	-0.750740000	-0.269900000
C	3.444415000	0.478678000	0.601702000
C	3.624697000	1.784367000	-0.054379000
C	0.420553000	-0.450902000	-1.338824000
C	-1.238627000	-1.785676000	-1.230401000
C	-0.474345000	-2.037264000	-0.093140000
C	-2.427835000	-2.525664000	-1.363214000
C	-1.894644000	-3.567650000	0.628699000
O	3.556355000	-2.340039000	1.553401000
O	5.174705000	-1.013682000	-0.200755000
O	2.051267000	0.277973000	0.945620000
H	1.283225000	-1.472917000	1.735690000
H	4.510459000	-2.339919000	1.384064000
H	2.690725000	-2.665033000	-0.308305000
H	5.443340000	-1.514803000	-0.979826000
H	3.463020000	-0.581813000	-1.299564000
H	4.050427000	0.406654000	1.511721000
H	2.883262000	2.134436000	-0.762605000
H	4.552258000	2.322852000	0.074447000
H	-3.113515000	-1.627549000	-3.064531000
H	-4.153013000	-2.840521000	-2.400511000
H	1.076518000	0.361184000	-1.618638000
H	-2.192203000	-4.303618000	1.368025000

23B-PC-complex

C	0.657742000	2.481488000	-0.368259000
N	-0.273539000	2.990708000	-1.362364000
C	2.057761000	3.138554000	-0.584985000
C	3.145148000	2.606718000	0.271915000
C	4.146803000	1.621998000	-0.201049000
O	4.842896000	1.055146000	0.693467000
H	0.762053000	1.402816000	-0.506170000

H	1.928840000	4.216259000	-0.425572000
H	2.313830000	2.972224000	-1.630841000
O	4.229693000	1.413365000	-1.446163000
C	0.217302000	2.757007000	1.075185000
O	-0.400042000	3.770966000	1.342982000
H	3.359007000	-0.757860000	-1.663839000
H	3.188971000	2.891548000	1.316960000
C	-1.546018000	2.270943000	-1.391706000
H	-1.370870000	1.240246000	-1.703582000
H	-2.071701000	2.247860000	-0.427193000
H	-2.207171000	2.733478000	-2.125289000
H	-0.448529000	3.970720000	-1.163452000
C	0.560266000	1.741939000	2.128994000
H	0.715495000	2.227531000	3.091569000
H	-0.305025000	1.075863000	2.213952000
H	1.425302000	1.139474000	1.855253000
N	-1.195440000	-1.367497000	-0.118299000
N	-2.734415000	-1.327369000	-1.752801000
N	-4.586072000	0.571212000	0.833608000
N	-2.419946000	-0.133300000	1.598042000
N	-5.414897000	0.093793000	-1.279253000
C	0.061229000	-1.611980000	0.565513000
C	0.393104000	-3.098981000	0.791100000
C	1.487600000	-3.364532000	-0.259194000
C	2.185805000	-2.009907000	-0.363096000
C	2.909884000	-1.751853000	-1.662038000
C	-1.534062000	-1.716097000	-1.407248000
C	-3.222594000	-0.681321000	-0.633045000
C	-2.281025000	-0.692929000	0.392492000
C	-4.427858000	-0.002351000	-0.372795000
C	-3.596704000	0.475221000	1.728551000
O	0.917842000	-3.238531000	2.101084000
O	2.412362000	-4.360290000	0.148560000
O	1.113412000	-1.059025000	-0.212472000
H	-0.017530000	-1.113475000	1.530868000
H	1.613054000	-3.912536000	2.050266000
H	-0.489141000	-3.730160000	0.658405000
H	2.091362000	-5.226680000	-0.128351000
H	1.032930000	-3.623846000	-1.218733000
H	2.874840000	-1.912291000	0.483945000
H	2.219197000	-1.837346000	-2.503730000
H	3.702053000	-2.493114000	-1.784636000
H	-5.299702000	-0.286185000	-2.202246000
H	-6.238712000	0.630335000	-1.068250000
H	-0.844483000	-2.244282000	-2.045073000
H	-3.779520000	0.960037000	2.681553000

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H	-0.112683000	0.604788000	-1.603668000
C	1.390494000	-1.360484000	-1.414153000
H	1.841967000	-1.654438000	-0.466238000
H	1.666345000	-2.105994000	-2.159978000
H	1.790783000	-0.392812000	-1.712383000
C	-0.117206000	-1.380104000	-1.248704000
H	-2.277763000	0.921432000	-2.161542000
H	-2.213601000	1.381907000	1.846171000
O	-0.697013000	-2.426790000	-0.965701000
C	-2.373772000	1.116858000	-0.105141000
C	-2.125815000	0.220265000	-1.337657000
N	-0.721132000	-0.185546000	-1.434569000
C	-3.181138000	-0.891840000	-1.523454000
O	-2.880959000	2.228373000	-0.276950000
N	-2.044287000	0.692401000	1.127960000
H	-3.007836000	-1.673907000	-0.787471000
C	-3.052934000	-1.507675000	-2.918819000
H	-3.238098000	-0.753853000	-3.689368000
H	-2.064704000	-1.933931000	-3.081794000
H	-3.788076000	-2.304558000	-3.046773000
C	-4.591271000	-0.330256000	-1.316178000
H	-4.794279000	0.492439000	-2.006147000
H	-5.328425000	-1.113659000	-1.499323000
H	-4.742316000	0.038368000	-0.300714000
C	-1.459049000	-0.569736000	1.558522000
H	-0.371210000	-0.501435000	1.610864000
H	-1.847225000	-0.806525000	2.548274000
H	-1.728462000	-1.376068000	0.885301000
N	2.308511000	2.096511000	0.044001000
N	4.410658000	1.620751000	-0.584389000
N	3.947815000	-1.034877000	1.959161000
N	2.003210000	0.357096000	1.730866000
N	5.896383000	-0.720938000	0.741105000
C	0.991393000	2.689755000	0.029605000
C	0.945609000	4.205959000	0.295923000
C	0.611551000	4.796731000	-1.089280000
C	-0.237084000	3.676820000	-1.727915000
C	-0.293133000	3.675026000	-3.197372000
C	3.378198000	2.399480000	-0.772159000
C	4.007495000	0.744843000	0.406908000
C	2.704380000	1.021576000	0.809441000
C	4.639609000	-0.347101000	1.032381000
C	2.699563000	-0.652211000	2.249087000
O	-0.102244000	4.459941000	1.213538000

O	-0.142833000	5.990104000	-1.007918000
O	0.427462000	2.480346000	-1.266024000
H	0.408772000	2.169043000	0.790051000
H	-0.492925000	5.310985000	0.962052000
H	1.899381000	4.570651000	0.686014000
H	0.455073000	6.746874000	-0.995482000
H	1.525690000	4.941456000	-1.669113000
H	-1.241940000	3.724003000	-1.294616000
H	0.534282000	3.268737000	-3.762777000
H	-1.096314000	4.180946000	-3.711186000
H	6.412186000	-0.255988000	0.014826000
H	6.288264000	-1.539772000	1.173724000
H	3.325478000	3.201505000	-1.490614000
H	2.190646000	-1.245693000	3.001115000

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H	-0.604732000	1.029496000	0.193159000
C	-0.490383000	1.061461000	2.677446000
H	-0.732016000	2.103350000	2.464786000
H	-0.645467000	0.855337000	3.732877000
H	0.562155000	0.910124000	2.425610000
C	-1.352142000	0.129381000	1.858619000
H	-2.377350000	3.193748000	-0.216619000
H	-4.965365000	-1.806873000	-0.554457000
O	-2.050275000	-0.745003000	2.354395000
C	-3.406267000	-0.607295000	-0.231333000
C	-1.959234000	-0.408117000	-0.446894000
N	-1.262173000	0.319597000	0.501846000
C	-1.292138000	-0.648275000	-1.775185000
O	-4.104927000	0.296484000	0.248803000
N	-3.960874000	-1.776303000	-0.640473000
H	-1.980017000	-1.239362000	-2.380627000
C	0.017345000	-1.437357000	-1.618018000
H	0.719798000	-0.900349000	-0.981383000
H	-0.156755000	-2.416172000	-1.170031000
H	0.490676000	-1.584804000	-2.590155000
C	-1.047884000	0.670229000	-2.537675000
H	-0.352197000	1.320882000	-2.006933000
H	-0.619825000	0.455786000	-3.518358000
H	-1.980185000	1.218024000	-2.680656000
C	-3.275334000	-3.029322000	-0.909687000
H	-3.849337000	-3.850188000	-0.480554000
H	-3.153385000	-3.215489000	-1.979353000
H	-2.292998000	-3.024239000	-0.441411000
N	2.355790000	2.139089000	-0.762512000
N	3.053228000	1.244262000	-2.700328000

N	3.697139000	-1.637603000	-0.461679000
N	2.776276000	0.243186000	0.716665000
N	4.136514000	-1.632304000	-2.738650000
C	1.671633000	3.008018000	0.163899000
C	1.925552000	4.514218000	-0.021819000
C	0.587942000	5.020801000	-0.602462000
C	-0.427004000	4.068853000	0.025543000
C	-1.741297000	3.933642000	-0.703143000
C	2.526437000	2.291369000	-2.123907000
C	3.228154000	0.333906000	-1.674042000
C	2.793130000	0.866071000	-0.464925000
C	3.699319000	-0.992591000	-1.642233000
C	3.247031000	-0.999402000	0.623862000
O	2.156501000	5.077871000	1.257766000
O	0.301796000	6.357795000	-0.232343000
O	0.263464000	2.805638000	0.009824000
H	1.983526000	2.705359000	1.163182000
H	1.772062000	5.967953000	1.241619000
H	2.774024000	4.706251000	-0.682641000
H	0.661488000	6.957782000	-0.896322000
H	0.581009000	4.900668000	-1.688785000
H	-0.593764000	4.378485000	1.063951000
H	-1.576826000	3.628693000	-1.736989000
H	-2.259598000	4.893247000	-0.694878000
H	4.115846000	-1.181655000	-3.636481000
H	4.426909000	-2.593040000	-2.677346000
H	2.241750000	3.199881000	-2.629946000
H	3.263811000	-1.572973000	1.544294000

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H	3.226993000	3.087591000	-3.294997000
H	-1.731732000	1.434531000	-0.587064000
H	-1.502664000	2.516624000	-1.970439000
H	-1.424782000	-1.971840000	-1.143638000
H	1.114909000	-3.053369000	-1.349125000
H	3.901330000	-0.462056000	-2.463830000
H	4.469797000	-0.134449000	-0.944809000
H	-0.103198000	0.724941000	-3.063433000
H	-0.203803000	-0.470221000	-0.256779000
H	1.446624000	-1.267050000	-2.682155000
H	2.320264000	-0.065268000	-0.016773000
H	2.753337000	2.023190000	-1.206603000
C	2.486653000	2.424657000	-3.751270000
O	2.441250000	1.171714000	-3.058510000
O	-2.612264000	0.864996000	-2.393256000
C	-1.549268000	1.469763000	-1.668407000

O	-1.046480000	-1.448010000	-1.877567000
O	1.588252000	-2.336539000	-0.909570000
N	3.733517000	-0.614009000	-1.464879000
O	0.807281000	1.681811000	-1.451494000
C	-0.208721000	0.812443000	-1.977191000
C	-0.065984000	-0.571213000	-1.338656000
C	1.332256000	-1.122322000	-1.602582000
C	2.127654000	1.272119000	-1.698561000
H	-2.501876000	-0.094138000	-2.304123000
H	2.775354000	2.201220000	-4.774923000
H	1.507834000	2.906618000	-3.740909000
C	2.362098000	-0.121023000	-1.102692000
H	3.798707000	-1.615985000	-1.263371000
N	-1.214235000	-4.854835000	0.734695000
N	0.894402000	-5.353133000	1.315650000
N	-0.370634000	-8.779904000	0.691542000
N	-2.053911000	-7.106113000	0.314257000
N	1.791673000	-8.295849000	1.375936000
C	-2.412330000	-4.086052000	0.407462000
C	-3.502845000	-4.198957000	1.475047000
C	-3.226759000	-2.966980000	2.354300000
C	-2.780827000	-1.916462000	1.316938000
C	-1.912874000	-0.846931000	1.832608000
C	0.022615000	-4.393786000	1.128606000
C	0.200795000	-6.512758000	1.029985000
C	-1.110614000	-6.223743000	0.661420000
C	0.561884000	-7.874089000	1.037655000
C	-1.594153000	-8.355167000	0.356486000
O	-4.755375000	-4.081246000	0.827896000
O	-4.377585000	-2.501768000	3.029316000
O	-2.059614000	-2.716205000	0.328810000
H	-2.783889000	-4.435308000	-0.556266000
H	-5.363282000	-3.668614000	1.459459000
H	-3.426390000	-5.137916000	2.028304000
H	-4.445045000	-2.942411000	3.884593000
H	-2.409919000	-3.177162000	3.048200000
H	-3.676027000	-1.507842000	0.841991000
H	-0.908589000	-1.082742000	2.157472000
H	-2.300365000	0.147765000	1.990211000
H	2.506591000	-7.637975000	1.631877000
H	2.008252000	-9.277581000	1.360814000
H	0.218276000	-3.340619000	1.229975000
H	-2.300146000	-9.133064000	0.085624000

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H	3.471147000	2.598475000	-3.666304000
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H	-1.594527000	1.886968000	-0.653090000
H	-1.355602000	2.875978000	-2.104085000
H	-1.427743000	-1.771304000	-0.959660000
H	0.904370000	-2.973193000	-1.049998000
H	3.745786000	-0.797589000	-2.207188000
H	4.241625000	-0.292154000	-0.710115000
H	-0.239689000	0.942163000	-3.216670000
H	-1.442779000	-0.226361000	1.193852000
H	1.279092000	-1.413668000	-2.494781000
H	2.051466000	0.124815000	0.018011000
H	2.839199000	1.939608000	-1.450535000
C	2.648822000	1.978517000	-4.034351000
O	2.432615000	0.862552000	-3.162727000
O	-2.679892000	1.361431000	-2.359605000
C	-1.500464000	1.857404000	-1.744477000
O	-1.383309000	-1.028231000	-1.604694000
O	1.095228000	-2.158121000	-0.571188000
N	3.493687000	-0.770620000	-1.214652000
O	0.869203000	1.819111000	-1.692926000
C	-0.262473000	1.038290000	-2.120066000
C	-0.235069000	-0.314560000	-1.474541000
C	1.066126000	-1.056018000	-1.475778000
C	2.122722000	1.209595000	-1.842584000
H	-2.779015000	0.438657000	-2.086307000
H	2.906867000	1.565743000	-5.005877000
H	1.744490000	2.583144000	-4.118803000
C	2.165556000	-0.094137000	-1.040833000
H	3.435575000	-1.730034000	-0.860014000
N	-1.105649000	-4.902803000	0.787220000
N	0.930314000	-5.440919000	1.561576000
N	-0.207940000	-8.806565000	0.509253000
N	-1.863423000	-7.114637000	0.090414000
N	1.858852000	-8.371742000	1.467215000
C	-2.281954000	-4.116811000	0.424523000
C	-3.422926000	-4.251445000	1.438057000
C	-3.183735000	-3.038835000	2.356468000
C	-2.676009000	-1.981291000	1.379692000
C	-1.798700000	-0.904377000	1.969724000
C	0.071017000	-4.473261000	1.360696000
C	0.289435000	-6.574237000	1.100280000
C	-0.976577000	-6.259993000	0.612274000
C	0.667438000	-7.929038000	1.032112000
C	-1.393267000	-8.360512000	0.077999000
O	-4.645602000	-4.113705000	0.738058000
O	-4.368296000	-2.576782000	2.980619000
O	-1.917727000	-2.748269000	0.404050000

H	-2.607407000	-4.440886000	-0.563831000
H	-5.268128000	-3.678995000	1.340316000
H	-3.375598000	-5.205403000	1.968093000
H	-4.499720000	-3.055658000	3.807396000
H	-2.412929000	-3.275930000	3.094049000
H	-3.536436000	-1.540038000	0.868800000
H	-0.937162000	-1.337646000	2.479439000
H	-2.378399000	-0.327758000	2.691842000
H	2.529430000	-7.735459000	1.860656000
H	2.087275000	-9.348537000	1.400232000
H	0.237609000	-3.431258000	1.569064000
H	-2.054168000	-9.116140000	-0.333539000

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N	-1.219711000	1.370131000	-0.098946000
N	0.450519000	0.463917000	1.096437000
N	-0.865059000	2.833119000	3.627552000
N	-2.096078000	2.923604000	1.566679000
N	0.952713000	1.433729000	3.973862000
C	-2.148416000	1.607411000	-1.172829000
C	-1.524356000	1.954082000	-2.548223000
C	-2.138243000	0.886462000	-3.494042000
C	-3.373812000	0.424299000	-2.720444000
C	-0.179740000	0.466644000	-0.049024000
C	-0.208352000	1.414164000	1.856139000
C	-1.252994000	1.983330000	1.134279000
C	-0.026844000	1.885288000	3.170757000
C	-1.829781000	3.287270000	2.818171000
O	-1.912423000	3.262980000	-2.935627000
O	-2.517203000	1.427604000	-4.748937000
O	-2.930446000	0.431476000	-1.360473000
H	-2.779455000	2.435272000	-0.856246000
H	-2.211343000	3.198965000	-3.858015000
H	-0.435128000	1.892386000	-2.516987000
H	-1.814890000	1.274781000	-5.391792000
H	-1.441078000	0.056034000	-3.616482000
H	-4.162572000	1.172655000	-2.856416000
H	1.544593000	0.677143000	3.678904000
H	1.000951000	1.748754000	4.927611000
H	0.056017000	-0.165239000	-0.890423000
H	-2.475921000	4.050258000	3.239278000
C	-3.877298000	-0.949071000	-3.093155000
H	-4.125806000	-0.946163000	-4.155838000
H	-3.101517000	-1.696031000	-2.913962000
S	-5.379012000	-1.379691000	-2.145220000
C	-5.908056000	-2.844393000	-3.077497000

H	-6.118555000	-2.587370000	-4.115457000
H	-5.148736000	-3.624923000	-3.036007000
H	-6.819851000	-3.208992000	-2.606241000
N	-6.637765000	2.561734000	0.336474000
N	-5.223332000	2.973363000	-1.353400000
N	-4.259176000	5.747318000	0.903133000
N	-6.026788000	4.401172000	1.819827000
N	-3.232810000	5.315986000	-1.136097000
C	-7.695017000	1.934526000	1.127332000
C	-9.063266000	2.588092000	0.905629000
C	-9.667577000	1.696336000	-0.191458000
C	-9.125550000	0.302781000	0.200853000
C	-9.033243000	-0.674947000	-0.895279000
C	-6.169722000	2.188714000	-0.902188000
C	-5.051883000	3.920310000	-0.361932000
C	-5.926560000	3.682748000	0.696372000
C	-4.159799000	4.998362000	-0.210134000
C	-5.163177000	5.415468000	1.830332000
O	-9.804074000	2.474448000	2.106932000
O	-11.081873000	1.677327000	-0.176844000
O	-7.811117000	0.581053000	0.739503000
H	-7.402259000	2.012382000	2.174960000
H	-10.736056000	2.388007000	1.856573000
H	-8.965237000	3.632479000	0.597838000
H	-11.416184000	2.389604000	-0.734735000
H	-9.281545000	1.989525000	-1.170344000
H	-9.769020000	-0.074454000	1.004123000
H	-8.181000000	-0.660672000	-1.560500000
H	-9.869177000	-1.323200000	-1.111831000
H	-2.960335000	4.628023000	-1.828320000
H	-2.537104000	5.995256000	-0.872681000
H	-6.543744000	1.311729000	-1.403322000
H	-5.189479000	6.054334000	2.706974000

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N	-0.947587000	1.380028000	0.254255000
N	0.260041000	-0.314950000	1.092482000
N	2.349999000	2.522526000	2.238381000
N	0.421177000	3.253751000	1.004568000
N	2.847622000	0.293510000	2.643265000
C	-2.003496000	2.115710000	-0.440372000
C	-1.558775000	2.607995000	-1.825063000
C	-2.104109000	1.504017000	-2.748336000
C	-3.400603000	1.114387000	-2.037983000
C	-0.808826000	0.020277000	0.413166000
C	0.864239000	0.888180000	1.400405000

