

SUPPLEMENTARY MATERIAL

COPY

3/15/01
KB#24TABLE S1: Optimized Geometry of the Intermediates and some important products

HMR			
N1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	1.4428518675
N3	1.3797804977	0.0000000000	1.9639052322
C4	2.5348460500	-0.3787395369	1.1652729223
N5	2.3382170213	-1.5797469576	0.3698728476
C6	2.1252047901	-1.6013285505	-1.0808030313
N7	0.7786059174	-1.8020642138	-1.5600554469
C8	-0.2946118690	-1.1703701232	-0.8417376961
N9	0.1614713670	1.2243946928	-0.6475719934
N11	2.3803578339	-2.8068824160	1.0294996771
N12	1.4852417129	-0.0255620009	3.3469014962
O13	0.3427717780	2.2078310511	0.0647806221
O14	0.1330784470	1.1967265403	-1.8755999841
O17	2.2043264269	-3.8083140573	0.3418766457
O18	2.5741058931	-2.7666282742	2.2419447853
O19	2.6064555016	-0.0434912133	3.8400508620
O20	0.4141975364	0.0163717009	3.9546697540
H21	-1.0514064417	-0.8819827422	-1.5761204946
H22	-0.7455222757	-1.9205909712	-0.1768705279
H23	-0.5139874269	0.8825307229	1.8215427396
H24	-0.5342584264	-0.8928184721	1.7787671242
H25	2.7750607114	0.4208660160	0.4606007013
H26	3.3582076744	-0.5033734109	1.8669452885
H27	2.4864545858	-0.6362168476	-1.4648560316
H28	2.7466304809	-2.3913646821	-1.5044076592

HMR_o			
N1	0.1267358405	0.4521574550	-0.0490562653
C2	0.0287814430	0.1174529579	1.3605770655
N3	1.3346365634	-0.0114674796	1.9960237057
C4	2.3198227365	-0.9674027012	1.4761920120
N5	1.7433330730	-2.2026141562	0.9522247835
C6	2.1456887519	-2.7332480296	-0.3745302491
N7	1.1329022119	-2.9790387356	-1.3689430015
C8	-0.1008444548	-2.9014346182	-1.0998228998
N9	0.9595164099	1.5806271989	-0.2639136140
N11	1.3774640677	-3.1507443947	1.9155498740
N12	1.3443150629	0.2157128347	3.3963307972
O13	0.4574270132	2.6645777268	-0.0240592087
O14	2.0528531385	1.3472670682	-0.7574546419
O17	1.1679022210	-4.2914019345	1.5193831856
O18	1.2583740990	-2.7375975843	3.0679122524
O19	2.3933018914	-0.0023175433	3.9809736777
O20	0.3140639737	0.6686233135	3.8828197256
H21	-0.8206209561	-3.1059482527	-1.8928397461
H22	-0.5087313183	-2.6399978018	-0.1169783494
H23	-0.5149608930	0.9149285824	1.8802381113
H24	-0.5561162613	-0.8050481794	1.4198620350
H25	2.8367243172	-0.4951337332	0.6414084743
H26	3.0198092306	-1.1545495256	2.2901894187
H27	2.8404172336	-1.9994182649	-0.7916508719
H28	2.6883200668	-3.6706677343	-0.2220504556

INT204

N1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	1.4349075048
N3	1.3897672509	0.0000000000	1.9568445775
C4	2.5305265952	-0.2131356860	1.0671515931
N5	2.7788232587	-1.5842519961	0.6933382704
C6	1.9524593996	-2.4318886392	-0.0259396573
N7	0.8371154606	-2.3077444794	-0.6273316729
C8	-0.1067009011	-1.2502567079	-0.7941765857
N9	0.0803487413	1.2337098734	-0.6447585298
N12	1.5234232628	-0.4488386154	3.2530438292
O13	0.2572657263	2.2163966956	0.0755436900
O14	-0.0229039858	1.2433552340	-1.8681417321
O19	2.6550092590	-0.7599195483	3.6330534641
O20	0.4934825874	-0.4805944141	3.9285563454
H21	-0.1123038124	-0.9288107609	-1.8363021947
H22	-1.0953377207	-1.6725068916	-0.5738494797
H23	-0.5249745483	0.8741177902	1.8164723059
H24	-0.5129310438	-0.9056567511	1.7708634150
H25	2.3541249399	0.3995244440	0.1852217971
H26	3.4148311890	0.1639852448	1.5756518507
H27	3.4448791002	-2.0662417710	1.2836777592
H28	2.4055713828	-3.4259855443	-0.0836540219

