JOC The Journal of Organic Chemistry

J. Org. Chem., 1998, 63(23), 8331-8336, DOI:10.1021/jo981190n

Terms & Conditions

Electronic Supporting Information files are available without a subscription to ACS Web Editions. The American Chemical Society holds a copyright ownership interest in any copyrightable Supporting Information. Files available from the ACS website may be downloaded for personal use only. Users are not otherwise permitted to reproduce, republish, redistribute, or sell any Supporting Information from the ACS website, either in whole or in part, in either machine-readable form or any other form without permission from the American Chemical Society. For permission to reproduce, republish and redistribute this material, requesters must process their own requests via the RightsLink permission system. Information about how to use the RightsLink permission system can be found at http://pubs.acs.org/page/copyright/permissions.html



ACS Publications

MOST TRUSTED. MOST CITED. MOST READ.

Copyright © 1998 American Chemical Society

© 1998 American Chemical Society, J. Org. Chem., Omoto jo981190n Supporting Info Page 1

Table S1. The Coordinates of Atoms in **1** (RHF/6-31G*)

Total Energy (au): -369.06965

atom	x	y	z
B	.000000	.000000	.000000
O	1.360739	.000000	.000000
O	-.515245	1.258501	.000000
C	-.878955	-1.311462	-.032579
C	-.316236	-2.431645	.803295
C	-.929478	-3.004805	1.820709
H	-1.896260	-1.081703	.268222
H	-.931846	-1.635152	-1.074336
H	.674691	-2.762706	.536877
H	-.465727	-3.795088	2.384161
H	-1.917638	-2.708843	2.130899
C	1.821908	1.332676	.061910
C	.543802	2.190444	-.051983
H	2.339971	1.485547	1.000564
H	2.518962	1.510145	-.746602
H	.492856	2.733729	-.987600
H	.440336	2.897811	.760298

Table S2. The Coordinates of Atoms in **1** (RHF/6-31G**)

Total Energy (au): -369.08462

atom	x	y	z
B	.000000	.000000	.000000
O	1.360666	.000000	.000000
O	-.515102	1.258745	.000000
C	-.881095	-1.308424	-.037343
C	-.290103	-2.459710	.732567
C	-.870335	-3.077750	1.742525
H	-1.884786	-1.085364	.311194
H	-.977325	-1.591821	-1.088114
H	.693480	-2.776161	.422353
H	-.386215	-3.889690	2.256367
H	-1.849416	-2.797480	2.094538
C	1.821712	1.333031	.063337

C	.544471	2.190378	-.055708
H	2.336291	1.487653	1.004719
H	2.522372	1.512257	-.742824
H	.495920	2.729852	-.994771
H	.442227	2.902940	.753334

Table S3. The Coordinates of Atoms at the Transition State for the Reaction of **1** with Formaldehyde (RHF/6-31G*)

Total Energy (au): -482.90366

atom	x	y	z
B	.000000	.000000	.000000
O	.000000	.000000	1.431800
O	1.334029	.000000	-.447546
O	-.766680	1.238511	-.512084
C	-1.909103	1.446697	-.021276
C	-3.142885	-.118628	-.719603
C	-2.273348	-1.019302	-.173365
C	-.943204	-1.262221	-.673570
H	-2.064943	1.311637	1.034879
H	-2.527816	2.177015	-.514558
H	-3.046692	.156677	-1.755330
H	-4.107690	.044650	-.270410
H	-2.506581	-1.405953	.805726
C	1.332080	.006094	1.868343
C	2.138077	.401520	.624858
H	1.457007	.702270	2.690985
H	1.609633	-.984824	2.220366
H	3.102459	-.090450	.570195
H	2.303135	1.476516	.591669
H	-.860674	-1.199387	-1.750788
H	-.507698	-2.180480	-.301112

Table S4. The Coordinates of Atoms in **1** (MP2/6-31G**)

Total Energy (au): -370.20243

atom	x	y	z
B	.000000	.000000	.000000
O	1.380555	.000000	.000000
O	-.549624	1.263712	.000000
C	-.841257	-1.326025	.038347
C	-.539874	-2.078426	1.304814
C	-1.418020	-2.286074	2.293202
H	-1.906150	-1.102261	-.028438
H	-.572604	-1.938334	-.827237
H	.475949	-2.444403	1.412682
H	-1.138810	-2.815015	3.193165
H	-2.438253	-1.931945	2.224402
C	1.797344	1.368987	.169430
C	.542045	2.195149	-.139689
H	2.134577	1.505481	1.198045
H	2.625100	1.580012	-.505408
H	.543384	2.577791	-1.161363
H	.395888	3.025373	.549005