C	0.126600000	1.953802000	0.890159000
C	2.035349000	1.221141000	2.107997000
C	1.544828000	3.441857000	1.693602000
O	-2.203845000	3.842400000	-2.099596000
O	-2.397638000	1.969437000	-4.053173000
O	-3.102954000	1.253151000	-0.635395000
H	-2.281900000	2.957200000	0.194345000
H	-2.422449000	3.845813000	-3.044437000
H	-0.474801000	2.720709000	-1.882901000
H	-1.612826000	1.884044000	-4.607773000
H	-1.407837000	0.662378000	-2.773053000
H	-4.175295000	1.838863000	-2.303027000
H	2.601871000	-0.680193000	2.609120000
H	3.642898000	0.579381000	3.188216000
H	-1.541353000	-0.662594000	0.018816000
H	1.852039000	4.472871000	1.833814000
C	-3.858552000	-0.293902000	-2.339858000
H	-3.973349000	-0.397680000	-3.419791000
H	-3.125526000	-1.021192000	-1.989491000
S	-5.468383000	-0.657861000	-1.558238000
C	-5.762391000	-2.238728000	-2.127608000
H	-9.085892000	-1.792940000	-0.584320000
H	-5.125802000	-2.695342000	-2.870452000
H	-6.663349000	-2.727093000	-1.790121000
N	-7.674579000	2.809427000	-0.091411000
N	-5.845090000	3.381354000	-1.258994000
N	-5.160373000	5.267663000	1.856905000
N	-7.233732000	4.057848000	1.961319000
N	-3.749290000	5.249986000	0.015357000
C	-8.941036000	2.185006000	0.240472000
C	-10.108704000	2.588373000	-0.679423000
C	-10.277361000	1.346576000	-1.575323000
C	-9.869855000	0.211285000	-0.638697000
C	-9.391293000	-1.048271000	-1.319987000
C	-6.957120000	2.694417000	-1.261429000
C	-5.813101000	3.986937000	-0.016661000
C	-6.943573000	3.645411000	0.723770000
C	-4.883204000	4.838591000	0.610892000
C	-6.291207000	4.864146000	2.445172000
O	-11.259810000	2.777824000	0.126576000
O	-11.612504000	1.161166000	-2.016576000
O	-8.798264000	0.773316000	0.139685000
H	-9.165072000	2.481745000	1.265281000
H	-12.017137000	2.469140000	-0.394113000
H	-9.878106000	3.494640000	-1.245009000
H	-11.743378000	1.638567000	-2.844380000

H	-9.589572000	1.396678000	-2.423251000
H	-10.719675000	-0.008741000	0.018344000
H	-8.544591000	-0.831967000	-1.972757000
H	-10.200344000	-1.469162000	-1.918931000
H	-3.414211000	4.803498000	-0.829279000
H	-3.085614000	5.767366000	0.568029000
H	-7.296709000	2.069446000	-2.070522000
H	-6.456938000	5.243341000	3.448204000

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H	-0.466268000	0.062947000	-0.678597000
C	-0.470244000	-2.888611000	-2.301913000
H	-1.460550000	-3.096167000	-2.712072000
H	0.259856000	-3.116973000	-3.076975000
H	-0.285621000	-3.521746000	-1.442989000
C	-0.380653000	-1.411917000	-2.005611000
H	-2.045746000	-2.855799000	1.639980000
H	-0.826474000	-0.756431000	1.228265000
H	1.563084000	-2.936495000	2.636584000
H	-1.913021000	-3.293892000	-0.046059000
O	-0.246333000	-0.607296000	-2.933745000
C	0.539507000	-2.385341000	1.025590000
C	-0.687724000	-1.593354000	0.544574000
N	-0.473348000	-0.948164000	-0.738104000
C	-1.979622000	-2.444776000	0.631060000
O	1.288610000	-2.964577000	0.244831000
N	0.737184000	-2.426947000	2.359594000
C	-3.205638000	-1.619804000	0.326995000
C	-3.672889000	-0.684275000	1.253231000
C	-3.871936000	-1.738658000	-0.891607000
C	-4.774881000	0.112625000	0.968005000
H	-3.169339000	-0.577447000	2.207277000
C	-4.977068000	-0.943894000	-1.182019000
H	-3.527274000	-2.460641000	-1.621296000
C	-5.431281000	-0.014452000	-0.253402000
H	-5.122515000	0.832049000	1.698822000
H	-5.479623000	-1.050046000	-2.135270000
H	-6.288660000	0.607161000	-0.478257000
C	0.021905000	-1.697638000	3.398763000
H	0.116199000	-0.618247000	3.269791000
H	-1.034034000	-1.965786000	3.429226000
H	0.461290000	-1.963360000	4.356886000
N	1.709533000	1.543146000	-0.042448000
N	3.060578000	0.094304000	-1.101091000
N	3.824295000	-0.856352000	2.397038000
N	2.211442000	0.919451000	2.267807000

N	4.805147000	-1.835064000	0.535731000
C	0.671888000	2.524063000	0.186418000
C	0.713529000	3.742570000	-0.747023000
C	-0.434425000	3.463035000	-1.735624000
C	-1.456531000	2.715195000	-0.866917000
C	-2.387467000	1.843677000	-1.607131000
C	2.177112000	1.044808000	-1.242907000
C	3.183622000	-0.065584000	0.266782000
C	2.349822000	0.819049000	0.942973000
C	3.948118000	-0.940371000	1.060599000
C	2.985894000	0.048948000	2.912146000
O	0.428630000	4.892788000	0.030107000
O	-1.012511000	4.648118000	-2.250493000
O	-0.607455000	1.904380000	0.003125000
H	0.775784000	2.845478000	1.221840000
H	-0.051292000	5.506463000	-0.546851000
H	1.682090000	3.841912000	-1.243668000
H	-0.543280000	4.910706000	-3.051305000
H	-0.091528000	2.807004000	-2.539249000
H	-1.991823000	3.443795000	-0.252332000
H	-1.983466000	1.096442000	-2.278165000
H	-3.450472000	1.876443000	-1.425960000
H	4.799372000	-2.008626000	-0.454625000
H	5.222306000	-2.523875000	1.138950000
H	1.811243000	1.412909000	-2.186950000
H	2.924232000	0.066225000	3.994900000

27-PC-complex

H	0.793776000	0.129616000	-1.673178000
C	-0.218089000	2.925050000	-0.055771000
H	-0.853778000	2.456601000	0.691290000
H	0.454286000	3.631144000	0.424061000
H	-0.856768000	3.474181000	-0.749120000
C	0.626009000	1.923472000	-0.794266000
H	-3.212924000	0.523161000	-1.702184000
H	-3.076798000	-2.977431000	1.831692000
H	-2.011113000	-2.770246000	-2.609060000
H	-2.289267000	1.965506000	-1.486696000
O	1.818701000	2.122814000	-0.998689000
C	-1.107461000	-1.135094000	-2.001305000
C	-1.165030000	0.182651000	-1.356633000
N	0.090635000	0.734370000	-1.249101000
C	-2.418019000	0.954706000	-1.093940000
O	-0.035358000	-1.517524000	-2.515405000
N	-2.210220000	-1.926482000	-2.093715000
C	-2.914514000	1.058345000	0.341453000

C	-3.969105000	1.928825000	0.623852000
C	-2.361271000	0.315708000	1.381070000
C	-4.458607000	2.054712000	1.917676000
H	-4.405363000	2.516085000	-0.176123000
C	-2.848815000	0.441329000	2.679412000
H	-1.551287000	-0.371282000	1.178299000
C	-3.897554000	1.310529000	2.953426000
H	-5.275815000	2.735927000	2.119444000
H	-2.407238000	-0.143355000	3.476598000
H	-4.275753000	1.409757000	3.962898000
C	-3.375034000	-1.986090000	-1.219821000
H	-3.144987000	-1.585785000	-0.237196000
H	-4.232582000	-1.451364000	-1.632712000
H	-3.654836000	-3.030938000	-1.096237000
N	1.430844000	-1.528190000	1.065011000
N	1.931082000	0.131555000	2.490670000
N	4.661106000	0.628954000	0.037501000
N	3.224309000	-1.202738000	-0.560067000
N	4.350119000	1.939657000	1.925528000
C	0.743262000	-2.668294000	0.469958000
C	1.219504000	-4.027730000	1.003543000
C	0.128759000	-4.375863000	2.031814000
C	-1.119552000	-3.766586000	1.396527000
C	-2.238410000	-3.436086000	2.354809000
C	1.115478000	-0.858379000	2.224958000
C	2.844747000	0.112273000	1.454723000
C	2.549947000	-0.910630000	0.557076000
C	3.958163000	0.915263000	1.146115000
C	4.259315000	-0.384058000	-0.737122000
O	1.203277000	-4.952391000	-0.071356000
O	-0.045489000	-5.771968000	2.206761000
O	-0.635626000	-2.558145000	0.778858000
H	0.904646000	-2.607109000	-0.606059000
H	0.956813000	-5.811637000	0.302982000
H	2.217066000	-3.957801000	1.444424000
H	0.562353000	-6.085599000	2.886907000
H	0.342506000	-3.882340000	2.983895000
H	-1.475435000	-4.447640000	0.615461000
H	-1.894394000	-2.750251000	3.130398000
H	-2.589655000	-4.353200000	2.829953000
H	3.784554000	2.227573000	2.704689000
H	5.093676000	2.542029000	1.616290000
H	0.263271000	-1.142362000	2.817871000
H	4.858839000	-0.559536000	-1.624253000

28-RC-complex

H	-0.169575000	1.685221000	3.546211000
C	2.573957000	0.224250000	2.291939000
H	2.749182000	0.761033000	1.359145000
H	3.522025000	0.081648000	2.803893000
H	2.132733000	-0.741630000	2.056491000
C	1.668242000	1.028638000	3.192457000
H	-1.347457000	1.189083000	1.781563000
H	-2.130837000	-2.316593000	1.935742000
O	2.098553000	1.549310000	4.223599000
C	-0.814445000	-0.852287000	2.180945000
C	-0.436437000	0.593068000	1.795814000
N	0.372348000	1.215443000	2.835816000
O	-0.077064000	-1.528723000	2.895457000
N	-1.966830000	-1.350951000	1.691985000
C	0.163957000	0.627362000	0.396673000
C	-0.618379000	1.217339000	-0.749388000
C	0.568835000	1.949001000	-0.193035000
H	0.793603000	-0.215794000	0.146244000
H	-1.599368000	1.621893000	-0.538636000
H	-0.528689000	0.741543000	-1.716690000
H	1.479552000	1.983545000	-0.775664000
H	0.382091000	2.831334000	0.405117000
C	-2.947973000	-0.706868000	0.831405000
H	-3.163128000	0.306727000	1.168617000
H	-2.619997000	-0.671231000	-0.207544000
H	-3.872475000	-1.277070000	0.886588000
N	-0.796805000	0.648652000	6.231570000
N	-0.003622000	2.408772000	7.375821000
N	2.726201000	-0.002564000	8.048613000
N	0.989669000	-0.952134000	6.684991000
N	2.671781000	2.167574000	8.867931000
C	-1.676757000	-0.164569000	5.413805000
C	-2.911539000	-0.711521000	6.150420000
C	-4.042207000	0.208408000	5.652918000
C	-3.582334000	0.511227000	4.210052000
C	-4.141368000	1.721672000	3.590010000
C	-0.974793000	1.956968000	6.624096000
C	0.865793000	1.341538000	7.493623000
C	0.392295000	0.238782000	6.787581000
C	2.102463000	1.184826000	8.145733000
C	2.147220000	-0.979765000	7.340961000
O	-3.126944000	-2.042250000	5.714022000
O	-5.304997000	-0.427503000	5.634911000
O	-2.155895000	0.645750000	4.346454000
H	-1.076055000	-0.988577000	5.029267000
H	-4.084455000	-2.191273000	5.730884000

H	-2.780604000	-0.669911000	7.234822000
H	-5.751248000	-0.275103000	6.476133000
H	-4.066302000	1.130776000	6.236803000
H	-3.812883000	-0.377350000	3.609152000
H	-3.683925000	2.681888000	3.783399000
H	-5.076540000	1.671108000	3.053213000
H	2.270400000	3.088874000	8.873485000
H	3.597961000	2.038943000	9.238125000
H	-1.832825000	2.524051000	6.302956000
H	2.697033000	-1.914224000	7.299961000

28-PC-complex

H	-0.612289000	-0.088554000	3.135636000
C	2.134269000	-1.149846000	1.518853000
H	2.954910000	-0.451818000	1.350903000
H	2.565340000	-2.089592000	1.861767000
H	1.608697000	-1.306525000	0.580849000
C	1.249645000	-0.631072000	2.624757000
H	-3.610263000	0.884059000	2.876435000
H	-3.622116000	-1.004794000	0.043199000
O	1.613190000	-0.667733000	3.797042000
C	-1.908539000	-0.734820000	0.984008000
C	-0.627573000	-0.026305000	1.084709000
N	-0.000586000	-0.154228000	2.319573000
O	-2.149850000	-1.681785000	1.754329000
N	-2.817529000	-0.397048000	0.024618000
C	-0.037063000	0.774272000	0.005635000
C	-0.104906000	2.309230000	0.060607000
C	1.204672000	1.611465000	0.185241000
H	-0.187937000	0.368494000	-0.986860000
H	-0.531819000	2.741173000	0.955812000
H	-0.357208000	2.814994000	-0.861353000
H	1.892940000	1.642379000	-0.648545000
H	1.677164000	1.623793000	1.156430000
C	-2.998443000	0.876986000	-0.663079000
H	-2.767913000	1.716440000	-0.009553000
H	-2.386886000	0.955831000	-1.562074000
H	-4.043742000	0.950969000	-0.956074000
N	-0.579911000	0.891692000	6.569285000
N	-0.442221000	2.982331000	7.373270000
N	2.380783000	1.454464000	9.223863000
N	1.274450000	-0.124318000	7.787870000
N	1.734311000	3.672159000	9.433631000
C	-1.049791000	-0.265834000	5.816473000
C	-2.060949000	-1.125589000	6.585951000
C	-3.407303000	-0.620851000	6.034607000

C	-3.065590000	-0.307642000	4.581114000
C	-3.946737000	0.708843000	3.898436000
C	-1.085517000	2.171333000	6.570710000
C	0.542450000	2.196313000	7.939265000
C	0.473795000	0.893110000	7.451244000
C	1.560799000	2.461802000	8.874723000
C	2.195452000	0.248787000	8.673529000
O	-1.851160000	-2.479465000	6.223582000
O	-4.428597000	-1.603371000	6.085878000
O	-1.710451000	0.203668000	4.651498000
H	-0.169642000	-0.848916000	5.546041000
H	-2.720785000	-2.907243000	6.224669000
H	-1.962913000	-0.988556000	7.665787000
H	-4.872735000	-1.556677000	6.940822000
H	-3.708822000	0.289245000	6.559950000
H	-3.050946000	-1.238625000	4.009742000
H	-3.942765000	1.656646000	4.439476000
H	-4.969664000	0.331300000	3.860213000
H	1.169914000	4.452298000	9.146635000
H	2.507774000	3.829413000	10.056585000
H	-1.915070000	2.441224000	5.939721000
H	2.888320000	-0.521731000	8.995021000

Cartesian coordinates of Substrates• radical and Ado-H for substrates **1-28**.

1A•

H	7.131665000	0.128468000	0.176429000
H	4.116280000	-1.581563000	0.224081000
H	3.966084000	-0.391882000	1.488280000
H	2.644874000	1.094456000	-0.062472000
H	2.793826000	-0.101788000	-1.331415000
H	1.560428000	-1.763106000	0.088234000
H	1.412469000	-0.564352000	1.359227000
H	0.111495000	0.911300000	-0.183812000
H	0.248527000	-0.288496000	-1.454228000
H	-0.979431000	-1.943112000	-0.041405000
H	-1.134335000	-0.752039000	1.240698000
H	-1.499262000	2.226296000	1.330305000
H	-2.925967000	1.274041000	2.052845000
H	-3.657335000	-2.053142000	-0.240207000
H	-2.249813000	-0.449509000	-1.579859000
H	-2.319432000	1.773312000	-0.929132000
H	-4.796275000	1.776608000	-0.045691000
O	5.317547000	1.048700000	-0.906455000
O	6.352095000	-0.337506000	0.520535000
C	5.254955000	0.165622000	-0.083557000

C	3.998899000	-0.508101000	0.400732000
C	2.725432000	0.019896000	-0.247098000
C	1.474849000	-0.686463000	0.272264000
C	0.189905000	-0.164870000	-0.367480000
C	-1.060915000	-0.869507000	0.156113000
C	-2.374531000	1.609674000	1.184756000
O	-5.811174000	-0.614513000	0.032158000
C	-4.643622000	-0.264675000	-0.098943000
N	-3.536180000	-1.073799000	-0.034888000
C	-2.340489000	-0.365096000	-0.489536000
C	-2.745022000	1.119093000	-0.168000000
N	-4.202150000	1.016316000	-0.339009000

1B•

1	4.165794000	-1.587120000	0.222987000
1	4.025322000	-0.406479000	1.496574000
1	2.710816000	1.092343000	-0.036240000
1	2.853076000	-0.091331000	-1.312558000
1	1.618326000	-1.762667000	0.098873000
1	1.470381000	-0.569665000	1.374040000
1	0.170732000	0.913011000	-0.164945000
1	0.309436000	-0.281820000	-1.439254000
1	-0.920392000	-1.941682000	-0.031396000
1	-1.082538000	-0.750918000	1.249921000
1	-1.449187000	2.220509000	1.338707000
1	-2.886735000	1.277092000	2.051536000
1	-3.597864000	-2.054884000	-0.241251000
1	-2.184922000	-0.450141000	-1.575840000
1	-2.258736000	1.772345000	-0.926158000
1	-4.741403000	1.773789000	-0.057075000
8	5.338995000	1.076730000	-0.892884000
8	6.442929000	-0.322832000	0.468994000
6	5.395293000	0.144512000	-0.052493000
6	4.073515000	-0.511286000	0.407131000
6	2.792291000	0.018004000	-0.225699000
6	1.535679000	-0.685580000	0.285859000
6	0.249605000	-0.162858000	-0.351742000
6	-1.003754000	-0.867967000	0.165548000
6	-2.327574000	1.609794000	1.187264000
8	-5.754903000	-0.617579000	0.015516000
6	-4.586651000	-0.267066000	-0.109152000
7	-3.479134000	-1.074879000	-0.037840000
6	-2.281000000	-0.365572000	-0.485961000
6	-2.688953000	1.118207000	-0.167524000
7	-4.145006000	1.014301000	-0.347919000

2A•

O	4.330373000	-0.531169000	-0.448864000
P	2.809684000	-0.447297000	-0.047934000
O	2.590975000	1.135499000	0.191237000
O	2.128828000	-0.764512000	-1.431390000
O	2.375609000	-1.251460000	1.105983000
C	1.415241000	1.639737000	0.703231000
C	0.327686000	1.895616000	-0.262339000
C	-0.923923000	2.524164000	0.341353000
O	-0.123947000	0.600647000	-0.839162000
C	-1.511233000	0.397241000	-0.567794000
C	-1.821536000	1.307466000	0.624198000
N	-1.794883000	-0.997394000	-0.383940000
O	-1.518378000	3.366033000	-0.633593000
O	-3.200890000	1.621765000	0.621018000
C	-1.399695000	-1.853030000	0.638721000
C	-2.012953000	-3.046814000	0.364329000
N	-2.767695000	-2.952725000	-0.789929000
C	-2.606398000	-1.729717000	-1.216662000
N	-0.607367000	-1.425720000	1.704438000
H	4.917915000	-0.728925000	0.293699000
H	1.199012000	-0.436416000	-1.441936000
H	1.285053000	1.576210000	1.775130000
H	0.690310000	2.487781000	-1.103933000
H	-0.695604000	3.083181000	1.253114000
H	-2.104236000	0.726259000	-1.424133000
H	-1.516977000	0.817280000	1.548181000
H	-2.463861000	3.411408000	-0.427666000
H	-3.489294000	1.795238000	1.524357000
H	-1.948202000	-3.957374000	0.937802000
H	-3.032443000	-1.297934000	-2.108499000
H	0.364714000	-1.255984000	1.451247000
H	-0.625748000	-2.102803000	2.455601000