INT158

N1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	1.4571495349
N3	1.2816394077	0.0000000000	2.1240596785
C4	2.3780875810	-0.4000374432	1.2591788241
N5	2.3876711057	-1.8540305883	1.1065860879
C6	1.4558708473	-2.6496344844	0.4646769496
N7	0.4516729720	-2.4380207734	-0.2943586340
C8	-0.1159031637	-1.2322878032	-0.8170009070
N9	0.1345200831	1.2128510005	-0.6399876946
O13	0.3370847663	2.1996678452	0.0737949927
O14	0.0442623302	1.2182709634	-1.8697766570
H21	0.3256276764	-0.9958382111	-1.7884228985
H22	-1.1823119637	-1.4253679196	-0.9868912946
H23	-0.5663167668	0.8636010713	1.8156696344
H24	-0.5422984245	-0.9072026968	1.7633583346
H25	2.3419915308	0.0646547571	0.2681961874
H26	3.3194738446	-0.1214132472	1.7373411728
H27	2.8835007876	-2.3430179723	1.8417366598
H28	1.6757693691	-3.7035427769	0.6610180155

INT157

N1	0.1524704369	-0.3789960374	0.0426076360
C2	0.3948558194	-0.2762020580	1.2800160610
N3	1.6646093841	-0.2140931652	1.9144922869
C4	2.8811948312	0.2544308003	1.2425256554
N5	3.6804573485	-0.7994170546	0.6698092373
C6	3.1164282001	-1.7513912230	-0.1749134748
N7	2.0563576553	-1.7436058211	-0.8799716846
C8	1.1336541094	-0.6180055767	-1.0291329942
N9	1.7843125900	-0.6373610871	3.2426862780
O10	2.9130562699	-0.5802064021	3.7316478193

O11	0.7668842399	-1.0298687806	3.8007439255
H12	1.6568203319	0.3216597132	-1.2644927812
H13	0.5282614682	-0.8502668215	-1.9081469078
H14	-0.4270761393	-0.1847666884	1.9846531546
H15	2.5468691401	0.9541472296	0.4796821986
H16	3.4826760552	0.7961788905	1.9693673331
H17	4.3676324320	-1.1825449183	1.3093160644
H18	3.7360442412	-2.6508327703	-0.2293958692

INT130

N3	0.0000000000	0.0000000000	0.0000000000
C4	0.0000000000	0.0000000000	1.4222934196
N5	1.4232020483	0.0000000000	1.9511711436
C6	2.2382309905	1.0034124263	1.8833716422
N7	1.8674338263	2.2971565078	1.7014356679
C8	1.3056386280	2.7681897369	0.6566451156
N9	0.5293631210	-1.1449578782	-0.4628684987
O10	1.0153136419	-2.0089800265	0.3488598136
O11	0.5541317680	-1.3190292169	-1.6857744329
H12	1.0088569556	3.8171171969	0.6687998003
H13	1.0892126036	2.1556979662	-0.2255423912
H15	-0.4768506295	0.9148440865	1.7788431030
H16	-0.4542560151	-0.8774170786	1.8953061720
H17	1.8071444675	-0.9466895447	1.9763365601
H18	3.2948302774	0.8312156279	2.0851664611

INT112

N1	0.0357703889	-0.0042353071	0.0530547292
C2	0.0195926540	0.1337841855	1.4225227475
N3	0.9389414132	0.1109134562	2.3138275581
C4	2.3324733020	-0.1099093652	1.9502173679
N5	2.6838820290	-1.4903982348	1.5831527473
C6	2.1852224325	-2.2207878063	0.5282839135
N7	1.5237482484	-1.9004947123	-0.5205562418
C8	1.1399408775	-0.5176116487	-0.7719345754
H21	1.9869309612	0.1721359122	-0.7077902551
H22	0.7770222526	-0.4599416892	-1.8019723084
H23	-0.9943600078	0.3295950549	1.7839265972
H24	-0.8821374501	-0.1600796472	-0.3433932148
H25	2.6740753535	0.5693490376	1.1633004368
H26	2.9404911887	0.1138588446	2.8312643179
H27	2.9698095602	-2.0643735322	2.3659571837
H28	2.4518635488	-3.2775826995	0.6236139250

INT222

N3	0.2818475125	-0.3552162149	0.1363690966
C4	-0.0520952020	-0.5501110115	1.5227173226
N5	1.1665052244	-0.1581692345	2.2874303025
C6	1.9335131647	0.9816993736	1.9098466695
N7	3.0865575302	0.6366437325	0.9873262819
C8	2.9683558102	0.0486504553	-0.1451479470
N10	4.5307666567	1.0033738718	1.4936382171
N11	1.8426663131	-1.0956697275	3.0627446941
N12	-0.7948249773	-0.3061863046	-0.6705446596
O15	4.5501622907	1.7456341713	2.4367580252
O16	5.4137694545	0.5113466727	0.8433477937
O17	1.2421965792	-2.1045578377	3.3955778111