Table S5. The Coordinates of Atoms in the Complex for the Reaction of **1** with Formaldehyde (MP2/6-31G**)

Total Energy (au): -484.39728

atom	x	y	z
B	.000000	.000000	.000000
O	.000000	.000000	2.723850
O	1.384023	.000000	.039199
O	-.550292	1.259991	-.070706
C	-.852920	-1.321401	-.076722
C	-.088672	-2.551757	.303458
C	-.414324	-3.370289	1.313288
H	-1.741228	-1.209894	.547629
H	-1.212188	-1.411478	-1.108155
H	.799588	-2.768021	-.281797
H	.178940	-4.243047	1.547915

H	-1.293768	-3.192544	1.919053
C	1.794136	1.378752	-.065377
C	.519192	2.178586	.219379
H	2.590273	1.574805	.651233
H	2.172883	1.553238	-1.074052
H	.418169	3.062859	-.407676
H	.449472	2.465388	1.269069
C	.817295	-.884532	2.947527
H	.754436	-1.509574	3.850162
H	1.647161	-1.088572	2.263028

Table S6. The Coordinates of Atoms at the Transition State for the Reaction of **1** with Formaldehyde (MP2/6-31G**)

Total Energy (au): -484.38317

atoms	x	y	z
B	.000000	.000000	.000000
O	.000000	.000000	1.440473
O	1.331050	.000000	-.489317
O	-.763067	1.332905	-.503739
C	-1.838506	1.583182	.118103
C	-3.248758	-.066704	-.540465
C	-2.310965	-.943437	-.072917
C	-1.014545	-1.135086	-.693909
H	-1.918354	1.349160	1.175564
H	-2.519258	2.309424	-.317749
H	-3.207126	.280501	-1.564829
H	-4.171123	.105536	-.001695
H	-2.446683	-1.350518	.924886
C	1.373345	.053149	1.839655
C	2.112190	.521717	.587255
H	1.492896	.731825	2.685984
H	1.705658	-.944572	2.142045
H	3.132248	.143297	.517481
H	2.138715	1.616236	.540640
H	-1.019490	-.998166	-1.773273
H	-.550476	-2.084069	-.430624

Table S7. The Coordinates of Atoms in **2** (RHF/6-31G*)

Total Energy (au): -408.10932

atom	x	y	z
B	.000000	.000000	.000000
O	1.358433	.000000	.000000
O	-.710464	1.156743	.000000
C	-.774289	-1.385786	-.026738
C	-.154310	-2.442645	.848751
C	-.750185	-3.040922	1.862621
H	-1.815927	-1.233124	.237450
H	-.766561	-1.736022	-1.061724
H	.866192	-2.702336	.617489
H	-.243532	-3.781413	2.456353
H	-1.766771	-2.816303	2.139366
C	2.096976	1.198908	.008631
C	-.069430	2.410643	-.006912
H	3.016092	1.010566	.547762
H	2.358637	1.455004	-1.013846
H	-.713138	3.106767	.514521
H	.023718	2.750842	-1.034147
C	1.299286	2.323539	.650864
H	1.178253	2.121984	1.711587
H	1.828115	3.266880	.551620

Table S8. The Coordinates of Atoms in **2** (RHF/6-31G**)

Total Energy (au): -408.12728

atom	x	y	z
B	.000000	.000000	.000000
O	1.358314	.000000	.000000
O	-.710506	1.157039	.000000
C	-.777683	-1.382418	-.032006
C	-.121260	-2.474462	.768893
C	-.675234	-3.120765	1.776514
H	-1.804581	-1.234643	.287725
H	-.823846	-1.690583	-1.079770
H	.890378	-2.719891	.486103

H	-.142588	-3.885849	2.314123
H	-1.680782	-2.911492	2.102641
C	2.096866	1.199273	.005723
C	-.069372	2.411137	-.009029
H	3.017582	1.013342	.544575
H	2.357841	1.455043	-1.018074
H	-.711566	3.109399	.513102
H	.023313	2.751618	-1.037285
C	1.299788	2.324334	.646771
H	1.180044	2.124266	1.708354
H	1.828668	3.267643	.545245