2B•

O	3.944407000	-0.050260000	1.284794000
P	3.296371000	-0.524473000	-0.130910000
O	2.425862000	0.823305000	-0.568003000
O	4.380415000	-0.621404000	-1.137409000
O	2.325313000	-1.630167000	0.129749000
C	1.404063000	1.283260000	0.198432000
C	0.210291000	1.747333000	-0.532668000
C	-0.816503000	2.454863000	0.347550000
O	-0.511025000	0.588019000	-1.117994000
C	-1.802785000	0.489317000	-0.551943000
C	-1.761094000	1.311137000	0.740489000

N	-2.183046000	-0.892054000	-0.381761000
O	-1.506502000	3.421548000	-0.434658000
O	-3.070870000	1.744213000	1.067157000
C	-1.583466000	-1.867566000	0.399775000
C	-2.387097000	-2.973297000	0.275168000
N	-3.457091000	-2.703333000	-0.557948000
C	-3.299066000	-1.463366000	-0.940022000
N	-0.451982000	-1.614062000	1.170089000
H	3.448975000	-0.410357000	2.030244000
H	1.338889000	0.936187000	1.223400000
H	0.497435000	2.378783000	-1.375027000
H	-0.350752000	2.923811000	1.218796000
H	-2.552109000	0.929397000	-1.217835000
H	-1.319888000	0.715181000	1.539642000
H	-2.380546000	3.534643000	-0.033309000
H	-3.128072000	1.890650000	2.018198000
H	-2.246238000	-3.936308000	0.739157000
H	-3.935036000	-0.912461000	-1.614709000
H	0.394016000	-1.411004000	0.634256000
H	-0.254268000	-2.397414000	1.778389000

2C•

O	3.851453000	0.001817000	1.338969000
P	3.321859000	-0.472965000	0.000217000
O	2.379119000	0.862505000	-0.595341000
O	4.340763000	-0.621611000	-1.107665000
O	2.290801000	-1.593885000	0.089567000
C	1.383792000	1.351778000	0.158888000
C	0.178887000	1.805084000	-0.558879000
C	-0.862211000	2.464517000	0.337407000
O	-0.540708000	0.645881000	-1.177599000
C	-1.788982000	0.462825000	-0.550467000
C	-1.746206000	1.279464000	0.745444000
N	-2.086214000	-0.941870000	-0.372380000
O	-1.613781000	3.404223000	-0.424615000
O	-3.067102000	1.653435000	1.110079000
C	-1.440890000	-1.885436000	0.415668000
C	-2.181751000	-3.033995000	0.274111000
N	-3.253308000	-2.823337000	-0.573250000
C	-3.158841000	-1.574112000	-0.948031000
N	-0.337942000	-1.579622000	1.206874000
H	1.318246000	1.023961000	1.191634000
H	0.440476000	2.451810000	-1.398516000
H	-0.402243000	2.951392000	1.201916000
H	-2.596390000	0.856872000	-1.177031000
H	-1.259999000	0.699676000	1.529686000

H	-2.485048000	3.468043000	-0.006981000
H	-3.099209000	1.805415000	2.061320000
H	-1.994898000	-3.988573000	0.739846000
H	-3.815273000	-1.057846000	-1.630730000
H	0.540667000	-1.404948000	0.691395000
H	-0.159116000	-2.337189000	1.853481000

3•

H	4.345306000	1.228870000	-0.712734000
H	-5.638997000	-0.192665000	0.017051000
H	-4.724782000	-1.284579000	1.085197000
H	-4.695489000	-1.556574000	-0.649021000
H	-2.173667000	-1.203606000	-0.945070000
H	-2.134809000	-1.303094000	0.789561000
H	-0.988093000	0.943913000	0.893581000
H	-1.031780000	1.041853000	-0.851352000
H	0.380398000	-1.024935000	-1.008159000
H	0.422165000	-1.130524000	0.740961000
H	1.566048000	1.104337000	0.846723000
H	1.492429000	1.225051000	-0.890557000
H	2.904319000	-1.190781000	-0.656332000
O	-3.613703000	1.324763000	-0.003992000
C	5.382268000	-0.455141000	0.148269000
C	4.173152000	0.478889000	0.078474000
C	-4.727397000	-0.778272000	0.116134000
C	-3.513270000	0.113054000	0.019728000
C	-2.172587000	-0.586144000	-0.038521000
C	-0.963178000	0.338452000	-0.017127000
C	0.358270000	-0.423323000	-0.092783000
C	1.582346000	0.494666000	-0.066988000
C	2.882974000	-0.220641000	-0.168154000
H	4.100813000	1.065749000	1.003667000
H	6.305887000	0.103343000	0.311339000
H	5.273204000	-1.173758000	0.963692000
H	5.491213000	-1.019943000	-0.780795000

4•

C	3.365152000	0.201904000	-0.059140000
C	1.859957000	0.255350000	0.003396000
O	1.262809000	1.327268000	-0.036273000
N	1.233567000	-0.964890000	0.093878000
C	-0.086777000	-1.359636000	0.157182000
C	-1.360225000	-0.647234000	0.093711000
O	-2.396769000	-1.335714000	0.169524000
N	-1.398963000	0.690816000	-0.046423000
C	-2.656400000	1.405776000	-0.107369000

H	3.680501000	0.553055000	-1.043318000
H	-0.199936000	-2.427704000	0.257783000
H	1.872029000	-1.746313000	0.130803000
H	-3.260413000	1.070406000	-0.953350000
H	-0.514200000	1.189637000	-0.073418000
H	-2.446554000	2.466934000	-0.221770000
H	-3.243046000	1.255611000	0.802046000
H	3.780751000	-0.789425000	0.110917000
H	3.765680000	0.892990000	0.682199000

5•

C	2.766433000	2.229437000	-0.061952000
N	1.895503000	1.375340000	-0.387404000
C	1.683329000	0.248318000	0.509789000
C	2.130812000	-1.120224000	-0.184152000
O	1.855864000	-1.264702000	-1.392426000
C	0.253013000	0.099067000	0.886126000
C	-0.841845000	0.261142000	-0.110461000
C	-2.224961000	-0.008232000	0.484132000
C	-3.319217000	0.177768000	-0.550382000
N	-4.675107000	-0.112889000	0.045382000
O	2.678762000	-1.934858000	0.591413000
H	3.357305000	2.169616000	0.860865000
H	2.297041000	0.335125000	1.415353000
H	0.052660000	-0.469758000	1.787412000
H	-0.811248000	1.267183000	-0.544077000
H	-0.662181000	-0.418508000	-0.957909000
H	-2.399445000	0.667749000	1.326118000
H	-2.261474000	-1.028916000	0.875918000
H	-3.358903000	1.199925000	-0.921598000
H	-3.201860000	-0.498779000	-1.394613000
H	-5.424187000	0.030546000	-0.633671000
H	-4.737283000	-1.078916000	0.371626000
H	-4.866332000	0.493065000	0.845639000
H	2.959100000	3.077844000	-0.716623000

6A•

C	-3.107384000	1.289375000	0.267574000
N	-1.908829000	0.950359000	0.472534000
C	-1.278393000	0.093983000	-0.532531000
C	-0.848724000	-1.241257000	0.084106000
O	-0.320327000	-1.116558000	1.309925000
C	-0.060969000	0.743019000	-1.127331000
C	1.024009000	1.316711000	-0.307166000
O	-0.935075000	-2.298324000	-0.496636000
H	-3.688135000	0.970527000	-0.605519000

H	-1.972657000	-0.174275000	-1.336620000
H	0.132678000	0.510413000	-2.166090000
H	1.478642000	2.168475000	-0.825444000
H	0.653260000	1.682579000	0.649472000
H	-3.607308000	1.936192000	0.985612000
C	2.230405000	0.343726000	-0.005383000
O	2.334259000	-0.688835000	-0.705616000
O	2.997238000	0.724906000	0.908173000
H	0.002897000	-1.989278000	1.588464000

6B•

C	-2.474585000	2.182326000	-0.144149000
N	-1.592331000	1.386732000	0.284015000
C	-1.279822000	0.219543000	-0.531615000
C	-1.733972000	-1.113846000	0.228657000
O	-2.346602000	-1.937179000	-0.484986000
C	0.174738000	0.107431000	-0.802565000
C	1.163786000	0.336385000	0.280213000
O	-1.401230000	-1.218903000	1.427116000
H	-3.002309000	2.045031000	-1.096184000
H	-1.834607000	0.229824000	-1.477058000
H	0.482481000	-0.457274000	-1.672155000
H	1.131682000	1.362950000	0.659618000
H	0.908600000	-0.278322000	1.158158000
H	-2.741649000	3.057028000	0.446467000
C	2.585853000	0.014187000	-0.090094000
O	2.959388000	-0.531541000	-1.102034000
O	3.443926000	0.400769000	0.877995000
H	4.342269000	0.152311000	0.605640000

6C•

C	-2.251475000	2.358398000	-0.200396000
N	-1.539676000	1.451183000	0.312716000
C	-1.274229000	0.271684000	-0.505912000
C	-1.727282000	-0.984145000	0.254398000
O	-2.153998000	-1.929850000	-0.599403000
C	0.191212000	0.101126000	-0.762716000
C	1.182409000	0.324862000	0.316265000
O	-1.655131000	-1.143074000	1.447017000
H	-2.681062000	2.298385000	-1.206268000
H	-1.809902000	0.291882000	-1.461533000
H	0.497787000	-0.377844000	-1.680800000
H	1.169228000	1.361602000	0.671400000
H	0.936647000	-0.262371000	1.213169000
H	-2.458824000	3.257747000	0.375225000
C	2.599187000	-0.016730000	-0.073040000

O	2.955682000	-0.480727000	-1.129117000
O	3.454524000	0.260460000	0.928881000
H	4.351652000	0.021989000	0.643100000
H	-2.355349000	-2.735313000	-0.093922000

6D•

C	-2.125413000	2.343744000	-0.364769000
N	-1.416743000	1.463449000	0.197246000
C	-1.178028000	0.220873000	-0.526335000
C	-1.862493000	-1.009983000	0.215990000
O	-1.877949000	-1.000797000	1.464547000
C	0.275755000	-0.081113000	-0.663052000
C	1.243933000	0.070110000	0.451669000
O	-2.287205000	-1.903783000	-0.552965000
H	-2.559276000	2.223134000	-1.366030000
H	-1.636487000	0.253083000	-1.523695000
H	0.557073000	-0.738563000	-1.476052000
H	1.079413000	1.001572000	0.995022000
H	1.084222000	-0.731896000	1.195925000
H	-2.331833000	3.280419000	0.151227000
C	2.733382000	-0.036759000	0.038302000
O	3.031556000	-0.900986000	-0.823845000
O	3.533759000	0.733925000	0.628770000

7A•

C	-0.803476000	-0.929368000	-0.048504000
C	-0.394127000	0.396959000	0.076159000
C	-1.355183000	1.437436000	0.111085000
N	0.143052000	-1.897891000	-0.137554000
C	1.484948000	-1.650304000	0.395486000
C	1.920495000	-0.249552000	0.084321000
N	0.957711000	0.708269000	0.069298000
C	3.289828000	0.071190000	-0.081043000
O	3.512317000	1.409793000	-0.299052000
O	4.224181000	-0.733092000	-0.036779000
O	-1.119882000	2.648304000	0.182526000
N	-4.314794000	-0.659046000	-0.196030000
H	-3.392737000	1.683866000	0.046237000
H	-0.196174000	-2.847410000	-0.101519000
H	2.184228000	-2.353866000	-0.049722000
H	1.495069000	-1.816418000	1.482386000
H	1.211765000	1.681089000	-0.032106000
H	-4.554733000	-1.634204000	-0.129669000
H	-5.026681000	0.002346000	0.064747000
N	-2.102905000	-1.299291000	-0.119156000
C	-3.005161000	-0.345154000	-0.080906000

N	-2.675478000	0.971649000	0.038658000
H	4.469275000	1.531484000	-0.380010000

7B•

C	-0.756188000	-0.918613000	-0.062847000
C	-0.357312000	0.411508000	0.044666000
C	-1.335291000	1.434455000	0.088007000
N	0.198462000	-1.889309000	-0.160659000
C	1.547771000	-1.616692000	0.361783000
C	1.972059000	-0.220920000	0.039777000
N	0.991369000	0.730254000	0.053673000
C	3.370870000	0.203599000	-0.090244000
O	3.577409000	1.446703000	-0.265978000
O	4.263677000	-0.694695000	-0.015371000
O	-1.124199000	2.654257000	0.154504000
N	-4.289683000	-0.695866000	-0.167054000
H	-3.375761000	1.656359000	0.040542000
H	-0.145323000	-2.831288000	-0.043849000
H	2.253132000	-2.316194000	-0.080385000
H	1.558089000	-1.788059000	1.450748000
H	1.279023000	1.690477000	-0.072651000
H	-4.499789000	-1.671778000	-0.030331000
H	-4.978841000	-0.058645000	0.199217000
N	-2.057783000	-1.307622000	-0.098701000
C	-2.969007000	-0.369421000	-0.059854000
N	-2.651369000	0.951903000	0.033274000

8A•

O	-4.056112000	-1.381204000	1.745364000
O	-4.104573000	1.972632000	-1.098394000
C	-1.246106000	0.607616000	-0.529875000
C	-0.606281000	0.596426000	0.895460000
C	0.833496000	1.040448000	0.842223000
C	4.209390000	-0.325318000	-0.155468000
C	2.617217000	-2.130436000	-0.300617000
O	1.132515000	2.193077000	1.113090000
H	-5.418843000	0.533618000	-1.794956000
O	5.782314000	1.437970000	-0.019428000
O	-5.543835000	-0.294710000	-1.305766000
C	1.884999000	0.071100000	0.395348000
O	6.530336000	-0.574006000	-0.668447000
C	3.195708000	0.532978000	0.256277000
C	3.915095000	-1.663825000	-0.434517000
H	-4.584930000	-2.267704000	-0.056906000
H	-3.706818000	1.451153000	0.866474000
H	-5.709620000	0.133027000	0.718927000

H	-4.589004000	2.695694000	-0.680013000
H	-3.570300000	-2.175123000	2.001750000
C	5.614646000	0.135097000	-0.313040000
C	1.606079000	-1.269553000	0.112127000
H	-1.205475000	1.620944000	-0.932018000
H	-1.141986000	1.295309000	1.536367000
H	-0.662665000	-0.033725000	-1.194632000
H	-0.705718000	-0.403387000	1.317652000
H	3.408076000	1.568827000	0.473990000
H	4.710308000	-2.323073000	-0.753968000
H	2.388744000	-3.165447000	-0.516231000
H	0.601834000	-1.655760000	0.210706000
O	-2.868092000	-1.177041000	-0.250039000
C	-3.836192000	0.971353000	-0.112368000
C	-4.954013000	-0.098583000	-0.034571000
C	-4.167754000	-1.346967000	0.351728000
C	-2.651833000	0.155406000	-0.503027000
H	6.719274000	1.657456000	-0.146269000

8B•

O	-3.996276000	-1.414818000	1.727795000
O	-4.083773000	1.965523000	-1.085438000
C	-1.207860000	0.625394000	-0.524476000
C	-0.572672000	0.616879000	0.901019000
C	0.869709000	1.064549000	0.851350000
C	4.257750000	-0.284045000	-0.154003000
C	2.655367000	-2.099093000	-0.269300000
O	1.153843000	2.222726000	1.124474000
H	-5.380924000	0.520301000	-1.792359000
O	5.882246000	1.453733000	-0.064533000
O	-5.500304000	-0.312959000	-1.310106000
C	1.921182000	0.100603000	0.410799000
O	6.550543000	-0.592151000	-0.703884000
C	3.233992000	0.560795000	0.257298000
C	3.952898000	-1.622389000	-0.415442000
H	-4.518316000	-2.288300000	-0.082798000
H	-3.677486000	1.432080000	0.874388000
H	-5.665648000	0.092869000	0.718953000
H	-4.576153000	2.679127000	-0.660127000
H	-3.496306000	-2.202959000	1.974655000
C	5.691088000	0.239906000	-0.321662000
C	1.640101000	-1.244394000	0.141268000
H	-1.175032000	1.639914000	-0.924888000
H	-1.111804000	1.315081000	1.540192000
H	-0.615037000	-0.009016000	-1.187553000
H	-0.671444000	-0.382625000	1.323755000

H	3.459615000	1.597281000	0.461165000
H	4.750281000	-2.279254000	-0.735507000
H	2.432135000	-3.138406000	-0.475124000
H	0.637687000	-1.633766000	0.248381000
O	-2.813140000	-1.178679000	-0.266843000
C	-3.802629000	0.958557000	-0.108070000
C	-4.909239000	-0.123533000	-0.038286000
C	-4.109370000	-1.367464000	0.334082000
C	-2.609765000	0.159344000	-0.507051000

9•

H	0.885393000	-1.838141000	-0.711685000
C	3.413407000	-0.369546000	0.922298000
H	2.810755000	-0.153906000	1.804319000
H	4.328025000	-0.881173000	1.210652000
H	3.675649000	0.582286000	0.459265000
C	2.680433000	-1.246778000	-0.055948000
H	-1.109865000	-0.211890000	1.773339000
H	1.796643000	2.842151000	-0.168553000
H	-0.932922000	-1.689465000	0.829355000
O	3.238203000	-2.123945000	-0.701878000
C	0.802395000	1.270456000	0.532870000
C	0.463294000	-0.148946000	0.370007000
N	1.314931000	-1.075793000	-0.198988000
C	-0.904986000	-0.600228000	0.772278000
O	0.351126000	1.903006000	1.500047000
N	1.593252000	1.879379000	-0.391051000
C	-1.987044000	-0.093364000	-0.192203000
H	-1.966389000	0.996574000	-0.238091000
H	-1.814977000	-0.483621000	-1.197017000
S	-3.638574000	-0.625592000	0.373070000
C	-4.648850000	0.114110000	-0.941824000
H	-5.688256000	-0.129039000	-0.725616000
H	-4.530505000	1.197534000	-0.955811000
H	-4.380127000	-0.298712000	-1.914138000
C	1.882647000	1.440639000	-1.749684000
H	2.808828000	0.865140000	-1.814431000
H	1.068749000	0.834277000	-2.142972000
H	1.986486000	2.321791000	-2.379588000

10A•

C	-2.241781000	1.035990000	-0.367243000
C	-2.807311000	-0.078123000	0.492469000
O	-2.273262000	-0.149796000	1.722531000
C	-1.309475000	0.359698000	-1.451465000
C	-0.153832000	-0.403284000	-0.895191000

C	-0.106571000	-1.757174000	-0.681234000
C	1.105421000	0.120491000	-0.439490000
N	1.098845000	-2.105687000	-0.118153000
C	1.866824000	-0.978132000	0.040252000
C	1.669758000	1.403206000	-0.400078000
C	3.153947000	-0.823766000	0.554729000
C	2.948480000	1.560356000	0.108851000
C	3.682700000	0.457295000	0.583407000
O	-3.639872000	-0.863911000	0.100237000
H	-0.963884000	1.160437000	-2.107694000
H	-1.940265000	-0.301344000	-2.048077000
H	-0.851993000	-2.507246000	-0.890032000
H	1.111475000	2.258015000	-0.759942000
H	3.394183000	2.546580000	0.144397000
H	3.717875000	-1.673958000	0.917218000
H	4.679467000	0.612184000	0.976837000
H	-3.092457000	1.426308000	-0.932321000
H	1.380054000	-3.042616000	0.113762000
C	-1.581762000	2.140371000	0.369804000
H	-1.011904000	1.955761000	1.266831000
H	-1.507401000	3.110306000	-0.101489000
H	-2.660393000	-0.916536000	2.176570000