O18	3.0095133109	-0.8018724053	3.3582597648
O19	-0.5686357625	-0.0864844870	-1.8731476123
O20	-1.9378859750	-0.4765130391	-0.1925601241
H21	3.8749714650	-0.1673891812	-0.7054786538
H22	1.8872571260	-0.2150813406	-0.3981661947
H25	-0.8938485942	0.0702300668	1.8525372881
H26	-0.2679214445	-1.5838694313	1.8122059356
H27	1.2794813007	1.6439371987	1.3426328739
H28	2.3817481522	1.4827578375	2.7633218711

RDR_o

C1	0.0552950779	0.0098385143	-0.6367913127
N2	0.0891869513	0.1118705671	2.8096876095
C3	1.5574519782	-0.0039578602	2.6953861093
N4	1.9818389552	-0.4887290919	1.3993487068
C5	2.2238410720	0.3823403751	0.2356844814
N6	1.1666443183	0.6135818954	-0.7205109234
N7	-0.5013176047	-1.1115208550	3.1907730575
N8	2.1400418718	-1.8693136679	1.2468902069
O9	-1.1334800441	-1.7006083657	2.3292720782
O10	-0.3954189720	-1.3905092561	4.3752422651
O11	1.8971031348	-2.5657285498	2.2307691011
O12	2.5177009102	-2.2578924465	0.1486729654
H13	-0.2173624953	-0.7015198712	0.1497143235
H14	-0.7004264928	0.2180729893	-1.3952090993
H15	1.9392870681	1.0124173521	2.8053107411
H16	1.9529976173	-0.6489308336	3.4835690594
H17	2.5200630067	1.3521920693	0.6476784940
H18	3.0771205948	-0.0305225573	-0.3060605555

INT249

N1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	1.4677245529
N3	1.2127340785	0.0000000000	2.2469881910
C4	2.3927578760	-0.3821757320	2.0080507179
N5	2.9840331119	-0.7603308561	0.7704245491
C6	2.7520153810	-0.1055803752	-0.5031248015
N7	1.8385650030	-0.8989377679	-1.3136377854
C8	0.4813350042	-1.1071166455	-0.8046501168
N9	-0.2853203847	1.1931974731	-0.6765092401
N10	1.9897823601	-0.7829199026	-2.7131857289
N11	4.1391480179	-1.5870942213	0.8549438316
O13	-0.6590219107	2.1551332826	-0.0152303390
O14	-0.1379195403	1.1592159865	-1.8968894707
O15	1.1399286560	-1.3299322295	-3.4022926849
O16	2.9912952160	-0.1996616555	-3.1105603912
O17	4.7857155635	-1.7316155611	-0.1718336102
O18	4.3604915228	-2.0982920411	1.9452332336
H21	-0.1664491529	-1.2940358172	-1.6584786324
H22	0.4749016168	-1.9788440989	-0.1449323956
H23	-0.5829715665	0.8730710123	1.7557096922
H24	-0.5573391586	-0.8890770418	1.7903158730
H25	3.0863886921	-0.4604512680	2.8415409566
H27	2.3633690937	0.8954285895	-0.2893302107
H28	3.6915155101	-0.0218630347	-1.0407636849

INT202

N1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	1.4806712189
N3	1.3462277814	0.0000000000	2.0324990872
C4	1.9768341496	1.0830963634	2.2572045672
N5	1.6009795351	2.3925080128	1.8989733149
C6	0.8599508418	2.6907660957	0.6528450939
N7	1.3614009544	1.9274971711	-0.4797317644
C8	0.9022256419	0.7732318447	-0.7579012346
N9	-0.5270398945	-1.1599007905	-0.6542897158
N11	2.4004810007	3.4449955289	2.4525363250
O13	-1.1069851564	-1.9776940341	0.0437286732
O14	-0.3867524658	-1.2041424080	-1.8687561749
O17	2.2650890802	4.5590710391	1.9700109938
O18	3.1176982536	3.1384121056	3.3946956488
H22	1.2221773809	0.2867220780	-1.6739576539
H23	-0.6163184303	0.8312922394	1.8384573379
H24	-0.4884874372	-0.9279023880	1.7693418186
H25	2.9287217090	1.0374148832	2.7771517981
H27	-0.2105657236	2.5497938069	0.8319879980
H28	1.0320113205	3.7468328709	0.4577478713
INT155			
N1	-0.0732914880	0.0389210697	0.0049335054
C2	-0.0029258812	0.0969206496	1.2840834191
N3	1.1156679702	0.0404712894	2.0986841504
C4	2.1268969324	0.8159953268	2.1595218139
N5	2.3368617183	1.9877003749	1.4414101924
C6	1.6072842118	2.2939598106	0.1909192068
N7	1.8182192478	1.2688672384	-0.8218702482
C8	1.0377456300	0.2482451216	-0.8023964952
N11	3.5635810455	2.6842609671	1.6911588148
O17	3.8282395358	3.6086475964	0.9408094533
O18	4.2210017873	2.3121509294	2.6538874383
H22	1.1785701401	-0.5033702027	-1.5812177758
H23	-0.9381641426	0.0490279566	1.8447850606
H25	2.9240197503	0.5889516386	2.8590595545
H27	0.5552750446	2.4326987242	0.4673634813
H28	2.0073488380	3.2399313707	-0.1629497007
INT108			
N1	0.0110658745	-0.0487243584	0.0079282906
C2	0.0375737367	-0.0621154914	1.2903262538
N3	1.1622447411	-0.0205469210	2.1105819648
C4	1.9302527743	1.0066981368	2.1051504946
N5	1.7014950889	2.2266966532	1.4733110910
C6	1.6091976385	2.2856035479	0.1953066850
N7	1.8785408659	1.2681827354	-0.7167896180
C8	1.1757761626	0.1952559063	-0.7158484401
H22	1.4447504477	-0.5899232015	-1.4242675405
H23	-0.9045133665	-0.2220703977	1.8171855508
H25	2.8191067108	0.9809854510	2.7375565090
H27	1.3932154666	3.2557102970	-0.2552311811
INT296			
N1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	2.4897950037
N3	1.4624280577	0.0000000000	2.3848668005