Table S9. The Coordinates of Atoms at the Transition State for the Reaction of **2** with Formaldehyde (RHF/6-31G*)

Total Energy (au): -521.94222

atoms	x	y	z
B	.000000	.000000	.000000
O	.000000	.000000	1.427443
O	1.248725	.000000	-.640647
O	-.817646	1.241556	-.495090
C	-1.950713	1.434949	.024755
C	-3.173767	-.153105	-.587355
C	-2.280947	-1.028548	-.035731
C	-.967814	-1.283746	-.574098
H	-2.073542	1.323314	1.088094
H	-2.596813	2.146913	-.461434
H	-3.111777	.082058	-1.635526
H	-4.127027	.017138	-.116337
H	-2.479685	-1.380231	.963556
C	.999218	.739089	2.070787
C	2.276813	.747425	-.062694
H	.770406	1.805093	2.022557
H	.998933	.457036	3.117984
H	3.203325	.474799	-.555180
H	2.114507	1.810747	-.241393
H	-.925894	-1.260378	-1.654857
H	-.514552	-2.185626	-.183719
C	2.360716	.484555	1.436409
H	2.645141	-.550501	1.602898
H	3.116199	1.118933	1.894481

Table S10. The Coordinates of Atoms in **2** (MP2/6-31G**)

Total Energy (au): -409.39020

atoms	x	y	z
B	.000000	.000000	.000000
O	1.376700	.000000	.000000
O	-.755970	1.147817	.000000
C	-.731724	-1.397639	.061609
C	-.467787	-2.024189	1.401825
C	-1.388300	-2.201587	2.357775
H	-1.803676	-1.273037	-.093788
H	-.343947	-2.044785	-.729540
H	.559299	-2.315561	1.597505
H	-1.132020	-2.633070	3.314995
H	-2.421936	-1.920791	2.203157
C	2.081308	1.248393	.037398
C	-.096421	2.421504	.028188
H	3.016846	1.069720	.566618
H	2.321963	1.545896	-.986965
H	-.761751	3.110788	.546856
H	.026417	2.775410	-.999034
C	1.250581	2.319558	.718641
C	1.099898	2.049293	1.765466
C	1.768223	3.280276	.689038

Table S11. The Coordinates of Atoms in the Complex for the Reaction of **2** with Formaldehyde (MP2/6-31G**)

Total Energy (au): -523.58483

atoms	x	y	z
B	.000000	.000000	.000000
O	.000000	.000000	2.874248
O	1.377769	.000000	.060140
O	-.752500	1.138220	-.143372
C	-.761107	-1.389092	-.001314
C	.068762	-2.559269	.422359
C	-.231792	-3.382988	1.436599
H	-1.654394	-1.304377	.620826

H	-1.120998	-1.546222	-1.025058
H	.983823	-2.729869	-.136076
H	.407697	-4.214038	1.700447
H	-1.137150	-3.253008	2.015921
C	2.067369	1.259439	.047114
C	-.109362	2.419131	-.118426
H	2.987717	1.122860	.614905
H	2.338421	1.498908	-.985092
H	-.805946	3.114889	.348339
H	.058687	2.745603	-1.148841
C	1.202129	2.354416	.641307
H	.997112	2.118797	1.685504
H	1.717863	3.315544	.593443
C	.819771	-.898262	3.018810
H	.739261	-1.625949	3.839493
H	1.672854	-1.018097	2.342370

Table S12. The Coordinates of Atoms at the Transition State for the Reaction of **2** with Formaldehyde (MP2/6-31G**)

Total Energy (au); -523.57089

atoms	x	y	z
B	.000000	.000000	.000000
O	.000000	.000000	1.434255
O	1.232493	.000000	-.693221
O	-.823695	1.325067	-.493964
C	-1.892287	1.556663	.147600
C	-3.272941	-.126377	-.423172
C	-2.314054	-.971613	.061097
C	-1.032949	-1.177568	-.584415
H	-1.942995	1.340216	1.210687
H	-2.600274	2.260888	-.282182
H	-3.257925	.174687	-1.462770
H	-4.186820	.056592	.126641
H	-2.423226	-1.336517	1.078087
C	1.022092	.795018	2.034411
C	2.254623	.802054	-.112399
H	.775682	1.861848	1.940947
H	1.040378	.551530	3.097807
H	3.186371	.568648	-.629317
H	2.037790	1.865892	-.278714
H	-1.068214	-1.089735	-1.668122
H	-.551605	-2.108937	-.291263