10B•

C	-2.251771000	1.023761000	-0.316986000
C	-2.906398000	-0.094236000	0.546449000
O	-2.587809000	-0.181008000	1.756920000
C	-1.313239000	0.356231000	-1.385989000
C	-0.157633000	-0.409445000	-0.827489000
C	-0.116266000	-1.755850000	-0.575925000
C	1.118062000	0.111548000	-0.415580000
N	1.101218000	-2.103203000	-0.029844000
C	1.882791000	-0.980145000	0.077356000
C	1.694088000	1.389661000	-0.423975000
C	3.183792000	-0.822068000	0.555230000
C	2.986680000	1.550662000	0.048504000
C	3.724163000	0.454754000	0.535042000
O	-3.712057000	-0.841533000	-0.067013000
H	-0.946745000	1.142913000	-2.051383000
H	-1.939634000	-0.308977000	-1.982347000
H	-0.875368000	-2.502989000	-0.739898000
H	1.131061000	2.238549000	-0.790326000
H	3.440456000	2.534033000	0.046686000
H	3.750090000	-1.666623000	0.927664000
H	4.731778000	0.611559000	0.899355000
H	-3.060510000	1.468590000	-0.909850000

H	1.378519000	-3.035674000	0.222800000
C	-1.577054000	2.090817000	0.457031000
H	-1.163802000	1.882517000	1.432598000
H	-1.358731000	3.044713000	-0.007656000

11A•

C	-2.471066000	0.806707000	0.591426000
C	-3.073656000	0.218294000	-0.677192000
O	-3.111754000	-1.128076000	-0.678813000
C	-0.994719000	1.043599000	0.375702000
C	0.001666000	0.072114000	0.234779000
C	-0.096396000	-1.328776000	0.211945000
C	1.427588000	0.352725000	0.074700000
N	1.146941000	-1.880779000	0.057279000
C	2.097621000	-0.886294000	-0.029916000
C	2.170957000	1.532490000	0.016486000
C	3.477899000	-0.976229000	-0.190494000
C	3.547937000	1.454405000	-0.145095000
C	4.193260000	0.211787000	-0.247262000
O	-3.459100000	0.874899000	-1.617857000
H	-0.687090000	2.078603000	0.310539000
H	-0.968259000	-1.954212000	0.268005000
H	1.684668000	2.496832000	0.095870000
H	4.134747000	2.362858000	-0.192756000
H	3.972208000	-1.936173000	-0.268103000
H	5.268146000	0.178845000	-0.372304000
H	-2.939999000	1.787429000	0.673902000
H	1.332985000	-2.867681000	0.004228000
C	-2.804041000	0.003889000	1.859186000
H	-2.348545000	-0.983635000	1.845939000
H	-2.429067000	0.540618000	2.730987000
H	-3.883200000	-0.118273000	1.966777000
H	-3.460653000	-1.422608000	-1.536276000

11B•

C	2.502868000	-0.856282000	0.462524000
C	3.087089000	-0.000369000	-0.712897000
O	3.299760000	1.219480000	-0.505935000
C	1.034221000	-1.110108000	0.261282000
C	0.038649000	-0.126632000	0.186799000
C	0.176981000	1.268683000	0.219091000
C	-1.396314000	-0.362258000	0.049636000
N	-1.058235000	1.863408000	0.116433000
C	-2.035561000	0.899596000	0.011403000
C	-2.174651000	-1.517460000	-0.041957000
C	-3.416982000	1.029992000	-0.113702000

C	-3.552644000	-1.397842000	-0.170101000
C	-4.166180000	-0.135179000	-0.204822000
O	3.283534000	-0.618890000	-1.789920000
H	0.712774000	-2.140654000	0.168001000
H	1.081081000	1.849662000	0.270228000
H	-1.711756000	-2.496417000	-0.014672000
H	-4.164572000	-2.288007000	-0.243983000
H	-3.887240000	2.004942000	-0.139870000
H	-5.242312000	-0.068341000	-0.304592000
H	3.006195000	-1.822981000	0.390067000
H	-1.219872000	2.855540000	0.107513000
C	2.815483000	-0.260148000	1.843737000
H	2.337327000	0.710074000	1.968153000
H	2.460330000	-0.923483000	2.636422000
H	3.891583000	-0.120859000	1.968572000

12A•

O	0.406643000	-2.211876000	0.562481000
N	2.396093000	-1.218459000	0.180065000
C	0.347156000	-0.018392000	-0.464702000
C	-2.145291000	-0.323748000	1.257082000
H	0.242444000	3.365194000	1.080697000
C	-2.128445000	-0.609525000	-0.224584000
N	-1.000467000	-0.336480000	-0.935979000
H	-2.127932000	0.753716000	1.427651000
C	1.050896000	-1.259252000	0.136965000
H	-1.068918000	-0.600653000	-1.908345000
H	0.887723000	0.250568000	-1.378682000
H	2.827302000	-2.044260000	0.568398000
H	-3.062116000	-0.735756000	1.671336000
H	0.686974000	0.984632000	1.528619000
O	-3.125817000	-1.036820000	-0.804751000
H	-1.284961000	-0.762269000	1.757327000
C	0.432669000	1.130023000	0.490734000
C	3.273976000	-0.201330000	-0.385826000
H	3.276374000	-0.229689000	-1.477798000
H	2.982584000	0.795501000	-0.056750000
H	4.284764000	-0.393282000	-0.034877000
S	-0.040375000	2.698987000	-0.050377000

12B•

O	0.402048000	-1.892565000	0.631169000
N	2.395363000	-0.941794000	0.172494000
C	0.345848000	0.273583000	-0.447201000
C	-2.188544000	-0.010282000	1.228672000
H	0.050745000	3.293471000	0.670478000

C	-2.141814000	-0.309080000	-0.250497000
N	-0.996803000	-0.056527000	-0.936757000
H	-2.157870000	1.068143000	1.392516000
C	1.049159000	-0.960240000	0.165247000
H	-1.050368000	-0.314325000	-1.911872000
H	0.890268000	0.560310000	-1.352712000
H	2.823028000	-1.764812000	0.570592000
H	-3.122241000	-0.402030000	1.624439000
H	0.471365000	1.303965000	1.569932000
O	-3.132462000	-0.732365000	-0.846981000
H	-1.348011000	-0.461019000	1.751422000
O	0.044868000	2.619112000	-0.020494000
C	0.425713000	1.418791000	0.496715000
C	3.274784000	0.056945000	-0.422051000
H	3.252962000	0.018606000	-1.513465000
H	3.003335000	1.060283000	-0.094795000
H	4.290369000	-0.146099000	-0.091561000

13A•

H	0.040191000	0.482349000	-1.628045000
H	-6.097338000	-0.695262000	-0.623111000
H	-5.830071000	-0.718310000	1.086814000
C	2.740592000	-2.027508000	-0.034822000
O	2.390849000	2.790018000	0.669064000
O	-0.349303000	2.652320000	-0.243248000
C	2.008396000	-0.789179000	-0.532537000
O	-1.306891000	-0.072846000	1.930615000
H	-1.812908000	0.058712000	-2.409438000
H	-4.247788000	-0.361070000	-2.225653000
C	-2.047397000	-0.124528000	0.953394000
N	-1.497860000	0.044089000	-0.353078000
O	3.951564000	-2.105089000	-0.081515000
O	1.952974000	-2.993041000	0.413708000
C	-0.084972000	0.311004000	-0.553254000
O	4.011690000	0.616678000	-0.210859000
C	0.435863000	1.547824000	0.179979000
C	1.905311000	1.745144000	-0.173675000
C	-4.150819000	-0.416291000	-0.024859000
C	2.673190000	0.471705000	-0.024268000
O	0.644448000	-0.843598000	-0.165229000
N	-5.464218000	-0.626965000	0.153949000
N	-3.383427000	-0.337794000	1.051893000
C	-2.299540000	-0.058025000	-1.451723000
C	-3.624286000	-0.286328000	-1.348502000
H	2.100673000	-0.835293000	-1.636797000
H	1.959433000	2.079135000	-1.225276000

H	0.349138000	1.389483000	1.254211000
H	4.418457000	-0.271746000	-0.216074000
H	0.044190000	3.450074000	0.132700000
H	3.288203000	3.013387000	0.393640000
H	2.505679000	-3.745223000	0.688984000

13B•

H	-0.099375000	-1.234840000	1.395270000
H	-5.559387000	1.853794000	-0.504526000
H	-5.991827000	0.249170000	-0.020701000
C	2.217221000	1.875876000	-0.241899000
O	2.864862000	-1.826643000	-1.377652000
O	-0.023350000	-2.150430000	-1.162776000
C	2.019665000	0.849273000	0.886095000
O	-2.100052000	-2.206773000	0.698773000
H	-0.842386000	1.833457000	-0.287475000
H	-3.199807000	2.556496000	-0.709583000
C	-2.426340000	-1.033778000	0.452600000
N	-1.405165000	-0.069779000	0.311700000
O	3.453629000	2.388528000	-0.180548000
O	1.401143000	2.160045000	-1.082046000
C	-0.023822000	-0.470590000	0.619654000
O	3.970576000	-0.674777000	1.068841000
C	0.683771000	-1.057909000	-0.604597000
C	2.096771000	-1.492502000	-0.212148000
C	-3.987118000	0.601561000	-0.082221000
C	2.745500000	-0.410459000	0.555338000
O	0.629675000	0.673025000	1.140469000
N	-5.280074000	0.934340000	-0.211324000
N	-3.705175000	-0.640212000	0.301753000
C	-1.689858000	1.182671000	-0.135075000
C	-2.967697000	1.562691000	-0.359369000
H	2.446159000	1.287000000	1.793055000
H	2.013291000	-2.388559000	0.422812000
H	0.757049000	-0.280594000	-1.370103000
H	4.296553000	0.061976000	1.603461000
H	-0.670790000	-2.475700000	-0.507533000
H	2.412604000	-2.565687000	-1.807611000
H	3.590402000	2.988243000	-0.932719000

13C•

H	0.055232000	0.393219000	-1.623060000
H	-6.097477000	-0.713333000	-0.618656000
H	-5.841185000	-0.684531000	1.092830000
C	2.773625000	-2.104067000	0.009632000
O	2.401153000	2.791300000	0.591024000

O	-0.343841000	2.613953000	-0.337259000
C	2.022455000	-0.835856000	-0.484935000
O	-1.322857000	-0.026065000	1.948498000
H	-1.794255000	-0.036442000	-2.395400000
H	-4.234251000	-0.433346000	-2.218508000
C	-2.053191000	-0.109501000	0.965224000
N	-1.493790000	0.010384000	-0.340063000
O	4.038596000	-2.012760000	-0.099464000
O	2.129493000	-3.073360000	0.422501000
C	-0.070467000	0.256142000	-0.541855000
O	4.011370000	0.533269000	-0.112759000
C	0.441925000	1.527390000	0.140532000
C	1.914468000	1.705665000	-0.205418000
C	-4.152834000	-0.422441000	-0.016986000
C	2.663238000	0.434283000	0.008737000
O	0.645143000	-0.882111000	-0.115795000
N	-5.469478000	-0.622103000	0.160043000
N	-3.392399000	-0.313664000	1.061803000
C	-2.288536000	-0.119578000	-1.438051000
C	-3.616962000	-0.335586000	-1.339173000
H	2.089722000	-0.874388000	-1.592061000
H	1.978907000	1.996237000	-1.271644000
H	0.343595000	1.419040000	1.219852000
H	4.314224000	-0.432195000	-0.140276000
H	0.054126000	3.427761000	-0.003576000
H	3.346244000	2.883150000	0.417818000

13D•

H	-0.143173000	-1.273070000	1.482633000
H	-5.459229000	1.903024000	-0.659919000
H	-5.942688000	0.307891000	-0.193480000
C	2.199997000	1.953635000	-0.198433000
O	2.901062000	-1.953601000	-1.188840000
O	0.061152000	-2.269203000	-0.996388000
C	1.997877000	0.879718000	0.925306000
O	-2.135285000	-2.225553000	0.687457000
H	-0.741195000	1.778361000	-0.253949000
H	-3.078884000	2.555140000	-0.773031000
C	-2.423676000	-1.043965000	0.423870000
N	-1.380928000	-0.104558000	0.321604000
O	3.417241000	2.267588000	-0.344473000
O	1.221260000	2.379234000	-0.833174000
C	-0.010994000	-0.515968000	0.705950000
O	4.138938000	-0.152640000	0.462848000
C	0.735907000	-1.135969000	-0.472301000
C	2.154380000	-1.524682000	-0.045268000

C	-3.928797000	0.620187000	-0.175452000
C	2.799227000	-0.344615000	0.602243000
O	0.631606000	0.609086000	1.247335000
N	-5.210546000	0.978211000	-0.356673000
N	-3.688693000	-0.626967000	0.221108000
C	-1.618335000	1.153199000	-0.134182000
C	-2.880342000	1.557759000	-0.411732000
H	2.413108000	1.335870000	1.830151000
H	2.069911000	-2.374075000	0.653139000
H	0.816589000	-0.386660000	-1.266848000
H	4.234131000	0.810352000	0.231948000
H	-0.660119000	-2.520198000	-0.385054000
H	2.413470000	-2.698501000	-1.565992000

14A•

O	-2.280243000	1.325777000	-0.065099000
C	-0.505315000	-0.196069000	0.524822000
N	-1.540140000	-1.191924000	0.763636000
C	-1.085949000	1.155357000	-0.060245000
H	-2.282607000	-0.733590000	1.279325000
H	-0.111527000	0.125047000	1.496210000
H	0.422447000	-1.330410000	-1.150120000
C	0.619708000	-0.703918000	-0.293120000
C	2.011557000	-0.405560000	-0.071791000
O	2.916154000	-0.823543000	-0.779799000
O	2.248796000	0.382495000	1.006556000
H	3.206241000	0.524121000	1.069943000
C	-0.106806000	2.191115000	-0.527718000
H	0.718856000	2.286509000	0.178083000
H	0.320778000	1.860701000	-1.478857000
H	-0.606022000	3.147064000	-0.669487000
C	-2.120083000	-1.812132000	-0.431361000
H	-3.026763000	-2.339701000	-0.137296000
H	-2.382361000	-1.096637000	-1.220532000
H	-1.434378000	-2.550230000	-0.849507000

14B•

8	-2.313024000	1.252901000	-0.097487000
6	-0.468830000	-0.181296000	0.504232000
7	-1.450788000	-1.235606000	0.759265000
6	-1.107529000	1.124310000	-0.048498000
1	-2.221507000	-0.811043000	1.263504000
1	-0.051007000	0.142296000	1.466750000
1	0.508468000	-1.136609000	-1.254222000
6	0.690152000	-0.615348000	-0.323253000
6	2.097540000	-0.298147000	0.023458000

8	2.979502000	-0.752733000	-0.761157000
8	2.307976000	0.392886000	1.062028000
6	-0.163986000	2.219473000	-0.463092000
1	0.711795000	2.238281000	0.186224000
1	0.193567000	1.998487000	-1.473223000
1	-0.676476000	3.179854000	-0.470788000
6	-1.993809000	-1.891268000	-0.433272000
1	-2.854924000	-2.491229000	-0.137493000
1	-2.317383000	-1.193944000	-1.216852000
1	-1.253887000	-2.567628000	-0.863274000

15•

15	-5.144355000	-0.460845000	-0.769229000
8	-5.639393000	-1.331732000	-1.975660000
8	-6.215338000	-0.522802000	0.381335000
8	-4.740960000	0.882207000	-1.217694000
8	-3.962768000	-1.329360000	-0.140271000
15	-2.849636000	-1.104340000	1.004173000
8	-3.626463000	-0.587817000	2.270963000
8	-2.026084000	-2.298100000	1.144921000
8	-2.138558000	0.247203000	0.593963000
15	-1.343087000	0.734900000	-0.747859000
8	-2.307677000	1.813773000	-1.335648000
8	-0.932624000	-0.385009000	-1.594486000
8	-0.136835000	1.544522000	-0.167190000
6	-0.283836000	2.669546000	0.734364000
6	1.111140000	3.076386000	1.185748000
8	1.730057000	1.997253000	1.908022000
6	2.062975000	3.364805000	0.072054000
8	1.662202000	4.210128000	-0.907861000
6	2.900819000	2.167771000	-0.182392000
8	4.222021000	2.487832000	-0.581857000
6	2.819302000	1.461224000	1.189993000
7	2.642585000	0.015904000	1.052775000
6	1.671788000	-0.794835000	1.603977000
7	1.836906000	-2.055955000	1.300024000
6	2.969741000	-2.085361000	0.511503000
6	3.640279000	-3.172007000	-0.125373000
8	3.372615000	-4.367539000	-0.121110000
7	4.768685000	-2.708809000	-0.845851000
6	5.188894000	-1.410195000	-0.951703000
7	6.264060000	-1.163530000	-1.729829000
7	4.564772000	-0.412889000	-0.358081000
6	3.480180000	-0.803610000	0.349475000
1	-0.881329000	2.367756000	1.594800000
1	-0.768420000	3.493779000	0.211251000

1	0.992522000	3.922712000	1.870782000
1	2.318318000	4.218043000	-1.618834000
1	2.426702000	1.531974000	-0.945862000
1	4.659776000	1.627830000	-0.727311000
1	3.747552000	1.636630000	1.740009000
1	0.879847000	-0.382111000	2.204034000
1	6.876017000	-1.909339000	-2.014533000
1	6.665464000	-0.241843000	-1.684469000
1	5.281477000	-3.433501000	-1.330221000
1	-3.266445000	1.523107000	-1.366555000
1	-3.896594000	-1.288175000	2.882496000
1	-6.931850000	0.125087000	0.313416000
1	-6.035170000	-2.187555000	-1.753856000

16•

6	-1.277187000	-0.794845000	0.577512000
6	-1.405371000	0.732384000	0.638362000
6	-0.359560000	1.375687000	-0.274381000
6	1.027599000	0.873385000	0.073995000
6	1.060043000	-0.667655000	0.047718000
8	0.045360000	-1.200495000	0.900994000
7	-2.719629000	1.264801000	0.296818000
8	-0.373087000	2.792093000	-0.135961000
8	1.998814000	1.313751000	-0.885022000
6	2.353056000	-1.248663000	0.514737000
8	3.534327000	-0.735467000	0.063842000
8	-1.668356000	-1.211980000	-0.701350000
6	-1.788117000	-2.626086000	-0.845951000
1	-1.900188000	-1.269334000	1.343754000
1	-1.178118000	1.028121000	1.665076000
1	-0.573229000	1.099386000	-1.314769000
1	1.298192000	1.225963000	1.075488000
1	0.862439000	-0.962539000	-0.994523000
1	-3.386728000	1.098481000	1.040525000
1	-3.072674000	0.807165000	-0.537175000
1	-1.309912000	3.041228000	-0.107847000
1	2.062730000	2.275738000	-0.839062000
1	2.408681000	-1.812240000	1.435238000
1	3.343523000	0.045975000	-0.488731000
1	-2.141009000	-2.810367000	-1.858402000
1	-0.824765000	-3.120015000	-0.700294000
1	-2.510779000	-3.029632000	-0.128993000

17A•

8	-3.119094000	-1.011157000	-0.484061000
8	-0.945842000	-0.224246000	0.345483000

1	3.093615000	0.426443000	-0.883942000
8	-2.953021000	0.265450000	1.790108000
6	1.360273000	1.404359000	-0.084931000
8	2.818315000	-1.964094000	0.519858000
1	3.892613000	-0.079223000	1.480681000
1	0.833402000	1.448460000	0.871441000
6	0.852433000	-1.369082000	-0.777404000
1	-0.017052000	-3.092675000	-1.135702000
1	3.977334000	1.464632000	0.989209000
6	1.828053000	2.785935000	-0.486662000
1	-2.571333000	2.254445000	-0.056574000
8	-2.716208000	1.415458000	-0.515293000
1	2.357992000	-2.815408000	0.454565000
6	-0.184318000	-0.243413000	-0.884764000
1	-4.074043000	-0.933895000	-0.615783000
15	-2.481687000	0.137647000	0.407022000
8	0.293881000	-2.610918000	-0.360485000
8	0.426273000	0.981720000	-1.107732000
1	2.357040000	2.749391000	-1.440988000
6	2.506183000	0.386845000	0.054667000
1	1.278438000	-1.480200000	-1.788692000
1	-0.859877000	-0.418360000	-1.721610000
1	2.496268000	3.196455000	0.270464000
6	1.929858000	-0.983866000	0.177748000
7	3.328218000	0.722356000	1.223063000
1	0.974052000	3.456374000	-0.584785000