C4	2.5027699717	0.5023448923	1.4379778700
N5	2.9429801014	-0.4554403623	0.4799434571
C6	2.5950080435	-0.4361604945	-0.9508642222
N7	1.5144488316	-1.3245036335	-1.3076263126
C8	0.0803171934	-0.9705318410	-1.0546339197
N9	0.0450278689	1.2658453107	-0.4200320707
N10	1.7432557264	-2.2613797752	-2.3088569091
N11	3.7139131270	-1.5100926456	0.9778180621
N12	1.5819692841	0.0674978007	3.7013760587
O13	0.0212171486	2.1471752812	0.4955126875
O14	0.1615366023	1.5802929342	-1.6216639746
O15	0.7481602941	-2.8808183190	-2.6841217118
O16	2.8894563359	-2.4113234327	-2.7274561483
O17	4.1310222364	-2.3231484682	0.1711807158
O18	3.8874374213	-1.5138726656	2.1998905352
O19	2.4910112131	0.1738972506	4.4555176009
O20	0.2539995910	-0.0039820352	3.9989898181
H21	-0.3734593286	-0.6285520903	-1.9888966950
H22	-0.4165682247	-1.8836562922	-0.7224240810
H23	-0.4588022814	0.9344068151	2.1626309454
H24	-0.4973555468	-0.9227512281	2.2197575910
H25	2.0514082372	1.3601241802	0.9347822791
H26	3.3245778047	0.8145457756	2.0854963139
H27	2.3407214716	0.5983190941	-1.1924533137
H28	3.4676694971	-0.7467540463	-1.5208826420

RDX_oring

N1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	1.4764549260
N3	1.3225394151	0.0000000000	2.0772662220
C4	2.0902145416	1.2059457690	2.3390718060
N5	2.7367862361	1.7818721390	1.1562736345
C6	1.9538558119	2.6779190160	0.2796721584
N9	0.3955990873	1.0365565296	-0.5707318509
N11	4.0965736226	2.1051044985	1.2467678078
N12	2.0434191989	-1.2135576283	2.0017149718
O13	0.5942478337	1.2543857572	-1.7407870671
O14	0.6162315306	2.2642133223	0.3407037572
O17	4.5064777378	2.8773849892	0.3807706974
O18	4.7564624988	1.5959024003	2.1417925275
O19	3.2168708030	-1.1729491696	2.3451955983
O20	1.4165339792	-2.1978945992	1.6317410912
H23	-0.5447066831	0.8558867211	1.8767132431
H24	-0.5004871767	-0.9228302176	1.7557896015
H25	1.3947313242	1.9278554004	2.7748305011
H26	2.8792120996	0.9679232833	3.0469919528
H27	2.3509818656	2.6469221056	-0.7360687768
H28	1.9621728119	3.7105855723	0.6472432436