C	2.368685	.533405	1.380122
H	2.646354	-.510177	1.535847
H	3.139247	1.165971	1.828251

Table S13. The Coordinates of Atoms in **3** (RHF/6-31G*)

Total Energy (au): -349.22534

atom	x	y	z
B	.000000	.000000	.000000
O	1.371312	.000000	.000000
N	-.470241	1.325902	.000000
C	-.842211	-1.343114	-.016456
C	-.408356	-2.307221	1.057839
C	-1.168994	-2.753582	2.039009
H	-1.906157	-1.139844	.071143
H	-.692331	-1.810800	-.991076
H	.619480	-2.628760	1.006188
H	-.788547	-3.432283	2.781876
H	-2.200773	-2.460440	2.139514
C	1.848291	1.324793	.114298
C	.637205	2.251491	-.129716
H	2.255859	1.463293	1.109172
H	2.642943	1.481152	-.603244
H	.672098	2.705610	-1.117543
H	.596172	3.053941	.600061
H	-1.404541	1.652490	-.080557

© 1998 American Chemical Society, J. Org. Chem., Omoto jo981190n Supporting Info Page 10

Table S14. The Coordinates of Atoms in **3** (RHF/6-31G**)

Total Energy (au): -349.24437

atom	x	y	z
B	.000000	.000000	.000000
O	1.371339	.000000	.000000
N	-.471119	1.325036	.000000
C	-.840926	-1.342789	-.019138
C	-.394467	-2.318031	1.038981
C	-1.145548	-2.780861	2.019385
H	-1.904030	-1.140545	.081083
H	-.699166	-1.798177	-1.001081
H	.635045	-2.634108	.975872
H	-.754702	-3.467539	2.749792
H	-2.178123	-2.493032	2.130266
C	1.847833	1.325088	.115195
C	.636459	2.250546	-.129055
H	2.254875	1.464885	1.111205
H	2.643416	1.484347	-.602026
H	.672626	2.705040	-1.117463
H	.596168	3.053878	.600734
H	-1.405089	1.648237	-.079164

Table S15 The Coordinates of Atoms at the Transition State for the Reaction of **3** with Formaldehyde (RHF/6-31G*)

Total Energy (au): -463.05154

atoms	x	y	z
B	.000000	.000000	.000000
O	.000000	.000000	1.428515
N	1.417403	.000000	-.418238
O	-.790850	1.248532	-.517671
C	-1.918096	1.466244	-.000336
C	-3.179244	-.112634	-.642148
C	-2.290109	-1.006039	-.116345
C	-.978546	-1.255248	-.657269
H	-2.046601	1.341334	1.060677
H	-2.552324	2.188634	-.486328

H	-3.119875	.151458	-1.683708
H	-4.127724	.056507	-.161408
H	-2.487578	-1.380237	.875192
C	1.324663	.067666	1.891582
C	2.157630	.551348	.701892
H	1.384930	.732917	2.746454
H	1.649507	-.920031	2.208828
H	3.179754	.184573	.749135
H	2.199364	1.642879	.690484
H	-.933863	-1.199911	-1.737759
H	-.530110	-2.170430	-.294707
H	1.656816	.393893	-1.303582

Table S16. The Coordinates of Atoms in **3** (MP2/6-31G**)

Total Energy (au): -350.35669

atom	x	y	z
B	.000000	.000000	.000000
O	1.391077	.000000	.000000
N	-.484241	1.328060	.000000
C	-.812083	-1.350785	.040471
C	-.503986	-2.090133	1.311644
C	-1.392171	-2.352648	2.278012
H	-1.886622	-1.175397	-.040453
H	-.513194	-1.958278	-.819132
H	.528350	-2.397014	1.444060
H	-1.105194	-2.867529	3.183707
H	-2.429753	-2.058551	2.185836
C	1.821140	1.364960	.168992
C	.625510	2.248824	-.217149
H	2.090791	1.513898	1.216828
H	2.699414	1.541877	-.449669
H	.687357	2.573468	-1.260825
H	.567189	3.138644	.412101
H	-1.428891	1.636997	-.148194