17B•

8	2.679461000	1.260685000	0.177504000
8	0.895388000	-0.547690000	0.251781000
1	-3.167857000	0.166061000	-0.782295000
8	2.895245000	-0.831167000	1.715683000
6	-1.808651000	-1.287793000	0.024447000
8	-1.979726000	2.412852000	0.405235000
1	-3.589464000	1.074154000	1.556035000
1	-1.279189000	-1.447237000	0.967029000
6	-0.477395000	1.085122000	-0.967156000
1	1.252802000	1.896967000	-0.410320000
1	-4.220207000	-0.379187000	1.208150000
6	-2.742942000	-2.447207000	-0.250039000
1	3.243526000	-1.911639000	-0.674442000
8	3.163987000	-0.962744000	-0.834456000
1	-1.253956000	3.024037000	0.193461000
6	0.162213000	-0.312082000	-0.946166000
15	2.479817000	-0.205595000	0.433639000
8	0.426523000	2.173054000	-0.888798000

8	-0.846611000	-1.279711000	-1.053812000
1	-3.277580000	-2.294738000	-1.189937000
6	-2.537421000	0.067267000	0.124775000
1	-0.967322000	1.163067000	-1.953258000
1	0.814536000	-0.450057000	-1.810646000
1	-3.471529000	-2.550005000	0.554749000
6	-1.522582000	1.158643000	0.100279000
7	-3.345170000	0.112025000	1.350226000
1	-2.178286000	-3.377605000	-0.316627000

17C•

8	2.603276000	1.238255000	0.393596000
8	0.898516000	-0.634796000	0.240273000
1	-3.143471000	0.236796000	-0.786456000
8	2.940844000	-0.966169000	1.648558000
6	-1.841885000	-1.258664000	0.038846000
8	-1.849836000	2.452653000	0.368991000
1	-3.531165000	1.201649000	1.530962000
1	-1.313423000	-1.421926000	0.982065000
6	-0.405255000	1.040781000	-0.975922000
1	1.346488000	1.783167000	-0.338989000
1	-4.217309000	-0.232658000	1.211231000
6	-2.828881000	-2.382732000	-0.203085000
8	3.173730000	-0.883641000	-0.913964000
1	-1.087447000	3.011209000	0.134900000
6	0.181044000	-0.383104000	-0.930768000
15	2.559489000	-0.301751000	0.345224000
8	0.543888000	2.086874000	-0.891240000
8	-0.895685000	-1.304290000	-1.042786000
1	-3.364081000	-2.227584000	-1.142630000
6	-2.516107000	0.126689000	0.122344000
1	-0.888317000	1.134706000	-1.965885000
1	0.811922000	-0.558013000	-1.806484000
1	-3.555786000	-2.439100000	0.608122000
6	-1.454907000	1.170286000	0.081482000
7	-3.323777000	0.226481000	1.346475000
1	-2.305226000	-3.337989000	-0.255326000

18•

1	-1.909114000	-0.498177000	2.167197000
6	4.477500000	-1.161884000	-0.268005000
6	1.433876000	-0.633345000	1.419493000
6	-2.058469000	-0.153534000	1.136255000
6	0.621961000	1.689104000	0.670086000
7	1.547277000	0.525201000	0.692302000
7	2.432208000	-1.464803000	1.234137000

8	-2.088678000	3.155465000	-0.577077000
7	3.260865000	1.312569000	-0.856784000
6	2.719958000	0.425058000	-0.012226000
6	-1.666554000	1.318288000	1.050801000
6	3.252964000	-0.816321000	0.333714000
8	-5.329537000	-1.181218000	-0.542851000
8	-3.411327000	-0.285051000	0.769565000
8	-3.259550000	-2.661520000	-0.179185000
6	4.412162000	0.873997000	-1.359379000
1	-1.404207000	-0.750654000	0.491796000
1	4.665937000	-3.026279000	0.551977000
1	0.396201000	1.999420000	-1.565130000
7	5.036796000	-0.286101000	-1.121432000
1	-2.085331000	1.124773000	-1.066413000
6	-0.099598000	1.829595000	-0.622769000
8	-0.361285000	1.536854000	1.657947000
1	-2.380503000	1.918006000	1.615909000
8	-3.127976000	-0.654739000	-1.752650000
1	1.244204000	2.559989000	0.905135000
6	-1.563275000	1.818013000	-0.397163000
1	4.913850000	1.538746000	-2.054880000
1	0.597029000	-0.795244000	2.076165000
7	5.111252000	-2.320809000	-0.008330000
1	5.937361000	-2.562632000	-0.528337000
15	-3.814040000	-1.290245000	-0.544464000
1	-3.039940000	3.071186000	-0.716534000

19•

1	-0.291318000	-1.410052000	-1.872325000
6	-1.423177000	-1.686514000	1.272685000
1	-2.075960000	-0.816808000	1.371075000
1	-1.924872000	-2.549720000	1.701680000
1	-0.497146000	-1.497523000	1.809712000
6	-1.171500000	-1.967345000	-0.187810000
1	0.565511000	1.894831000	0.427345000
1	0.807430000	0.422508000	-1.444299000
1	3.640300000	-0.232073000	0.701482000
1	-0.348693000	0.718415000	1.361859000
8	-1.696092000	-2.926712000	-0.749436000
6	1.759268000	-0.598936000	0.197846000
6	0.498846000	-0.042726000	-0.508990000
7	-0.403110000	-1.106642000	-0.915954000
16	-1.668043000	1.684387000	-0.405653000
6	-0.129379000	1.060709000	0.353807000
8	1.730397000	-1.688410000	0.761164000
7	2.872544000	0.159622000	0.174520000

6	-1.983641000	3.044091000	0.576576000
1	-1.244705000	3.426333000	1.264814000
1	-2.899652000	3.583346000	0.389268000
6	3.097065000	1.465750000	-0.428404000
1	2.905117000	2.277172000	0.277039000
1	4.135504000	1.525756000	-0.748663000
1	2.471803000	1.607572000	-1.306575000

20•

7	0.343643000	-0.448699000	-0.469178000
1	4.250968000	-2.229817000	-0.934393000
1	-4.118435000	2.720093000	0.284613000
8	2.729127000	2.343597000	-0.024270000
1	4.276411000	1.618153000	1.296941000
6	2.022958000	1.181070000	0.382588000
6	-4.926522000	0.346092000	0.242029000
6	3.557126000	-0.491687000	-0.414193000
7	-3.559800000	0.196455000	0.126594000
1	1.314976000	-2.351589000	-0.289798000
8	-3.794993000	-2.052756000	0.653463000
7	-0.774928000	-2.297218000	0.122257000
8	4.090120000	0.741092000	1.663360000
1	1.258721000	1.411063000	1.124724000
6	-2.732650000	1.281420000	-0.174489000
1	2.131536000	3.099519000	-0.030848000
1	2.578563000	-0.590296000	1.485411000
6	-1.638829000	-1.217040000	0.081025000
6	-0.956868000	-0.066089000	-0.282309000
6	1.445386000	0.445855000	-0.836731000
6	-3.033118000	-1.154094000	0.330004000
7	-3.319043000	2.503467000	-0.289033000
1	1.063333000	1.146455000	-1.578138000
6	0.389831000	-1.805308000	-0.207361000
8	3.769627000	-1.852501000	-0.187551000
1	4.459000000	-0.012901000	-0.802259000
8	2.511011000	-0.290839000	-1.384619000
1	-5.401063000	1.224540000	-0.154690000
1	-2.662537000	3.261782000	-0.392740000
6	3.066845000	0.176151000	0.881607000
7	-1.443333000	1.180051000	-0.394767000
1	-5.481328000	-0.522344000	0.543978000

21A•

6	0.646310000	-0.985235000	0.576898000
15	-0.678431000	0.092332000	-0.007317000
8	2.432432000	0.612999000	-0.020489000

8	-1.966382000	-0.163666000	0.902465000
1	0.372874000	-2.026211000	0.403683000
1	1.673549000	1.228751000	0.017319000
8	-0.252677000	1.513442000	-0.061736000
1	0.683808000	-0.833134000	1.667667000
8	-1.103889000	-0.569445000	-1.388649000
1	2.725324000	-1.413949000	-0.146004000
6	1.950105000	-0.663270000	-0.080409000
1	-1.705054000	-0.031614000	-1.923857000
1	-2.028398000	0.435558000	1.659272000

21B•

6	-0.580893000	-1.164060000	-0.336854000
15	0.782807000	0.052773000	-0.102522000
8	-2.296328000	0.602524000	-0.119625000
8	2.069441000	-0.463264000	-0.656771000
1	-0.318790000	-2.106708000	0.144922000
1	-1.486035000	1.094762000	-0.418131000
8	0.223967000	1.382758000	-0.569292000
1	-0.596791000	-1.349007000	-1.422141000
8	0.968149000	0.119552000	1.527706000
1	-2.466080000	-1.177826000	0.928891000
6	-1.898552000	-0.677482000	0.156401000
1	0.280426000	0.663864000	1.930863000

21C•

6	-0.587955000	-1.128336000	-0.411821000
15	0.803471000	0.055589000	0.037321000
8	-2.241914000	0.646646000	-0.045845000
8	2.002709000	-0.328806000	-0.822338000
1	-0.365956000	-2.131602000	-0.040739000
1	-1.350991000	1.116525000	-0.242656000
8	0.174671000	1.420388000	-0.373244000
1	-0.564837000	-1.177664000	-1.510933000
8	1.033642000	-0.061254000	1.541267000
1	-2.443045000	-1.199506000	0.875447000
6	-1.925396000	-0.681228000	0.071881000

22A•

1	3.305672000	-0.984550000	-2.022214000
1	3.799890000	-1.033419000	-0.412751000
6	1.988559000	-0.169468000	-0.567320000
7	2.998566000	-1.181723000	-1.071832000
6	0.866090000	-0.848083000	0.120429000
6	2.801699000	0.760110000	0.423894000
8	3.934687000	0.316610000	0.741652000

1	1.140080000	-1.635998000	0.814588000
1	1.665183000	0.430180000	-1.412495000
8	2.228367000	1.796547000	0.778608000
6	-0.489067000	-0.477625000	0.046955000
6	-1.452403000	-1.187519000	0.816748000
6	-0.980706000	0.582129000	-0.764872000
6	-2.793868000	-0.874905000	0.772813000
1	-1.118774000	-1.998645000	1.452370000
6	-2.322296000	0.894684000	-0.808490000
1	-0.295369000	1.170708000	-1.358650000
6	-3.242387000	0.170378000	-0.043290000
1	-3.504146000	-1.436265000	1.368532000
1	-2.681743000	1.703935000	-1.430945000
8	-4.552990000	0.528515000	-0.130121000
1	-5.094252000	-0.034206000	0.438483000
1	2.659260000	-2.141261000	-1.036423000

22B•

1	-4.106642000	0.204403000	-0.710700000
1	-3.701887000	0.194432000	0.851161000
6	-2.103672000	0.024286000	-0.369726000
7	-3.429904000	0.577179000	-0.051576000
6	-1.056459000	0.712974000	0.494321000
6	-2.019298000	-1.520464000	-0.148149000
8	-2.495484000	-1.948322000	0.934172000
1	-1.337968000	0.655971000	1.547501000
1	-1.901394000	0.220269000	-1.423840000
1	-1.175075000	1.943085000	0.228357000
8	-1.479268000	-2.198950000	-1.055182000
6	0.370045000	0.371438000	0.290910000
6	1.206853000	0.096019000	1.377423000
6	0.953067000	0.370444000	-0.984909000
6	2.558991000	-0.181464000	1.209154000
1	0.791464000	0.091622000	2.378347000
6	2.299187000	0.098301000	-1.169366000
1	0.342328000	0.590201000	-1.851109000
6	3.109817000	-0.181763000	-0.069628000
1	3.183231000	-0.399296000	2.068480000
1	2.736992000	0.100626000	-2.159544000
8	4.431697000	-0.446333000	-0.308389000
1	4.889436000	-0.616783000	0.524076000
6	-1.250034000	3.363856000	-0.137691000
1	-1.470159000	3.321129000	-1.199206000
1	-0.256789000	3.723924000	0.110066000
1	-2.050761000	3.757244000	0.478601000

22C•

1	3.626856000	-0.697628000	-1.793204000
1	3.326548000	-1.734833000	-0.546540000
6	1.945506000	-0.134884000	-0.622181000
7	2.882324000	-1.148083000	-1.256327000
6	0.837735000	-0.832814000	0.085079000
6	2.707439000	0.742004000	0.372811000
8	3.704054000	0.071586000	0.962222000
1	1.133821000	-1.623289000	0.764688000
1	1.598556000	0.506835000	-1.425773000
8	2.383330000	1.871990000	0.617712000
6	-0.515962000	-0.465118000	0.026569000
6	-1.462775000	-1.195485000	0.799894000
6	-1.021660000	0.607303000	-0.760923000
6	-2.803404000	-0.888190000	0.782250000
1	-1.114182000	-2.015850000	1.414557000
6	-2.362285000	0.915367000	-0.776458000
1	-0.351456000	1.209325000	-1.358583000
6	-3.267350000	0.172305000	-0.007933000
1	-3.502952000	-1.462249000	1.377873000
1	-2.735591000	1.734287000	-1.376994000
8	-4.573617000	0.527420000	-0.066754000
1	-5.108919000	-0.044751000	0.498966000
1	4.134937000	0.633204000	1.628577000
1	2.362512000	-1.759372000	-1.889372000

22D•

1	-3.887940000	-0.726330000	1.520720000
1	-3.475496000	-1.724368000	0.304132000
6	-2.064525000	-0.294771000	0.697300000
7	-3.108509000	-1.229382000	1.110348000
6	-0.914610000	-1.029980000	0.074618000
6	-2.510772000	0.784100000	-0.300767000
8	-3.344743000	0.302940000	-1.240523000
1	-1.731880000	0.255341000	1.579174000
1	-1.167155000	-1.950028000	-0.440045000
8	-2.132189000	1.932134000	-0.278717000
6	0.422842000	-0.598058000	0.053826000
6	0.865492000	0.619987000	0.639305000
6	1.417432000	-1.400956000	-0.575668000
6	2.193959000	0.994677000	0.606205000
1	0.150621000	1.281802000	1.107368000
6	2.741344000	-1.027268000	-0.606281000
1	1.118587000	-2.333884000	-1.038074000
6	3.143683000	0.175622000	-0.012468000
1	2.504467000	1.929684000	1.058128000

1	3.485288000	-1.650796000	-1.085159000
8	4.466672000	0.493566000	-0.073138000
1	4.630608000	1.337249000	0.367545000
1	-3.554515000	1.017767000	-1.863622000

23A•

6	0.878520000	-0.384100000	-0.003680000
7	1.958271000	-1.311863000	0.274828000
6	-0.252842000	-0.596554000	1.053294000
6	-1.479623000	0.193138000	0.816131000
6	-2.531303000	-0.309273000	-0.036666000
8	-3.570395000	0.554585000	-0.151727000
1	0.469565000	-0.613958000	-0.990407000
1	0.164160000	-0.353764000	2.033440000
1	-0.485556000	-1.661412000	1.021299000
8	-2.512891000	-1.388244000	-0.608669000
6	1.317209000	1.092099000	0.026172000
8	2.137029000	1.462208000	0.841374000
1	-1.602398000	1.178006000	1.245694000
1	-4.231413000	0.153448000	-0.737971000
6	2.983550000	-1.354225000	-0.768818000
1	2.537740000	-1.709258000	-1.700029000
1	3.460706000	-0.384728000	-0.967322000
1	3.760570000	-2.060692000	-0.476405000
1	2.387792000	-1.051658000	1.157180000
6	0.705553000	2.019251000	-0.984739000
1	0.931821000	3.056516000	-0.747344000
1	1.116877000	1.768866000	-1.967514000
1	-0.374093000	1.871265000	-1.052405000

23B•

6	0.794435000	-0.378430000	0.055600000
7	1.923865000	-1.261266000	0.302285000
6	-0.275979000	-0.575686000	1.171638000
6	-1.560548000	0.131942000	0.938791000
6	-2.531568000	-0.305219000	-0.092620000
8	-3.548226000	0.430905000	-0.263405000
1	0.328500000	-0.662174000	-0.890343000
1	0.170231000	-0.275731000	2.123943000
1	-0.453133000	-1.653722000	1.197598000
8	-2.268055000	-1.367518000	-0.727622000
6	1.185945000	1.104913000	-0.000036000
8	2.079628000	1.529945000	0.706907000
1	-1.782831000	1.041054000	1.485420000
6	2.892384000	-1.298357000	-0.793302000
1	2.410889000	-1.698921000	-1.687971000

1	3.320080000	-0.318686000	-1.048561000
1	3.712575000	-1.965701000	-0.525981000
1	2.391659000	-0.952747000	1.148868000
6	0.428999000	1.988017000	-0.951935000
1	0.669386000	3.035973000	-0.783365000
1	0.703063000	1.707268000	-1.973318000
1	-0.646268000	1.822520000	-0.858147000

24•

1	1.226142000	1.626039000	0.242168000
6	3.471996000	0.565941000	-0.184972000
1	3.903176000	0.297731000	0.782548000
1	4.134313000	0.198316000	-0.965925000
1	3.408837000	1.652657000	-0.238184000
6	2.130642000	-0.111626000	-0.319671000
1	-1.713034000	-2.732939000	0.605495000
8	2.007992000	-1.258916000	-0.722695000
6	-0.515222000	-1.139127000	0.680266000
6	-0.259730000	0.208661000	0.123882000
7	1.049511000	0.647298000	0.068144000
6	-1.348268000	1.245554000	0.042953000
8	0.113310000	-1.549352000	1.663864000
7	-1.509692000	-1.870950000	0.122620000
1	-2.298708000	0.711011000	0.063245000
6	-1.285649000	2.061040000	-1.257269000
1	-0.360621000	2.637555000	-1.321474000
1	-1.340126000	1.414680000	-2.134203000
1	-2.119102000	2.764310000	-1.297637000
6	-1.330980000	2.171356000	1.277657000
1	-0.419033000	2.771835000	1.318080000
1	-2.175769000	2.861063000	1.237016000
1	-1.400137000	1.595102000	2.201172000
6	-2.144293000	-1.657671000	-1.166879000
1	-2.250327000	-2.614222000	-1.678301000
1	-3.133826000	-1.204432000	-1.071113000
1	-1.521903000	-1.011771000	-1.783388000

25•

1	2.297201000	3.179165000	-0.165762000
1	-2.646929000	0.385864000	1.597735000
1	-2.525282000	1.992932000	0.860172000
1	-1.653488000	-2.569341000	-0.598416000
1	0.843289000	-3.202769000	-0.927212000
1	3.099279000	-0.423441000	-0.572219000
1	3.490389000	-0.594752000	1.024798000
1	-1.092571000	1.038931000	-0.943813000

1	0.779502000	-1.120889000	-1.348161000
1	1.256331000	-0.983667000	1.659215000
1	1.750946000	1.414565000	1.367424000
6	1.589293000	2.725604000	-0.864810000
8	1.545248000	1.305192000	-0.683013000
8	-3.582672000	0.668015000	-0.250105000
6	-2.516525000	0.923015000	0.652219000
8	-1.917763000	-1.636744000	-0.575678000
8	0.623131000	-2.766546000	-0.095761000
7	2.846782000	-0.906105000	0.295105000
8	-0.170811000	1.172803000	0.914525000
6	-1.153507000	0.571020000	0.050971000
6	-0.901839000	-0.900385000	-0.046318000
6	0.495270000	-1.360435000	-0.312588000
6	1.167118000	0.894694000	0.600425000
1	-3.597491000	-0.280465000	-0.432599000
1	1.921340000	2.895647000	-1.885591000
1	0.600485000	3.163738000	-0.720879000
6	1.418250000	-0.617241000	0.648745000
1	2.984100000	-1.912179000	0.167958000