TABLE S2: Optimized Geometry of the Transition States

TS1			
N1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	1.4413425631
N3	1.3226720911	0.0000000000	2.1106784755
C4	2.6236828704	0.1460646865	1.4762068833
N5	3.0397883443	-1.0210628266	0.7101073997
C6	3.0753425289	-1.0701304574	-0.7476686011
N7	1.8856197502	-1.4667539856	-1.4562855901
C8	0.8224337389	-1.8183127269	-0.8006206079
N9	0.4849248279	1.1896237996	-0.5974902320
N11	3.4338202560	-2.1560285463	1.4221347720
N12	1.2467312415	0.1601332206	3.4963002587
O13	0.5644647464	2.1919788161	0.1238384573
O14	0.7100348120	1.1443949755	-1.7955592027
O17	3.7226829939	-3.1500014488	0.7595977469
O18	3.4455979177	-2.0571093622	2.6436085388
O19	2.2804168230	0.3615633290	4.1204665257
O20	0.1124260699	0.0786986785	3.9681757991
H21	-0.0610092494	-2.0845987248	-1.3732543706
H22	0.8601897275	-2.1481842342	0.2426074686
H23	-0.5691769117	0.8738181493	1.7777644663
H24	-0.5465951748	-0.8951116223	1.7441275168
H25	2.6246695066	0.9915098017	0.7858412156
H26	3.3256929979	0.3388549960	2.2853861658
H27	3.3300398326	-0.0650559969	-1.1064151591
H28	3.8833422898	-1.7416141080	-1.0506086099
TS2			
N1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	1.3224494257
N3	1.9042116165	0.0000000000	1.8799926184
C4	2.9406281291	0.1226723298	0.8524283845
N5	3.4252943209	-1.1114907060	0.2654900055
C6	2.6957269461	-1.8165096636	-0.8073003990
N7	2.1113252871	-3.1034118416	-0.5114067667
C8	2.3514568874	-3.7008409722	0.5794970572
N9	-0.0838036141	1.3162887895	-0.5574691348
N11	4.7991688630	-1.3728978579	0.3791228382
N12	2.1613899145	-0.9815993860	2.8659672653
O13	-1.0956453482	1.9604030220	-0.3377705397
O14	0.8537034113	1.6334115150	-1.2809607231
O17	5.2006667703	-2.3707269142	-0.2095295638
O18	5.4797226325	-0.6030441599	1.0514451890
O19	3.3414771607	-1.1404067485	3.1617137253
O20	1.1964342728	-1.5185938191	3.3946223214
H21	1.8982401255	-4.6788381428	0.7457971416
H22	2.9894286827	-3.3060972020	1.3790003842
H23	-0.2753205459	0.8856267319	1.8921154572
H24	-0.1761830686	-0.9662646052	1.7819965336
H25	2.5124929753	0.7758416210	0.0888764690
H26	3.8015114952	0.6173191984	1.3125053533
H27	1.8867340002	-1.1463125444	-1.1081570135
H28	3.3719922816	-1.9484428043	-1.6563717077

TS3

N1	-0.0383526423	0.0161243181	0.0058057244
C2	-0.0356797010	0.0563523748	1.4477031947
N3	1.3524673111	0.0016046175	1.9199131680
C4	2.3430644266	0.9286368826	1.3797707053
N5	3.2615731044	0.4343440249	0.3537383220
C6	2.8876688917	-0.4649458294	-0.7335739247
N7	1.8703773530	-1.2336266480	-1.0765318697
C8	0.4926468560	-1.1556207780	-0.7129086687
N9	-0.1279452591	1.2139878909	-0.6988943056
N10	4.6677936624	-0.5286029887	1.4196891906
N11	1.5763723315	-0.5717510955	3.1702427736
O12	-0.3957698437	2.2344777474	-0.0614482592
O13	0.0610423063	1.1470392776	-1.9101620174
O14	4.9049526731	-1.6278232840	0.9830379446
O15	5.2705722480	0.1786317640	2.1841435881
O16	2.7177234884	-0.5114175927	3.6153564972
O17	0.6106980382	-1.1093184324	3.7101190025
H18	-0.0949378103	-1.2556824262	-1.6290796427
H19	0.2476604666	-2.0142800333	-0.0730338694
H20	-0.5481300191	0.9619450158	1.7757732718
H21	-0.5552893028	-0.8189833093	1.8332654997
H22	1.8091801460	1.8056827944	0.9996858940
H23	2.9904301614	1.2550713639	2.1954330344
H24	2.7921011323	0.7513918888	-0.9813749477
H25	3.8226035001	-0.7435444639	-1.2229627598

TS4

N1	-0.0060831933	-0.0238214134	0.0146317518
C2	0.0135006395	0.0074064754	1.4459151829
N3	0.9833931382	0.0419866578	2.3561894554
C4	2.3730318236	0.0025573341	1.9347924440
N5	2.8319944257	-1.3535354088	1.5843178537
C6	2.2636780484	-2.1586150586	0.6272886359
N7	1.5230593878	-1.9039121424	-0.3906114728
C8	1.1707465200	-0.5472988800	-0.7610515951
N9	-0.1287819116	1.7624511404	-0.6306929439
O10	-0.4228247454	2.5474648846	0.2425897142
O11	-0.0581407266	1.9229810856	-1.8288659125
H12	2.0173674030	0.1449675875	-0.7082599504
H13	0.8214435706	-0.5563958006	-1.7944162740
H14	-0.9723429490	0.2854500539	1.8229651245
H15	-0.3200414894	-1.0954089552	0.8709818644
H16	2.5968760144	0.6912801966	1.1163688715
H17	2.9847472674	0.3106309770	2.7864815448
H18	3.2054213150	-1.8731384439	2.3693086687
H19	2.5238714252	-3.2097378146	0.7757008458

TS5

N1	0.2153995155	-0.0043760588	-0.0677320610
C2	0.0110995785	0.0863911940	1.2135058555
N3	0.8964733494	-0.1584572234	2.2045282636
C4	2.1827079450	-0.0472689395	1.9574476380
N5	3.0417981165	-1.7348841558	1.1065091219
C6	2.7417135297	-2.4929689427	0.0934551201
N7	1.8831507618	-2.2158072511	-0.9119422852
C8	1.6580748375	-0.9668903103	-1.2460355931

H21	2.3895327548	-0.1807441410	-1.0467668061
H22	0.9985547696	-0.7946795314	-2.0928030482
H23	-0.9874745063	0.3575410198	1.5771705040
H24	-0.6307989931	0.1819720179	-0.6056434434
H25	2.5560251185	0.5955871219	1.1569574495
H26	2.8570905637	-0.1901323647	2.7982551262
H27	3.6726918406	-2.1971306996	1.7608968980
H28	3.1835861948	-3.4945346672	0.0284400222

TS6

N1	0.0086676878	-0.0153771947	-0.0073747350
C2	-0.0052641699	-0.0274021525	1.3279767237
N3	1.3480267330	-0.0136563892	1.8376454168
C4	2.3035681774	-0.7865947732	1.0284636488
N5	1.8871691225	-2.1565374247	0.7781082746
C6	0.9534493794	-2.6873870413	-0.1074509312
N7	-0.0727391972	-2.2697632708	-0.7427715462
C8	-0.7800429499	-1.0057508465	-0.7045178015
N9	-1.0937631183	1.8374900098	-0.2053584066
N10	1.4854316065	-0.0008115800	3.2181825234
O11	-1.1127056982	2.2363358283	1.0045688502
O12	-1.5052613411	2.5122652817	-1.1112470584
O13	2.5685268062	-0.3492306746	3.6862148751
O14	0.5066808791	0.3923649884	3.8518613585
H15	-0.9511941248	-0.6675894957	-1.7303326264
H16	-1.7570523029	-1.1976578240	-0.2330630892
H17	-0.5637419061	1.1933843461	1.4830543698
H18	-0.6886542491	-0.6870094447	1.8825935836
H19	2.4039909319	-0.2437634066	0.0893574726
H20	3.2520234743	-0.7985636306	1.5594074973
H21	2.4854178969	-2.8599206657	1.1887554679
H22	1.1665067850	-3.7505783644	-0.2562488574

TS7

N1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	1.1872780025
N3	1.7020056670	0.0000000000	2.1779879527
C4	2.9335730566	0.1503394279	1.4717997495
N5	3.5337530344	-1.0942754385	0.9309868908
C6	3.2625411733	-1.6128238941	-0.2553222709
N7	2.4797103353	-1.0584477312	-1.1375225861
C8	1.2171300311	-0.9683549450	-1.4043112137
N12	1.7931720837	-0.7623554692	3.2833459094
O19	2.8983625039	-1.2709763472	3.6021820335
O20	0.7494208504	-0.9278267605	3.9341809715
H21	0.9133656649	-0.2871351966	-2.1924812596
H22	0.5413989805	-1.7936445088	-1.1877110655
H24	-0.5779209576	0.0138986870	2.0980115191
H25	2.7289989390	0.8012240124	0.6189929914
H26	3.7117661714	0.5889624353	2.1040005965
H27	4.0908480190	-1.6282879464	1.5884405531
H28	3.8467492463	-2.4947452983	-0.5323084489

TS8

N3	0.1771417858	0.0207394979	0.0164320813
C4	0.0770203024	-0.0119717636	1.3538934166
N5	1.7583871073	0.0250370672	2.0976020713