26•

7	-0.860255000	-0.141685000	-0.359537000
7	-1.854613000	-1.992649000	0.428920000
7	-4.858595000	0.113609000	-0.089334000
7	-2.833206000	1.250375000	-0.708693000
7	-4.913181000	-2.046438000	0.753944000
6	0.179614000	0.782323000	-0.818145000
6	0.422010000	1.926874000	0.171695000
6	1.591902000	1.379508000	1.008574000
6	2.387029000	0.597134000	-0.038442000
6	-0.716857000	-1.427629000	0.108539000
6	-2.805911000	-1.029656000	0.156302000
6	-2.207824000	0.126820000	-0.339004000
6	-4.208618000	-1.005134000	0.278424000
6	-4.151526000	1.151394000	-0.551394000
8	0.827363000	3.063480000	-0.568927000
8	2.405531000	2.396812000	1.562773000
8	1.394154000	0.072730000	-0.939940000
1	-0.130026000	1.175669000	-1.787131000
1	1.445255000	3.559164000	-0.011075000
1	-0.466964000	2.139509000	0.769346000
1	2.057323000	2.648318000	2.426414000
1	1.213123000	0.707864000	1.783093000
1	3.025573000	1.299679000	-0.583326000
1	-4.454610000	-2.910505000	0.983450000

1	-5.917586000	-2.003630000	0.774873000
1	0.253233000	-1.889302000	0.171855000
1	-4.732684000	2.023288000	-0.832662000
6	3.219054000	-0.523109000	0.543755000
1	3.916562000	-0.095731000	1.265679000
1	2.585253000	-1.250218000	1.052049000
16	4.187791000	-1.381486000	-0.744460000
6	5.180355000	-2.395784000	0.202934000
1	5.255344000	-2.266145000	1.272350000
1	5.832742000	-3.077304000	-0.321338000

27•

1	2.743872000	-0.667107000	-0.604383000
6	0.474295000	-2.792814000	0.732188000
1	-0.457935000	-2.327923000	0.418485000
1	0.429391000	-3.861103000	0.539208000
1	0.589803000	-2.638087000	1.806064000
6	1.664510000	-2.243976000	-0.006226000
1	-0.026577000	1.205238000	1.686618000
1	2.186317000	3.412578000	-0.208621000
1	0.105333000	-0.499248000	1.904151000
8	2.491283000	-2.988525000	-0.525473000
6	2.016321000	1.455558000	-0.097183000
6	1.247139000	0.267422000	0.294669000
7	1.876666000	-0.884393000	-0.115037000
6	0.013385000	0.268065000	1.133861000
8	3.176858000	1.313663000	-0.534576000
7	1.506647000	2.710543000	0.041165000
6	-1.312987000	0.071609000	0.411435000
6	-2.489430000	0.049793000	1.163408000
6	-1.398064000	-0.085417000	-0.969996000
6	-3.722252000	-0.124665000	0.548114000
1	-2.436120000	0.169640000	2.239365000
6	-2.632883000	-0.261959000	-1.590118000
1	-0.497622000	-0.073378000	-1.571402000
6	-3.798487000	-0.281858000	-0.834241000
1	-4.624534000	-0.138655000	1.146602000
1	-2.679394000	-0.383621000	-2.664998000
1	-4.758681000	-0.419017000	-1.314898000
6	0.122786000	3.166397000	0.100168000
1	-0.544533000	2.472926000	-0.405681000
1	-0.224730000	3.311036000	1.125056000
1	0.061088000	4.123637000	-0.414546000

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1	1.036729000	1.718930000	-0.590443000
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6	2.582094000	-0.774057000	1.070508000
1	2.460020000	-1.690672000	0.494806000
1	3.593925000	-0.736644000	1.465286000
1	1.866013000	-0.797514000	1.891367000
6	2.377657000	0.435541000	0.198635000
1	-3.168181000	1.538940000	-0.083458000
8	3.313430000	1.140198000	-0.166949000
6	-1.232862000	1.152859000	-0.226239000
6	-0.132459000	0.205469000	0.012784000
7	1.100193000	0.796836000	-0.165616000
8	-1.008903000	2.228604000	-0.813676000
7	-2.490037000	0.839366000	0.177257000
6	-0.288297000	-1.262822000	0.123222000
6	-1.212827000	-1.983077000	-0.827958000
6	0.270067000	-2.137692000	-0.978275000
1	-0.232613000	-1.687006000	1.120073000
1	-1.737576000	-1.387043000	-1.562428000
1	-1.779353000	-2.815212000	-0.432879000
1	0.724150000	-3.075870000	-0.688985000
1	0.749485000	-1.640331000	-1.811095000
6	-2.895521000	-0.105465000	1.209790000
1	-3.188979000	-1.069858000	0.794940000
1	-2.092335000	-0.261679000	1.927334000
1	-3.745706000	0.315590000	1.744190000

Ado-H

7	0.220422000	-0.292879000	0.430681000
7	1.654634000	-1.892738000	-0.217838000
7	3.993743000	0.977958000	-0.091851000
7	1.753043000	1.603625000	0.513634000
7	4.606809000	-1.175437000	-0.697718000
6	-1.023549000	0.372399000	0.823467000
6	-1.679056000	1.127635000	-0.339830000
6	-2.696975000	0.094401000	-0.853457000
6	-3.130463000	-0.601833000	0.435681000
6	-3.642890000	-2.012903000	0.272420000
6	0.415224000	-1.614585000	0.104125000
6	2.318455000	-0.687542000	-0.100791000
6	1.443735000	0.319043000	0.302677000
6	3.659531000	-0.308083000	-0.301026000
6	3.044911000	1.838838000	0.294663000
8	-2.343179000	2.261455000	0.190728000
8	-3.822966000	0.688795000	-1.478639000
8	-1.941671000	-0.605758000	1.258693000
1	-0.778266000	1.063088000	1.631483000
1	-3.140291000	2.394522000	-0.344092000

1	-0.944839000	1.419774000	-1.094549000
1	-3.633037000	0.823786000	-2.414572000
1	-2.203784000	-0.615201000	-1.522969000
1	-3.887681000	0.023189000	0.920551000
1	-2.895460000	-2.645488000	-0.209421000
1	-4.541528000	-2.002549000	-0.346513000
1	4.390203000	-2.149306000	-0.816500000
1	5.560597000	-0.869950000	-0.786771000
1	-0.396121000	-2.320796000	0.143420000
1	3.376868000	2.860371000	0.447631000
1	-3.898229000	-2.445303000	1.240114000

Cartesian coordinates of RC, PC and TS for HAA, decay and cyclization reactions for PFL-AE and LAM from **Figure 3** and **Figure 4**.

PFL-AE

C	-6.668955000	-39.094448000	19.404607000
S	-5.185893000	-38.082989000	18.991291000
C	-2.257929000	-34.068201000	24.906886000
S	-1.917667000	-33.798648000	23.114547000
C	-4.154338000	-32.632969000	29.356146000
C	-5.461251000	-32.985012000	28.673525000
O	-6.517341000	-32.434428000	28.998044000
C	-3.675200000	-31.204177000	29.000336000
C	-3.252330000	-30.989563000	27.559323000
C	-4.199341000	-30.963297000	26.518349000
C	-1.910128000	-30.767991000	27.217403000
C	-3.833781000	-30.708185000	25.197298000
C	-1.524782000	-30.511270000	25.895946000
C	-2.489209000	-30.474104000	24.882369000
O	-2.178894000	-30.196325000	23.580805000
N	-5.411735000	-33.899656000	27.681283000
C	-6.533464000	-34.178830000	26.786050000
C	-7.868015000	-34.194518000	27.558314000
O	-8.121550000	-35.082096000	28.362601000
C	-6.339144000	-35.556891000	26.143828000
S	-7.629823000	-35.922063000	24.876369000
N	-8.758946000	-33.242315000	27.177578000
C	-10.047746000	-33.158618000	27.839459000
C	-11.122105000	-34.111588000	27.260258000
O	-12.228437000	-34.150353000	27.791574000
C	-10.552164000	-31.708369000	27.930822000
C	-10.663048000	-30.975338000	26.623858000
C	-10.787308000	-31.469459000	25.342130000
N	-10.593016000	-29.595072000	26.570379000
C	-10.658776000	-29.266265000	25.291503000

N	-10.776002000	-30.370882000	24.514415000
N	-10.750874000	-34.877442000	26.208059000
C	-11.619377000	-35.867478000	25.592829000
C	-11.694736000	-35.702978000	24.073312000
C	-12.400781000	-34.412119000	23.649098000
N	-12.308244000	-34.088353000	22.333375000
O	-13.021402000	-33.717403000	24.448428000
C	-9.880163000	-28.946450000	15.692044000
C	-9.642939000	-28.068780000	16.930469000
O	-8.464293000	-27.610827000	17.091475000
O	-10.618356000	-27.850897000	17.683996000
C	-6.650367000	-30.561492000	14.217745000
C	-5.347096000	-30.434290000	14.998617000
O	-5.020569000	-29.372245000	15.537021000
N	-4.606714000	-31.567957000	15.086647000
C	-3.300789000	-31.662072000	15.720692000
C	-2.802804000	-28.166726000	18.285687000
C	-3.888391000	-27.907497000	19.321181000
O	-4.914234000	-27.280803000	18.924463000
O	-3.720676000	-28.345074000	20.490955000
C	-2.160801000	-31.443721000	20.433922000
N	-3.408444000	-31.057783000	21.133315000
C	-7.076607000	-24.153286000	19.058776000
N	-8.102142000	-24.159243000	20.089509000
C	-9.182983000	-24.961010000	20.078245000
N	-10.082661000	-24.866713000	21.072208000
N	-9.396449000	-25.795221000	19.066817000
C	-9.359039000	-26.911872000	32.330059000
C	-9.665771000	-27.068918000	30.867862000
C	-9.888020000	-28.236411000	30.158633000
N	-9.780715000	-25.988269000	30.016455000
C	-10.056938000	-26.501997000	28.830093000
N	-10.139361000	-27.856939000	28.860762000
S	-7.495102000	-35.760628000	20.941237000
S	-4.500793000	-36.782226000	22.751444000
S	-3.959632000	-34.635443000	19.888028000
S	-5.664266000	-33.134551000	22.903182000
Fe	-3.905878000	-34.545685000	22.220268000
Fe	-6.212013000	-33.640881000	20.541086000
Fe	-6.427392000	-35.373114000	22.966891000
Fe	-5.282617000	-36.426179000	20.559930000
N	-6.931116000	-33.664951000	18.413823000
C	-7.238256000	-32.288279000	17.995151000
C	-6.234349000	-31.320537000	18.670127000
O	-5.539916000	-31.799258000	19.625466000
C	-8.706637000	-31.900057000	18.293805000

C	-9.316303000	-32.459676000	19.586163000
S	-8.278776000	-32.105599000	21.053144000
C	-9.235032000	-32.968859000	22.327055000
C	-9.725457000	-29.237923000	20.594489000
C	-8.830775000	-28.377280000	21.392055000
O	-8.888428000	-28.745075000	22.782913000
C	-7.318479000	-28.385609000	20.980559000
O	-6.939193000	-27.085404000	20.604431000
C	-6.624530000	-28.878158000	22.281001000
O	-5.356795000	-28.372818000	22.569234000
C	-7.631725000	-28.419881000	23.335046000
O	-6.176314000	-30.162427000	18.244341000
N	-6.924154000	-27.559533000	28.337938000
C	-7.004718000	-26.727666000	27.297642000
N	-7.199359000	-27.031910000	26.012502000
C	-7.318172000	-28.350288000	25.824632000
C	-7.289250000	-29.343073000	26.814658000
C	-7.080676000	-28.886781000	28.143201000
N	-7.044350000	-29.704102000	29.211994000
N	-7.464518000	-30.593216000	26.238544000
C	-7.575346000	-30.362603000	24.951077000
N	-7.499048000	-29.025634000	24.633402000
C	-13.942770000	-25.637293000	20.827335000
C	-13.164959000	-26.934675000	20.849757000
O	-11.962009000	-26.961229000	21.122722000
N	-13.852201000	-28.073409000	20.571837000
C	-13.194195000	-29.363333000	20.487355000
C	-13.072903000	-30.152091000	21.799075000
O	-12.313000000	-31.129570000	21.846999000
N	-13.847435000	-29.742714000	22.813884000
C	-13.980204000	-30.421112000	24.094318000
C	-2.438130000	-26.177569000	25.078540000
C	-3.509576000	-26.878364000	25.921226000
C	-2.429069000	-26.644210000	23.618583000
C	-5.404181000	-22.904772000	24.902314000
C	-6.361449000	-23.403856000	23.807800000
C	-5.787117000	-24.641103000	23.104751000
C	-7.754638000	-23.703156000	24.380603000
Na	-6.292791000	-28.181201000	17.234058000
H	-2.831478000	-30.960759000	29.667872000
H	-4.491045000	-30.503902000	29.253816000
H	-5.256160000	-31.125446000	26.737383000
H	-1.142661000	-30.779777000	27.998696000
H	-4.583337000	-30.668093000	24.403556000
H	-0.471955000	-30.332247000	25.653593000
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PFL-AE-TS-HAA

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C	0.865639000	-1.546565000	-4.707463000
O	-0.289620000	-0.833270000	-4.865526000
N	2.835423000	-5.015947000	-1.376146000
C	2.194111000	-4.615971000	-0.125644000
C	3.210183000	-4.612182000	1.033507000
O	3.675446000	-5.659743000	1.463963000
C	1.084829000	-5.620081000	0.206112000
S	0.104313000	-5.111319000	1.681879000
N	3.446671000	-3.396684000	1.592593000
C	4.428036000	-3.285515000	2.657247000
C	3.863272000	-3.578760000	4.068159000
O	4.625756000	-3.565561000	5.030054000
C	5.188890000	-1.949706000	2.602895000
C	4.333728000	-0.719890000	2.708363000
C	3.061859000	-0.584170000	3.222326000
N	4.755140000	0.502737000	2.219134000
C	3.757105000	1.348357000	2.423323000
N	2.712611000	0.730101000	3.027823000
N	2.541395000	-3.865107000	4.144538000
C	1.876446000	-4.237120000	5.382304000
C	0.596121000	-3.436687000	5.623957000
C	0.850333000	-1.951023000	5.894068000
N	-0.249579000	-1.151841000	5.874351000
O	1.972232000	-1.509966000	6.123643000
C	-4.814578000	5.635325000	2.849227000
C	-3.461227000	5.886525000	2.175089000
O	-3.440452000	5.824598000	0.903082000
O	-2.475937000	6.140693000	2.906894000
C	-7.636253000	3.940584000	0.534493000
C	-7.208849000	3.388178000	-0.820840000
O	-6.367312000	3.966539000	-1.516203000
N	-7.787391000	2.216316000	-1.182266000
C	-7.583244000	1.541431000	-2.454773000
C	-4.182402000	3.370773000	-4.348573000
C	-2.870446000	3.442655000	-3.576714000
O	-2.735935000	4.415509000	-2.778851000

O	-2.010661000	2.534278000	-3.749099000
C	-3.634881000	-0.624053000	-4.235039000
N	-2.603236000	-0.143053000	-3.283457000
C	-0.867733000	7.654489000	-1.882734000
N	0.335016000	7.477486000	-1.087432000
C	0.319973000	7.083154000	0.196974000
N	1.474840000	6.966612000	0.872998000
N	-0.837947000	6.870338000	0.812409000
C	10.548064000	-0.007689000	-0.669085000
C	9.277696000	0.573901000	-0.115342000
C	8.263775000	-0.074015000	0.569241000
N	8.975652000	1.917570000	-0.213682000
C	7.808765000	2.062129000	0.390481000
N	7.336107000	0.890546000	0.888297000
S	-3.364932000	-3.405737000	2.038166000
S	-2.913939000	-5.679312000	-0.770328000
S	-4.845464000	-2.714684000	-1.474216000
S	-1.148037000	-2.302307000	-0.817883000
Fe	-2.734986000	-3.622767000	-1.934474000
Fe	-3.295974000	-1.644547000	0.231651000
Fe	-1.697001000	-4.132487000	0.589914000
Fe	-4.532662000	-4.288174000	0.220802000
N	-5.012488000	-0.628750000	1.253370000
C	-4.778329000	0.822730000	1.264821000
C	-4.062243000	1.228407000	-0.050563000
O	-3.606563000	0.276100000	-0.763476000
C	-4.000232000	1.275521000	2.521895000
C	-2.877717000	0.350444000	3.018425000
S	-1.720649000	-0.142864000	1.682965000
C	-0.610489000	-1.239525000	2.603412000
C	-0.962750000	3.309108000	1.955297000
C	0.024054000	3.486552000	0.855167000
O	1.099018000	2.529718000	0.933146000
C	-0.657238000	3.285257000	-0.540633000
O	-0.564235000	4.470700000	-1.284767000
C	0.153582000	2.105811000	-1.142562000
O	0.341514000	2.108965000	-2.523614000
C	1.479880000	2.276305000	-0.404820000
O	-3.988232000	2.435770000	-0.311953000
N	6.035536000	0.669147000	-2.082322000
C	5.450363000	1.867688000	-2.110975000
N	4.257375000	2.212619000	-1.621914000
C	3.632024000	1.176482000	-1.054413000
C	4.124071000	-0.129461000	-0.923114000
C	5.411560000	-0.363086000	-1.474760000
N	6.045169000	-1.548469000	-1.412763000

N	3.192320000	-0.924704000	-0.271235000
C	2.173326000	-0.131734000	-0.033811000
N	2.378682000	1.156566000	-0.474411000
C	0.076030000	7.365791000	4.504219000
C	0.323038000	5.910463000	4.178886000
O	1.058664000	5.541774000	3.261060000
N	-0.356125000	5.011376000	4.948798000
C	-0.512966000	3.641586000	4.572463000
C	0.513500000	2.627914000	4.956999000
O	0.341170000	1.445471000	4.599143000
N	1.597457000	3.045450000	5.633326000
C	2.681864000	2.173091000	6.055288000
C	2.586678000	2.066281000	-6.325689000
C	3.370302000	1.457592000	-5.157382000
C	1.098065000	2.256361000	-6.012297000
C	4.336658000	5.775940000	-4.746232000
C	3.388956000	6.088497000	-3.576847000
C	2.112795000	5.240466000	-3.667164000
C	4.088250000	5.880849000	-2.225241000
Na	-4.132615000	4.607066000	-0.869605000
H	5.031267000	-3.973688000	-5.012453000
H	5.312121000	-2.995166000	-3.561578000
H	3.125547000	-2.182984000	-2.259650000
H	3.097605000	-3.521393000	-6.361918000
H	1.018013000	-0.946502000	-2.642776000
H	0.976230000	-2.290108000	-6.736823000
H	-0.669070000	-0.998382000	-5.745899000
H	5.480164000	-5.429281000	-3.115726000
H	5.742122000	-1.910713000	1.647598000
H	5.941144000	-1.973567000	3.410858000
H	2.398138000	-1.293109000	3.701993000
H	1.817813000	1.138826000	3.309378000
H	3.728919000	2.397472000	2.132625000
H	5.172283000	-4.087061000	2.514123000
H	0.059448000	-3.861476000	6.492906000
H	-0.086966000	-3.544973000	4.760695000
H	-0.092926000	-0.148097000	5.739807000
H	-1.137327000	-1.521398000	5.550020000
H	2.593269000	-4.062008000	6.196113000
H	-5.329618000	4.779770000	2.379527000
H	-4.692052000	5.453744000	3.929173000
H	-7.218777000	3.314488000	1.343912000
H	-6.779320000	2.055198000	-2.999657000
H	-4.144750000	2.619294000	-5.152533000
H	-4.990665000	3.116832000	-3.639243000
H	-4.150380000	-1.485521000	-3.789082000