C6	2.6260485061	0.9651391982	1.9920741923
N7	2.3162288126	2.2915368561	1.8164191248
C8	1.7691748499	2.7665789356	0.7685973772
N9	0.5861373925	-1.2020872588	-0.4954426571
O10	1.0425312105	-2.0828681089	0.2712548186
O11	0.5157694292	-1.3311999562	-1.7150687096
H12	1.5392108132	3.8325082740	0.7509346476
H13	1.5053894337	2.1580596791	-0.1017356558
H15	-0.3294305338	0.9017110379	1.7798231738
H16	-0.2133867068	-0.9303905519	1.8646873887
H17	2.1332632837	-0.9117127404	2.2314006206
H18	3.6915179309	0.7696581613	2.1405679405
TS9			
N1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	1.4493755641
N3	1.3854786983	0.0000000000	1.9585894501
C4	2.1051132979	-1.1318235309	1.9185679294
N5	1.6151550957	-2.3327452733	1.2655454737
C6	2.0363461956	-2.6491411572	-0.0744700325
N7	1.3372920923	-1.7804319461	-1.0500679599
C8	0.0132607216	-1.2125653089	-0.8039808339
N9	0.3172987040	1.2159280470	-0.6420719479
N10	1.7321822895	-1.9939526671	-2.3745384100
N11	0.6714864811	-3.1452079753	1.8884284887
N12	0.9794329316	0.0097708757	3.9763450755
O13	0.3738105378	2.2100697026	0.0687907410
O14	0.4791091841	1.1610301850	-1.8538241095
O15	1.0561701882	-1.5080692743	-3.2700602674
O16	2.7581787012	-2.6620178043	-2.5099780384
O17	0.2169829153	-4.0851315248	1.2417791322
O18	0.3586363206	-2.8286773403	3.0347948934
O19	1.8331520005	-0.8109535561	4.4242486031
O20	0.3426119575	0.7560247171	4.6637676825
H21	-0.4112306056	-0.9918506894	-1.7803004820
H22	-0.6159019580	-1.9395608389	-0.2832155542
H23	-0.4797357593	0.9065934474	1.8113428927
H24	-0.5789150316	-0.8704030614	1.7673583169
H25	3.1740647094	-0.9984874045	1.7338774483
H26	2.1458642452	-1.2615534324	3.3036056265
H27	3.1068684742	-2.4578427319	-0.1581118059
H28	1.8438180570	-3.7045906338	-0.2692359577
TS10			
N1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	1.4709495729
N3	1.2187153087	0.0000000000	2.2303569065
C4	2.4432643582	-0.2313186830	2.0212886741
N5	3.1739789795	-0.4503566939	0.8235382233
C6	2.7172013461	-0.1567209550	-0.5252811423
N7	1.8508781273	-1.2554021267	-0.9490987531
C8	0.5310755591	-1.1311209828	-0.7206238838
N9	-0.2006112492	1.2083967709	-0.6654733677
N10	1.8234309138	-0.9430186153	-2.9739040855
N11	4.4671045218	-1.0481000672	0.9547766267
O13	-0.5967604335	2.1643426137	-0.0075584263
O14	0.0364317373	1.2110998887	-1.8752126260

O15	0.6117372879	-1.1682448947	-3.2595014416
O16	2.7050403379	-0.8808917699	-3.7829007926
O17	5.1230429533	-1.1589912621	-0.0689884493
O18	4.8021136331	-1.3907993736	2.0796176088
H21	0.2118018226	-1.1114143292	-2.0803440705
H22	0.0140470047	-2.0601904249	-0.4661034155
H23	-0.5873316843	0.8665995755	1.7726418078
H24	-0.5484620878	-0.8977846503	1.7800822380
H25	3.1065652683	-0.2699955952	2.8803673976
H27	2.2351081301	0.8229331291	-0.5037254600
H28	3.5850526422	-0.1223892779	-1.1786317453
TS11			
N1	-0.5140791184	0.3150936188	0.0830908407
C2	-0.4672637247	0.1281567071	1.4154008507
N3	0.6908124466	0.1809486869	2.2518450457
C4	1.5182674233	1.1367767380	2.4088981974
N5	1.5380167727	2.3984826076	1.8092486453
C6	0.6881196633	2.7708246897	0.6679379258
N7	1.0276775554	2.0181669197	-0.5333966688
C8	0.4821571658	0.8726667399	-0.7074907031
N9	-0.3611760818	-1.7102761039	-0.4898968758
N11	2.6653456582	3.2381110916	2.0945532205
O13	-0.6436512082	-2.2840644976	0.5884749811
O14	-0.2300528871	-2.2619395040	-1.5510240670
O17	2.7464368031	4.2745441130	1.4557056829
O18	3.4290693652	2.8591506436	2.9714362194
H22	0.7037140657	0.3195120575	-1.6193466716
H23	-1.3996743616	0.3551729296	1.9468033570
H24	-0.6762864995	-1.1574672727	1.3030109355
H25	2.3301737241	1.0054045446	3.1165038432
H27	-0.3500281797	2.6440575199	0.9924301497
H28	0.8674351699	3.8262639926	0.4843413987
TS12			
N1	0.0407594628	0.0176356003	0.0672868751
C2	0.1757507731	-0.1015890561	1.3352308643
N3	1.3496291041	-0.0509547297	2.0843850977
C4	2.0723614424	1.0062101176	2.1320356808
N5	1.7086476530	2.2456564532	1.6098349581
C6	1.4593786194	2.4708063755	0.3063608156
N7	1.7259670956	1.5295228395	-0.7392748472
C8	1.0883274055	0.4166470251	-0.7548490160
N11	3.6188423552	3.1880707376	1.6827140506
O17	3.5846005383	3.8708514813	0.6296657985
O18	4.4775457492	3.2672590889	2.5224891690
H22	1.3040834189	-0.2755348849	-1.5710263053
H23	-0.7064664912	-0.3744412659	1.9167993652
H25	2.9759577914	0.9998774211	2.7380237838
H27	0.6417574051	3.1755806139	0.1079435332
H28	2.4395417979	3.3439219823	0.1988136640
TS13			
N1	0.1274343270	0.0170093992	0.0441184804
C2	0.0322794460	-0.0546403996	1.2266937606
N3	1.5723062525	0.0950878469	2.3559639829
C4	2.3544547221	0.9847974281	2.4632480104