H	-4.350396000	0.191066000	-4.420897000
H	-1.841321000	-0.834015000	-3.199922000
H	-3.003595000	0.036014000	-2.322289000
H	-2.208765000	0.774713000	-3.598665000
H	-1.308158000	6.690654000	-2.191522000
H	-1.615641000	8.228270000	-1.310689000
H	1.215486000	7.402236000	-1.585585000
H	1.476669000	6.509760000	1.798731000
H	2.349739000	7.268630000	0.459426000
H	-0.915331000	6.603791000	1.799343000
H	-1.692531000	6.578593000	0.323997000
H	10.580783000	-1.099242000	-0.508842000
H	11.437101000	0.431536000	-0.176880000
H	8.124785000	-1.119095000	0.838105000
H	6.419860000	0.748342000	1.367316000
H	7.253024000	2.996688000	0.489115000
H	0.099345000	7.553940000	5.591292000
H	-0.530176000	3.547962000	3.260214000
H	-1.519045000	3.271927000	4.811467000
H	-1.059826000	5.395526000	5.573238000
H	2.343205000	1.125453000	6.028453000
H	1.645015000	4.031008000	5.873733000
H	2.691468000	1.412829000	-7.214008000
H	4.437989000	1.319112000	-5.409120000
H	2.959516000	0.470336000	-4.875435000
H	3.323087000	2.099690000	-4.259677000
H	0.614697000	1.291296000	-5.777212000
H	0.952403000	2.907004000	-5.132168000
H	0.559860000	2.710174000	-6.865433000
H	4.688708000	4.727720000	-4.686868000
H	3.822893000	5.898979000	-5.717820000
H	3.098756000	7.156475000	-3.653182000
H	2.352372000	4.163752000	-3.619819000
H	1.412466000	5.439358000	-2.836266000
H	1.574494000	5.420813000	-4.615951000
H	5.002667000	6.496839000	-2.141631000
H	4.364628000	4.819008000	-2.087821000
H	3.422259000	6.148487000	-1.382578000
H	-5.719735000	-6.760919000	2.589452000
H	-5.415131000	-5.081406000	3.136018000
H	0.114421000	-4.532012000	-4.799619000
H	-0.033733000	-4.402204000	-3.024389000
H	2.243411000	-5.467713000	-2.065952000
H	1.752154000	-3.611751000	-0.248695000
H	1.554238000	-6.596346000	0.408249000
H	0.409892000	-5.734134000	-0.659933000

H	-5.729759000	1.383322000	1.257032000
H	-3.610650000	2.285666000	2.318073000
H	-4.713210000	1.380185000	3.359221000
H	-3.286833000	-0.586155000	3.434118000
H	-2.293290000	0.853458000	3.807709000
H	0.023684000	-1.754621000	1.866469000
H	-1.201085000	-2.007020000	3.125489000
H	-0.006923000	-0.647811000	3.303513000
H	-1.291373000	2.271366000	2.060485000
H	-1.775786000	4.041809000	1.913479000
H	0.461213000	4.495667000	0.860283000
H	-1.711828000	2.986959000	-0.423730000
H	-1.315227000	4.463041000	-1.944867000
H	-0.311392000	1.160759000	-0.789833000
H	-0.512370000	2.348134000	-2.976586000
H	2.024993000	3.131730000	-0.844439000
H	6.018928000	2.668040000	-2.601917000
H	6.962440000	-1.603949000	-1.842756000
H	5.575757000	-2.416755000	-1.133249000
H	1.249478000	-0.421364000	0.463227000
H	2.001618000	-3.920039000	3.280199000
H	3.784525000	-5.669535000	-3.609799000
H	2.982896000	2.431371000	7.084268000
H	3.559470000	2.275354000	5.391140000
H	1.623532000	-5.316384000	5.367344000
H	-0.713539000	-5.836013000	-3.874627000
H	-7.070090000	-5.774192000	3.244923000
H	-3.151020000	-0.936082000	-5.174269000
H	-0.930655000	7.623750000	4.128607000
H	0.830335000	7.990797000	4.003865000
H	-0.601209000	8.234912000	-2.774789000
H	5.227692000	6.434967000	-4.751868000
H	3.036388000	3.039035000	-6.613434000
H	-4.427871000	4.363137000	-4.768264000
H	-8.736719000	3.974186000	0.663179000
H	-7.295664000	0.482781000	-2.316764000
H	-8.505880000	1.565120000	-3.065175000
H	-5.456145000	6.526688000	2.713512000
H	10.666334000	0.177838000	-1.756839000
H	-5.793853000	-0.868340000	0.636741000
H	3.259312000	-2.562158000	1.021260000
H	-8.493238000	1.831116000	-0.562590000
H	-7.233176000	4.958168000	0.642879000
H	-5.237685000	-1.002394000	2.177868000

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C	-3.881671000	-7.431020000	2.212228000
S	-4.425952000	-6.779200000	0.578059000
C	1.514616000	-4.414320000	-4.030528000
S	-0.316758000	-4.295125000	-4.190578000
C	6.214135000	-2.733159000	-2.640145000
C	5.636281000	-2.707783000	-1.237037000
O	6.153142000	-2.026865000	-0.347063000
C	5.905711000	-1.454279000	-3.457820000
C	4.483889000	-1.336407000	-3.970085000
C	3.416603000	-1.037999000	-3.104103000
C	4.186259000	-1.496682000	-5.331818000
C	2.113107000	-0.874991000	-3.571185000
C	2.882233000	-1.345698000	-5.817749000
C	1.843070000	-1.023389000	-4.937409000
O	0.556228000	-0.831403000	-5.357121000
N	4.532739000	-3.455193000	-1.019255000
C	3.726731000	-3.428525000	0.201749000
C	4.566233000	-3.064411000	1.445948000
O	5.306002000	-3.884273000	1.973687000
C	3.114069000	-4.814802000	0.431386000
S	1.928972000	-4.824598000	1.846696000
N	4.300581000	-1.839957000	1.977819000
C	5.039923000	-1.403514000	3.148808000
C	4.461448000	-1.929141000	4.485786000
O	5.049194000	-1.667862000	5.531961000
C	5.246210000	0.123974000	3.167557000
C	3.987700000	0.946639000	3.184460000
C	2.780962000	0.669907000	3.791998000
N	3.894317000	2.164580000	2.536107000
C	2.659942000	2.599463000	2.733216000
N	1.949413000	1.724163000	3.490456000
N	3.329177000	-2.670781000	4.414040000
C	2.730686000	-3.325765000	5.567012000
C	1.212782000	-3.140760000	5.622932000
C	0.795136000	-1.697527000	5.917836000
N	-0.489043000	-1.372278000	5.620144000
O	1.573728000	-0.884915000	6.412322000
C	-7.049800000	3.341101000	2.708357000
C	-5.836817000	3.417034000	1.795035000
O	-6.006284000	3.136463000	0.594882000
O	-4.721479000	3.809839000	2.287098000
C	-8.632007000	0.689981000	-0.050989000
C	-7.908208000	0.424088000	-1.363839000
O	-7.244500000	1.293531000	-1.939584000
N	-8.028340000	-0.835962000	-1.842497000

C	-7.457820000	-1.296991000	-3.095041000
C	-4.695652000	1.782635000	-4.916609000
C	-3.545363000	2.267332000	-4.039385000
O	-3.813194000	3.165528000	-3.179031000
O	-2.423322000	1.727699000	-4.181944000
C	-2.645450000	-1.486575000	-4.450484000
N	-1.575106000	-1.133237000	-3.491519000
C	-3.250583000	6.778556000	-2.068767000
N	-3.885637000	7.101322000	-0.799501000
C	-4.016535000	6.223633000	0.204219000
N	-4.670970000	6.578709000	1.332626000
N	-3.500298000	5.005887000	0.115845000
C	9.591401000	4.360745000	0.378010000
C	8.121094000	4.267503000	0.675199000
C	7.446514000	3.269870000	1.357097000
N	7.222401000	5.236732000	0.277834000
C	6.041905000	4.820320000	0.703987000
N	6.120743000	3.636444000	1.365599000
S	-1.967774000	-4.189206000	1.913491000
S	-0.648939000	-6.402838000	-0.678003000
S	-3.218289000	-4.078951000	-1.752867000
S	0.121974000	-2.662465000	-0.850192000
Fe	-0.931597000	-4.432152000	-1.962227000
Fe	-2.182694000	-2.556481000	0.008280000
Fe	-0.032387000	-4.502180000	0.650037000
Fe	-2.663819000	-5.426000000	0.059156000
N	-4.230554000	-2.018657000	0.787394000
C	-4.398065000	-0.561458000	0.689021000
C	-3.704981000	-0.076583000	-0.609713000
O	-2.875747000	-0.882202000	-1.143681000
C	-3.867031000	0.156568000	1.954833000
C	-2.604472000	-0.432488000	2.599666000
S	-1.217089000	-0.521756000	1.409543000
C	0.094348000	-1.237009000	2.433823000
C	-0.932128000	3.308607000	1.750831000
C	-0.525337000	3.655268000	0.330564000
O	0.873195000	3.374145000	0.171933000
C	-1.276085000	2.878156000	-0.784401000
O	-1.755666000	3.813700000	-1.731665000
C	-0.190060000	1.927557000	-1.346459000
O	-0.273165000	1.552158000	-2.690675000
C	1.101305000	2.709204000	-1.051252000
O	-3.989107000	1.044326000	-1.043349000
N	6.175605000	2.586255000	-1.733654000
C	5.245103000	3.453364000	-2.136795000
N	3.924553000	3.389813000	-1.950457000

C	3.568223000	2.300212000	-1.263707000
C	4.427592000	1.317742000	-0.748416000
C	5.810367000	1.503733000	-1.015941000
N	6.772416000	0.669204000	-0.571494000
N	3.692582000	0.355863000	-0.069489000
C	2.444625000	0.744234000	-0.174108000
N	2.292970000	1.904414000	-0.904143000
C	-4.275209000	6.134340000	5.040518000
C	-3.274083000	5.059651000	5.418096000
O	-2.490547000	5.200897000	6.355880000
N	-3.316741000	3.951908000	4.606059000
C	-2.542443000	2.819552000	4.533339000
C	-1.264965000	2.427822000	5.116970000
O	-0.701293000	1.406153000	4.632645000
N	-0.707989000	3.126685000	6.122480000
C	0.583460000	2.773725000	6.682375000
C	2.117300000	3.150445000	-6.340146000
C	3.155091000	2.566018000	-5.376448000
C	0.705057000	2.612141000	-6.085908000
C	2.239828000	7.180400000	-4.450294000
C	1.201591000	6.732704000	-3.408692000
C	0.522972000	5.428913000	-3.847744000
C	1.830410000	6.570676000	-2.016425000
Na	-5.413536000	2.678158000	-1.502970000
H	6.598723000	-1.437701000	-4.315669000
H	6.159527000	-0.579199000	-2.834972000
H	3.605666000	-0.919145000	-2.036504000
H	4.989612000	-1.731454000	-6.038134000
H	1.303678000	-0.618116000	-2.885801000
H	2.674424000	-1.464508000	-6.886362000
H	0.476947000	-0.993538000	-6.312843000
H	7.306683000	-2.818825000	-2.518488000
H	5.834651000	0.401071000	2.275666000
H	5.870753000	0.346892000	4.050666000
H	2.457822000	-0.148261000	4.426428000
H	0.968945000	1.782751000	3.799503000
H	2.228023000	3.503388000	2.308176000
H	6.042804000	-1.863049000	3.112878000
H	0.801771000	-3.783889000	6.423746000
H	0.748832000	-3.488855000	4.681725000
H	-0.707965000	-0.372990000	5.535419000
H	-1.065828000	-2.015795000	5.087600000
H	3.196102000	-2.890806000	6.461910000
H	-7.421374000	2.302052000	2.749604000
H	-6.844954000	3.703780000	3.728028000
H	-8.180047000	0.084113000	0.755742000

H	-6.875651000	-0.475723000	-3.536629000
H	-4.321843000	1.358475000	-5.861936000
H	-5.234045000	0.987243000	-4.368083000
H	-3.231860000	-2.310789000	-4.019091000
H	-3.269677000	-0.598550000	-4.608930000
H	-0.919218000	-1.932136000	-3.389897000
H	-2.000078000	-0.907438000	-2.550697000
H	-1.032314000	-0.316670000	-3.804531000
H	-2.149086000	6.738828000	-1.988015000
H	-3.607507000	5.807516000	-2.451766000
H	-4.168843000	8.061031000	-0.634742000
H	-4.836729000	5.834887000	2.014205000
H	-5.299303000	7.374882000	1.331800000
H	-3.788079000	4.326694000	0.843946000
H	-2.885133000	4.712954000	-0.661114000
H	10.138552000	3.526118000	0.849620000
H	10.017095000	5.306252000	0.764345000
H	7.789368000	2.340101000	1.806039000
H	5.322889000	3.093751000	1.767180000
H	5.091018000	5.334290000	0.551205000
H	-4.370086000	6.844812000	5.874704000
H	-0.321053000	3.873675000	2.476118000
H	-2.895349000	2.139637000	3.761020000
H	-4.025802000	3.965372000	3.838763000
H	0.708153000	1.678164000	6.706370000
H	-1.207439000	3.965693000	6.440388000
H	2.412287000	2.922985000	-7.383381000
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H	2.921689000	2.828251000	-4.328943000
H	0.662209000	1.521209000	-6.251954000
H	0.385874000	2.778601000	-5.042251000
H	-0.040178000	3.089466000	-6.748933000
H	3.061672000	6.441292000	-4.517652000
H	1.783698000	7.261182000	-5.454720000
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H	1.273379000	4.624550000	-3.944233000
H	-0.235355000	5.087830000	-3.121078000
H	0.032253000	5.537650000	-4.832859000
H	2.307213000	7.508410000	-1.674234000
H	2.598053000	5.773848000	-2.024730000
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H	-3.663772000	-6.601101000	2.904602000
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H	2.911988000	-2.695664000	0.072983000
H	3.930727000	-5.520800000	0.650649000
H	2.599148000	-5.153476000	-0.483285000
H	-5.459260000	-0.275792000	0.579574000
H	-3.721534000	1.221718000	1.705923000
H	-4.657270000	0.128712000	2.726747000
H	-2.779789000	-1.459285000	2.962117000
H	-2.275978000	0.185868000	3.447705000
H	0.973685000	-1.369907000	1.787366000
H	-0.213434000	-2.230040000	2.791684000
H	0.327159000	-0.561522000	3.264211000
H	-0.801185000	2.232348000	1.945185000
H	-1.987443000	3.569153000	1.923780000
H	-0.682150000	4.731960000	0.141975000
H	-2.115384000	2.290721000	-0.378430000
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H	-0.208221000	1.026272000	-0.708214000
H	-1.122574000	1.831986000	-3.141047000
H	1.299015000	3.418562000	-1.872477000
H	5.612305000	4.325301000	-2.692392000
H	7.717986000	0.873959000	-0.880202000
H	6.546947000	-0.304179000	-0.333719000
H	1.591079000	0.220810000	0.252870000
H	2.960057000	-2.911863000	3.493724000
H	5.860232000	-3.617238000	-3.184451000
H	0.651512000	3.175333000	7.705934000
H	1.414989000	3.193420000	6.083567000
H	2.957307000	-4.411368000	5.552070000
H	1.804171000	-5.464887000	-3.866336000
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H	-2.189860000	-1.811403000	-5.395847000
H	-5.264406000	5.710455000	4.796119000
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H	-6.793721000	-2.164197000	-2.938839000
H	-8.254587000	-1.595911000	-3.798556000
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H	9.814850000	4.333893000	-0.709479000
H	-4.840562000	-2.502726000	0.122806000
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LAM-TS-HAA

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S	-49.953466000	10.482787000	-64.548098000
C	-48.731668000	11.707265000	-58.096225000
C	-48.204549000	10.511829000	-58.845242000
C	-47.522846000	10.486105000	-60.052641000
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C	-47.712542000	8.452192000	-59.241706000
N	-47.216871000	9.162495000	-60.288882000
C	-49.079849000	15.402187000	-61.182845000
S	-47.706661000	16.152657000	-62.162065000
C	-44.665428000	16.962165000	-59.793722000
C	-43.254482000	17.401703000	-59.435215000
O	-44.627996000	16.232701000	-61.008138000
C	-43.798270000	18.917754000	-63.570640000
N	-43.361189000	18.450500000	-64.877687000
C	-42.185617000	17.855778000	-65.132124000
N	-41.359523000	17.510294000	-64.130267000
N	-41.791132000	17.631942000	-66.387924000
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O	-40.983126000	16.148826000	-68.847194000
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C	-44.876645000	7.891976000	-64.792965000
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C	-45.965991000	9.347871000	-63.529552000
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N	-38.052107000	10.049513000	-66.200968000
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C	-38.816013000	9.991871000	-59.944455000
C	-37.548426000	11.444234000	-58.515802000
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C	-37.053310000	11.379361000	-60.884780000
O	-36.308658000	11.820294000	-61.930433000
C	-42.448605000	15.514596000	-55.359390000
C	-41.262062000	15.021833000	-56.205106000
O	-40.447724000	14.215640000	-55.714002000
O	-41.245820000	15.459180000	-57.403335000
C	-36.760024000	15.335108000	-56.460462000
C	-36.337208000	14.809614000	-57.849881000
O	-35.232894000	14.241296000	-57.955563000
O	-37.175880000	14.992027000	-58.789102000
N	-45.045793000	13.387518000	-68.060619000
C	-43.759218000	12.671336000	-68.024535000
C	-43.903750000	11.394660000	-67.156575000
O	-42.950052000	10.593179000	-67.167186000
C	-42.616232000	13.579906000	-67.530157000
C	-42.937388000	14.530757000	-66.370277000
S	-43.777595000	13.697191000	-64.972490000
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C	-40.501182000	12.179255000	-64.824211000
C	-40.829883000	11.174375000	-63.773741000
O	-41.162242000	11.832870000	-62.543329000
C	-42.082279000	10.308154000	-64.040160000
O	-41.921432000	9.333851000	-65.024147000
C	-42.391283000	9.775226000	-62.632496000
O	-41.599887000	8.634418000	-62.360719000
C	-41.953264000	10.976487000	-61.741063000
O	-44.985391000	11.271118000	-66.499720000
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C	-42.643359000	12.587471000	-57.735190000
N	-42.204253000	12.076944000	-58.889173000
C	-43.112191000	12.189497000	-59.866544000
C	-44.365891000	12.806684000	-59.761931000
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S	-48.180537000	12.346953000	-67.315774000
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Fe	-46.093665000	13.171606000	-66.100961000
Fe	-47.725051000	14.896768000	-64.147067000
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C	-35.786820000	15.168751000	-65.263595000
N	-36.990275000	15.428468000	-64.963178000
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C	-39.098056000	14.091860000	-61.546344000
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LAM-PC-HAA

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C	-47.513880000	10.485708000	-60.046961000
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C	-47.734244000	8.449124000	-59.250889000
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N	-42.032986000	17.591576000	-66.602304000
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O	-40.861364000	15.942306000	-68.948397000
C	-44.305362000	7.287090000	-66.041946000
C	-44.922538000	7.844206000	-64.792002000
C	-45.210401000	7.311202000	-63.545987000
N	-45.433830000	9.125005000	-64.751031000
C	-45.990882000	9.317338000	-63.530688000
N	-45.878412000	8.239734000	-62.769993000
C	-38.953023000	6.532466000	-63.508902000
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C	-37.726229000	9.923812000	-65.003889000
N	-38.216151000	10.090159000	-66.250533000
O	-37.391103000	10.899178000	-64.320809000
C	-43.242566000	8.214531000	-58.726439000
C	-43.845070000	7.450858000	-59.909614000
C	-44.231619000	9.199488000	-58.096242000
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C	-38.570114000	10.486851000	-58.643281000
C	-38.869086000	10.004993000	-59.928176000
C	-37.541038000	11.439689000	-58.538038000
C	-38.168368000	10.446715000	-61.052866000
C	-36.820122000	11.880217000	-59.649846000
C	-37.126600000	11.380108000	-60.923975000
O	-36.419580000	11.824179000	-61.991487000
C	-42.456641000	15.443655000	-55.376977000
C	-41.288864000	14.881467000	-56.208969000
O	-40.472415000	14.103767000	-55.677984000
O	-41.291708000	15.238535000	-57.433890000
C	-36.782296000	15.334414000	-56.434464000
C	-36.406180000	14.809724000	-57.838327000
O	-35.314053000	14.224771000	-57.976473000
O	-37.269599000	15.012521000	-58.750060000
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C	-43.917374000	12.619316000	-68.080784000
C	-44.037142000	11.349077000	-67.199028000
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C	-41.964172000	11.018965000	-61.809936000
O	-45.100627000	11.229775000	-66.512857000
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C	-43.091755000	12.169377000	-59.874248000
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C	-44.233672000	12.171911000	-61.767687000
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C	-39.057566000	15.188348000	-66.251469000
O	-40.120958000	15.753220000	-65.875367000
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C	-39.248140000	14.833332000	-62.959282000
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C	-40.057969000	14.593939000	-60.538045000
N	-39.731527000	14.033329000	-59.198687000
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PFL-AE-decay-TS

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N	-11.361516000	-34.973978000	21.680386000
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N	-4.606855000	-31.584424000	15.078254000
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C	-2.240755000	-31.271926000	20.526023000
N	-3.392300000	-31.186619000	21.452131000
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C	-9.544945000	-24.435935000	19.146760000
N	-10.747583000	-24.279111000	19.721792000
N	-9.267136000	-25.555666000	18.496222000
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C	-7.115237000	-28.100518000	23.734246000

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C	-6.885657000	-28.325099000	26.234320000
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C	-13.808226000	-30.421022000	22.797378000
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H	-3.411720000	-30.291288000	21.959298000
H	-6.614224000	-24.140768000	19.060229000
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H	-10.087659000	-25.933953000	32.686002000
H	-9.998854000	-29.166062000	30.536396000
H	-10.156350000	-28.510250000	28.048435000
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PFL-AE-decay-PC

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C	-9.372979000	-26.840455000	32.238070000
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N	-6.602872000	-26.862582000	26.473284000
C	-6.800097000	-28.148002000	26.152294000
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LAM-decay-TS

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N	-38.574301000	10.209136000	-66.195000000

O	-37.547831000	10.977185000	-64.345039000
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C	-38.911486000	10.041823000	-59.930547000
C	-37.512660000	11.401341000	-58.533122000
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C	-36.798481000	11.845058000	-59.647795000
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LAM-decay-PC

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H	-40.324320000	9.652995000	-57.666460000
H	-39.742747000	9.344608000	-60.073171000
H	-37.231747000	11.802418000	-57.556299000
H	-38.502316000	10.145223000	-62.051652000
H	-36.014389000	12.596867000	-59.525124000
H	-36.826369000	11.445900000	-62.843250000
H	-42.447259000	16.464265000	-55.610478000
H	-43.419879000	14.982989000	-55.732925000
H	-37.237056000	16.299620000	-56.445364000
H	-37.608859000	14.636582000	-55.960720000

H	-52.032524000	14.715070000	-68.497549000
H	-50.793353000	13.423598000	-68.628895000
H	-50.079253000	9.559694000	-62.373483000
H	-49.583518000	11.276953000	-62.393104000
H	-49.275828000	16.197005000	-60.288424000
H	-49.942102000	15.292952000	-61.688577000
H	-45.061110000	14.314612000	-68.394278000
H	-43.607444000	12.249996000	-69.016597000
H	-41.939913000	12.828836000	-67.183198000
H	-42.351292000	14.124705000	-68.313306000
H	-42.168799000	14.908098000	-65.984061000
H	-43.762505000	15.282341000	-66.705568000
H	-44.832600000	14.677839000	-63.017034000
H	-43.188614000	15.302211000	-63.374994000
H	-44.623281000	15.893122000	-64.319743000
H	-39.652158000	12.689462000	-64.551908000
H	-41.496152000	12.983992000	-64.700497000
H	-40.045247000	10.430196000	-63.743734000
H	-43.023892000	11.145105000	-64.074866000
H	-42.616752000	9.759967000	-65.714662000
H	-43.528783000	9.484425000	-62.406939000
H	-42.007543000	8.100526000	-61.646814000
H	-41.917552000	10.309139000	-60.485778000
H	-42.697402000	12.494125000	-56.667616000
H	-46.538666000	14.680376000	-57.684004000
H	-46.743679000	14.492774000	-59.402961000
H	-44.562050000	11.841453000	-62.814362000
H	-35.865416000	17.265469000	-65.555251000
H	-36.885747000	15.297594000	-65.701561000
H	-36.969842000	14.872288000	-63.348538000
H	-39.071765000	16.100356000	-62.685912000
H	-40.043601000	14.818694000	-63.421614000
H	-37.980906000	14.378988000	-61.164903000
H	-39.015285000	13.125160000	-61.872996000
H	-40.068900000	15.608523000	-60.389123000
H	-41.039619000	14.215421000	-60.947323000
H	-40.437013000	14.201340000	-58.516803000
H	-45.836233000	12.901932000	-68.715261000
H	-39.824946000	12.830189000	-59.385732000
H	-38.787646000	14.126948000	-58.979715000
H	-37.924788000	13.658108000	-64.185295000
H	-45.391846000	9.828569000	-65.489685000
H	-41.004588000	16.930437000	-70.758120000
H	-51.261512000	14.357696000	-70.081905000
H	-51.322622000	10.844298000	-62.551716000
H	-49.661421000	11.476915000	-57.534186000

H	-39.853004000	6.232533000	-62.953150000
H	-38.768273000	9.078868000	-57.002288000
H	-35.930670000	15.274702000	-55.730165000
H	-42.887764000	7.489049000	-57.966162000
H	-42.364047000	15.224418000	-54.297092000
H	-45.073781000	16.339107000	-58.968277000
H	-43.482213000	6.576202000	-65.842469000
H	-44.475205000	19.767615000	-63.736529000
H	-38.951031000	5.911374000	-64.412710000
H	-48.749492000	14.517893000	-60.609665000
H	-36.752741000	18.753593000	-64.810784000

PFL-AE-cyclization-TS

C	14.361315000	-57.255208000	51.127294000
S	14.376173000	-57.074706000	49.293663000
C	20.158635000	-52.994658000	46.360263000
S	18.523293000	-53.355805000	45.593095000
C	23.492288000	-49.784676000	48.336572000
C	22.526151000	-49.765719000	49.508688000
O	22.547973000	-48.829476000	50.309575000
C	23.062912000	-48.781301000	47.232355000
C	21.847017000	-49.177800000	46.416373000
C	20.561685000	-49.201283000	46.987641000
C	21.953375000	-49.517289000	45.058571000
C	19.436446000	-49.547578000	46.243065000
C	20.826922000	-49.839201000	44.289928000
C	19.558171000	-49.846389000	44.881701000
O	18.410433000	-50.108653000	44.189480000
N	21.626871000	-50.772290000	49.603629000
C	20.467652000	-50.742686000	50.497847000
C	20.831387000	-50.119528000	51.858052000
O	21.616050000	-50.675959000	52.614984000
C	19.984069000	-52.175715000	50.749944000
S	18.448143000	-52.230394000	51.776721000
N	20.128358000	-49.005161000	52.195039000
C	20.402632000	-48.351927000	53.463226000
C	19.672085000	-48.977438000	54.677950000
O	19.924610000	-48.552554000	55.801607000
C	20.202027000	-46.830492000	53.401285000
C	18.810393000	-46.357513000	53.096365000
C	17.606696000	-47.024756000	53.198460000
N	18.567906000	-45.051796000	52.712884000
C	17.254033000	-44.937106000	52.597786000
N	16.632328000	-46.106361000	52.890664000
N	18.798980000	-49.979361000	54.418339000
C	18.091104000	-50.709184000	55.457584000

C	16.591796000	-50.816584000	55.184234000
C	15.878758000	-49.464071000	55.230017000
N	14.692761000	-49.416106000	54.569067000
O	16.335889000	-48.498089000	55.829216000
C	8.324300000	-48.074774000	48.380224000
C	9.454088000	-47.512695000	47.515359000
O	9.281872000	-47.504707000	46.265756000
O	10.499136000	-47.120196000	48.102853000
C	8.213012000	-51.141527000	45.961817000
C	9.305943000	-51.358544000	44.922716000
O	9.675276000	-50.457402000	44.165723000
N	9.862450000	-52.597332000	44.918030000
C	10.895313000	-53.022184000	43.989237000
C	13.005381000	-49.488304000	42.416647000
C	13.687080000	-48.677804000	43.510381000
O	12.975410000	-47.931382000	44.228270000
O	14.941959000	-48.825744000	43.653761000
C	15.627245000	-52.062868000	43.985441000
N	15.722552000	-51.044539000	45.057101000
C	12.562498000	-44.125698000	43.909908000
N	13.106031000	-43.990053000	45.248012000
C	12.612012000	-44.542105000	46.370394000
N	13.286115000	-44.330414000	47.516861000
N	11.465227000	-45.218192000	46.375319000
C	23.793317000	-41.643079000	50.911687000
C	22.374162000	-42.077990000	51.137797000
C	21.905588000	-43.111997000	51.928868000
N	21.310789000	-41.462869000	50.510931000
C	20.236830000	-42.122351000	50.910394000
N	20.538744000	-43.125251000	51.773525000
S	14.793215000	-53.529000000	50.679658000
S	17.759702000	-54.919265000	49.170505000
S	15.029302000	-54.267412000	46.873495000
S	16.753486000	-51.288742000	48.381516000
Fe	17.140440000	-53.426468000	47.429730000
Fe	14.523616000	-52.322824000	48.480860000
Fe	16.957454000	-52.886459000	50.126510000
Fe	15.420553000	-55.062181000	49.027767000
N	12.373469000	-52.933663000	48.474619000
C	11.566468000	-51.801723000	47.996880000
C	12.374050000	-51.017056000	46.933253000
O	13.615263000	-51.294329000	46.830550000
C	11.085144000	-50.897924000	49.156185000
C	12.059024000	-50.728515000	50.327242000
S	13.680848000	-50.088411000	49.764903000
C	14.618499000	-50.110974000	51.321737000

C	16.135238000	-47.180832000	49.722017000
C	15.273894000	-46.697125000	48.595294000
O	15.902550000	-45.546558000	47.975909000
C	15.014230000	-47.647675000	47.399611000
O	13.747685000	-47.328484000	46.882155000
C	16.173432000	-47.283714000	46.395871000
O	15.728351000	-46.853058000	45.149667000
C	16.858974000	-46.090823000	47.083348000
O	11.755753000	-50.190879000	46.258137000
N	21.323233000	-44.444864000	48.914636000
C	20.484265000	-43.923739000	48.020129000
N	19.353502000	-44.459295000	47.547952000
C	19.080411000	-45.636572000	48.115471000
C	19.810498000	-46.264744000	49.144595000
C	21.026524000	-45.619120000	49.505353000
N	21.893537000	-46.127032000	50.410069000
N	19.211441000	-47.451546000	49.507763000
C	18.127098000	-47.555272000	48.728616000
N	18.048717000	-46.490780000	47.812554000
C	9.985584000	-44.626300000	49.743526000
C	11.107423000	-45.477060000	50.286836000
O	12.281961000	-45.331705000	49.939990000
N	10.800179000	-46.356434000	51.278039000
C	11.829730000	-47.231580000	51.795808000
C	12.885131000	-46.533048000	52.654105000
O	13.985631000	-47.078747000	52.830270000
N	12.544774000	-45.371357000	53.222411000
C	13.452599000	-44.603786000	54.057324000
C	19.301266000	-45.934268000	42.768053000
C	19.848131000	-46.001231000	44.198166000
C	18.193703000	-46.961930000	42.512109000
C	17.538784000	-41.917124000	43.595573000
C	16.395619000	-42.615562000	44.339075000
C	16.258605000	-44.060682000	43.855931000
C	16.614606000	-42.538804000	45.857794000
Na	10.915197000	-48.516781000	45.099918000
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H	20.425601000	-48.927438000	48.035232000
H	22.936400000	-49.513605000	44.575841000
H	18.454080000	-49.612687000	46.711695000
H	20.936166000	-50.077964000	43.226976000
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H	20.516691000	-46.432202000	54.382250000

H	17.368944000	-48.045493000	53.473507000
H	15.623327000	-46.316694000	52.864609000
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H	16.135910000	-51.471606000	55.950628000
H	16.417247000	-51.309305000	54.210395000
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H	18.268168000	-50.177984000	56.402572000
H	8.360477000	-49.178513000	48.338945000
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H	8.650342000	-51.179521000	46.975041000
H	11.353066000	-52.127348000	43.544788000
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H	15.600912000	-53.060675000	44.444466000
H	14.707643000	-51.881176000	43.409616000
H	16.611417000	-51.147879000	45.572520000
H	14.918925000	-51.116965000	45.736617000
H	15.662843000	-50.096127000	44.619867000
H	13.371787000	-43.946669000	43.185384000
H	12.195220000	-45.153134000	43.749908000
H	13.832838000	-43.295699000	45.383603000
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H	11.252673000	-45.952658000	47.101454000
H	10.886534000	-45.258763000	45.543142000
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H	19.210484000	-41.917017000	50.599365000
H	8.993465000	-45.077226000	49.901669000
H	12.373527000	-47.726010000	50.973514000
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H	9.829231000	-46.550278000	51.495494000
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H	11.637762000	-44.979817000	52.985974000
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H	20.259720000	-47.003467000	44.419646000
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H	18.567651000	-47.991415000	42.656092000
H	17.353720000	-46.829465000	43.216825000
H	17.796194000	-46.884543000	41.483099000
H	18.496297000	-42.439284000	43.784816000

H	17.367985000	-41.909441000	42.503425000
H	15.457160000	-42.072905000	44.098985000
H	17.193834000	-44.612969000	44.037989000
H	15.471345000	-44.620487000	44.380221000
H	16.055409000	-44.102803000	42.769384000
H	16.664167000	-41.489268000	46.201944000
H	17.556415000	-43.037125000	46.152601000
H	15.800894000	-43.033013000	46.419339000
H	15.323797000	-57.654008000	51.490743000
H	14.176151000	-56.280659000	51.607506000
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H	20.027002000	-52.472720000	47.322484000
H	21.620481000	-51.479948000	48.875267000
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H	20.783148000	-52.721731000	51.276733000
H	19.796778000	-52.682049000	49.788319000
H	10.669720000	-52.152334000	47.461686000
H	10.821924000	-49.911233000	48.737706000
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H	11.628615000	-50.031836000	51.063757000
H	15.685620000	-50.167040000	51.054989000
H	14.367435000	-51.024754000	51.881964000
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H	16.483696000	-46.408917000	50.411594000
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H	20.763991000	-42.943419000	47.615245000
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H	21.937551000	-47.141702000	50.544590000
H	17.675152000	-48.524673000	48.508301000
H	18.716161000	-50.326795000	53.461001000
H	23.623366000	-50.793769000	47.919238000
H	12.868546000	-43.956412000	54.729090000
H	14.125168000	-43.971352000	53.448440000
H	18.496610000	-51.734286000	55.549123000
H	20.706339000	-53.937258000	46.526393000
H	13.554341000	-57.954772000	51.405227000
H	16.510968000	-51.969233000	43.338101000
H	10.144989000	-44.471467000	48.667240000
H	10.015402000	-43.642738000	50.247437000

H	11.754456000	-43.390608000	43.725189000
H	17.649993000	-40.876066000	43.936212000
H	18.916207000	-44.914437000	42.562260000
H	12.227865000	-48.881002000	41.925496000
H	7.413321000	-51.907658000	45.910222000
H	11.682177000	-53.614482000	44.492249000
H	10.464867000	-53.642324000	43.183209000
H	7.347135000	-47.760420000	47.978386000
H	24.113028000	-41.794854000	49.859471000
H	12.379570000	-53.692827000	47.787912000
H	19.646407000	-48.488165000	51.451966000
H	9.450342000	-53.305386000	45.516880000
H	7.778283000	-50.142283000	45.816048000
H	12.028260000	-53.331434000	49.350555000

PFL-AE-cyclization-PC

C	14.358417000	-57.259444000	51.106907000
S	14.353140000	-57.095493000	49.271059000
C	20.149282000	-53.005229000	46.332296000
S	18.538033000	-53.387963000	45.523803000
C	23.489616000	-49.802477000	48.378186000
C	22.544090000	-49.832819000	49.567576000
O	22.613870000	-48.957932000	50.433220000
C	23.028829000	-48.766780000	47.316262000
C	21.819193000	-49.162357000	46.491106000
C	20.527235000	-49.188166000	47.047658000
C	21.942009000	-49.504093000	45.135016000
C	19.410937000	-49.531826000	46.288181000
C	20.826086000	-49.828279000	44.353177000
C	19.550247000	-49.832015000	44.929141000
O	18.410539000	-50.090335000	44.222648000
N	21.605755000	-50.807294000	49.601277000
C	20.445292000	-50.806633000	50.495174000
C	20.774347000	-50.164961000	51.857862000
O	21.513360000	-50.727654000	52.655171000
C	19.997571000	-52.249788000	50.755657000
S	18.437753000	-52.323034000	51.743277000
N	20.082552000	-49.031261000	52.150459000
C	20.341891000	-48.360945000	53.412528000
C	19.613904000	-48.983575000	54.630618000
O	19.860257000	-48.547379000	55.751469000
C	20.119214000	-46.842486000	53.326689000
C	18.717826000	-46.384981000	53.040900000
C	17.519610000	-47.042618000	53.229202000
N	18.459376000	-45.100307000	52.601958000
C	17.140901000	-44.988120000	52.538570000

N	16.533111000	-46.139544000	52.917689000
N	18.746342000	-49.993388000	54.379414000
C	18.053104000	-50.727893000	55.426317000
C	16.562602000	-50.899274000	55.137162000
C	15.790252000	-49.579399000	55.176430000
N	14.597257000	-49.586058000	54.526378000
O	16.209841000	-48.589741000	55.765570000
C	8.328451000	-48.072091000	48.371553000
C	9.443076000	-47.544890000	47.468147000
O	9.235637000	-47.543744000	46.225186000
O	10.515605000	-47.171159000	48.020909000
C	8.211484000	-51.140043000	45.956352000
C	9.299525000	-51.361877000	44.913413000
O	9.656737000	-50.466967000	44.142843000
N	9.865272000	-52.595820000	44.918713000
C	10.896503000	-53.021496000	43.988347000
C	13.051614000	-49.397342000	42.446775000
C	13.622504000	-48.491317000	43.533655000
O	12.842421000	-47.728953000	44.146322000
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C	15.606631000	-52.018220000	43.961947000
N	15.673862000	-50.955154000	44.992883000
C	12.574190000	-44.124304000	43.866448000
N	13.139611000	-44.052854000	45.201542000
C	12.673500000	-44.678153000	46.296346000
N	13.393531000	-44.605305000	47.428276000
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C	23.662319000	-41.628500000	50.859865000
C	22.258010000	-42.153041000	50.952832000
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N	21.233438000	-41.657042000	50.173546000
C	20.161382000	-42.351651000	50.514888000
N	20.427746000	-43.269039000	51.480018000
S	14.812935000	-53.544051000	50.617462000
S	17.758490000	-54.965586000	49.072569000
S	15.002074000	-54.297256000	46.815789000
S	16.785981000	-51.338794000	48.308611000
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Fe	14.542464000	-52.336797000	48.422873000
Fe	16.980879000	-52.934169000	50.046925000
Fe	15.411611000	-55.094163000	48.968394000
N	12.376774000	-52.902130000	48.443055000
C	11.590987000	-51.749455000	47.978376000
C	12.396433000	-51.007866000	46.882203000
O	13.628125000	-51.321711000	46.772169000
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O	16.058301000	-45.537495000	48.091958000
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O	13.964409000	-47.667500000	47.262879000
C	16.238869000	-47.211645000	46.466039000
O	15.472437000	-46.708757000	45.415548000
C	16.980729000	-46.039537000	47.127109000
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LAM-cyclization-TS

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LAM-cyclization-PC

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O	-40.472415000	14.103767000	-55.677984000
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C	-44.037142000	11.349077000	-67.199028000
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