N5	2.1786718986	2.5818578367	1.4454673535
C6	2.1540713804	2.7436724483	0.2674907011
N7	2.3369648336	1.2775488028	-0.9295411455
C8	1.6752033016	0.2971169417	-1.0451205572
H22	1.5528158791	-0.6143828737	-1.6077620124
H23	-0.6546514641	-0.2218979149	2.0406809796
H25	3.2303841173	1.3123891279	3.0005610139
H27	2.0907795998	3.4918163418	-0.5067405733

TS14

N1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	2.2934190228
N3	1.4594120214	0.0000000000	2.2497671676
C4	2.5194803994	0.4635105003	1.3139075043
N5	2.9434755687	-0.5150942823	0.3648095156
C6	2.5323642957	-0.5479088809	-1.0458209124
N7	1.4157818244	-1.4258127390	-1.3127051349
C8	0.0067868661	-1.0501956226	-0.9767694231
N9	0.0199973296	1.2400693326	-0.5078288780
N10	1.5667493463	-2.4015518233	-2.2902914962
N11	3.6764654299	-1.5924270038	0.8754026375
N12	1.5690068714	0.0740610917	3.5712907375
O13	0.0508985019	2.1747245437	0.3428040714
O14	0.0566880218	1.4553774733	-1.7333508837
O15	0.5403469661	-3.0185824288	-2.5754626041
O16	2.6803796335	-2.5830700880	-2.7769447946
O17	4.0425723940	-2.4399185932	0.0785712207
O18	3.8759754172	-1.5762427120	2.0919574756
O19	2.4996186463	0.1817151431	4.3046090990
O20	0.2731848397	0.0039019051	3.8940850155
H21	-0.5193687768	-0.7764434053	-1.8949580907
H22	-0.4660517429	-1.9329148063	-0.5408156952
H23	-0.4833708816	0.9431837725	2.0578642830
H24	-0.5113298685	-0.9348328733	2.1140899283
H25	2.1131792159	1.3324394595	0.7938396903
H26	3.3466370365	0.7516920802	1.9650816496
H27	2.2941149943	0.4814930502	-1.3226488583
H28	3.3683519178	-0.9058858020	-1.6420952484

TS15

C1	-0.3306093814	-0.6168212162	0.2171090712
N2	0.0871962251	-0.5387417079	1.6577420645
C3	1.3733458766	0.0200833867	1.9895914610
N4	2.4660138502	-0.9228241355	1.6542353098
C5	3.0011159313	-0.9944989588	0.4385388986
N6	0.8793926643	-0.8394145519	-0.5180169294
N7	-0.9342957207	-0.3546154900	2.5993043556
N8	2.6312256088	-2.0871169858	2.5529882642
N9	1.0093707937	-2.0605126821	-1.0408499107
O10	-2.0667612647	-0.5884953433	2.1948961723
O11	-0.6208009142	0.0029364511	3.7323839520
O12	1.9870905079	-2.0230336594	3.5771940639
O13	3.4096680443	-2.9374799292	2.1796183159
O14	2.2127395845	-2.4079724306	-1.2604463261
O15	0.0529539772	-2.7904221411	-1.3264447824
H16	-1.0548415183	-1.4250256617	0.1031754029
H17	-0.7973525472	0.3365238779	-0.0628687399

H18	1.5990443999	0.9252167188	1.4163392802
H19	1.3956657804	0.2314926692	3.0547808942
H20	3.0708765353	-0.0906554566	-0.1434836570
H21	3.6869484958	-1.8094725260	0.2691791037
TS16			
N1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	2.0260378724
N3	1.2242497866	0.0000000000	2.5104540027
C4	2.0506155429	1.2468028963	2.7407898911
N5	2.3352190585	2.0123510384	1.5739610560
C6	1.2478234876	3.0660264368	1.0814973011
N9	0.0202353110	1.0102875136	-0.5726883494
N11	3.1607164972	1.3893911940	0.6552026340
N12	1.8825454315	-1.3209404825	2.7215842707
O13	0.0341482358	1.7446812869	-1.5027688594
O14	0.0328993412	2.5488375574	1.0459787955
O17	3.4263323467	2.0011697328	-0.3741133188
O18	3.5782731936	0.2578976312	0.9506740177
O19	2.8736366429	-1.2972129858	3.4121418367
O20	1.3203343064	-2.2645371136	2.2102268622
H23	-0.4463484087	1.0001606508	1.9739623888
H24	-0.5478779963	-0.9324306128	2.0379717755
H25	1.4645091875	1.8795851948	3.4074907641
H26	2.9525104970	0.8982082895	3.2374831194
H27	1.6757364846	3.3996825029	0.1239473691
H28	1.3766632072	3.8716180342	1.8310814392