Table S17. The Coordinates of Atoms in the Complex for the Reaction of **3** with Formaldehyde (MP2/6-31G**)

Total Energy (au): -464.55098

atom	x	y	z
B	.000000	.000000	.000000
O	.000000	.000000	2.871644
O	1.391675	.000000	.032045
N	-.491466	1.329213	-.047750
C	-.822536	-1.348324	-.074121
C	-.037080	-2.547120	.361148
C	-.378277	-3.361707	1.369246
H	-1.740633	-1.265305	.512275
H	-1.134200	-1.476912	-1.117188
H	.882412	-2.740212	-.182206
H	.233320	-4.210226	1.642827
H	-1.287251	-3.204746	1.936035
C	1.815119	1.376825	-.061999
C	.600465	2.218146	.338862
H	2.677425	1.530711	.584906
H	2.105548	1.577614	-1.095700
H	.581238	3.172767	-.190083
H	.596517	2.410099	1.415766
H	-1.429264	1.596472	.201104
C	.827810	-.894168	2.993304
H	.782421	-1.611402	3.826552
H	1.650753	-1.019088	2.281844

Table S18. The Coordinates of Atoms of **3** at the Transition State for the Reaction of **3** with Formaldehyde (MP2/6-31G**)

Total energy (au): -464.53088

atom	x	y	z
B	.000000	.000000	.000000
O	.000000	.000000	1.436210
N	1.405868	.000000	-.440502
O	-.793285	1.344960	-.509712
C	-1.855237	1.597099	.134442

C	-3.275134	-.052350	-.461719
C	-2.324569	-.928018	-.016607
C	-1.049936	-1.127449	-.674384
H	-1.904217	1.377552	1.197189
H	-2.550955	2.316797	-.289995
H	-3.268860	.280716	-1.491642
H	-4.179758	.126299	.104406
H	-2.426625	-1.322964	.989896
C	1.363210	.133722	1.861686
C	2.123238	.662214	.647897
H	1.416695	.801530	2.723127
H	1.746811	-.847886	2.155081
H	3.181996	.393416	.681444
H	2.052347	1.758596	.612813
H	-1.090529	-.997521	-1.754511
H	-.576985	-2.073753	-.419292
H	1.621368	.365516	-1.357942

Table S19. The Coordinates of Atoms in **4** (RHF/6-31G*)

Total Energy (au): -329.38038

atom	x	y	z
B	.000000	.000000	.000000
N	1.416800	.000000	.000000
N	-.417370	1.358428	.000000
C	-.943262	-1.284979	.029644
C	-.376304	-2.467641	-.709545
C	.091685	-3.573223	-.160601
H	-1.112380	-1.555476	1.071288
H	-1.919238	-1.031758	-.382046
H	-.339300	-2.373314	-1.784881
H	.500522	-4.370139	-.756704
H	.080008	-3.727601	.905516
C	1.926108	1.348127	-.177374
C	.723977	2.234041	.207367
H	2.788467	1.551342	.449457
H	2.219124	1.531808	-1.210004
H	.674518	3.129243	-.404224
H	.802001	2.548968	1.246912
H	-1.323830	1.699878	.223557
H	2.005493	-.773337	-.207914

© 1998 American Chemical Society, J. Org. Chem., Omoto jo981190n Supporting Info Page 14

Table S20. The Coordinates of Atoms in **4** (RHF/6-31G**)

Total Energy (au): -329.40348

atom	x	y	z
B	.000000	.000000	.000000
N	1.415843	.000000	.000000
N	-.419157	1.357134	.000000
C	-.942617	-1.284443	.030872
C	-.362965	-2.478246	-.678688
C	.096113	-3.573943	-.103941
H	-1.131192	-1.536604	1.073975
H	-1.910004	-1.035634	-.403430
H	-.307676	-2.402434	-1.755270
H	.514964	-4.379585	-.681515
H	.066176	-3.709366	.964695
C	1.925284	1.348349	-.172762
C	.721077	2.234139	.205931
H	2.784192	1.552788	.459599
H	2.225091	1.533804	-1.203916
H	.673517	3.127660	-.409480
H	.797182	2.554144	1.244897
H	-1.326896	1.696239	.214738
H	2.004095	-.774728	-.196021

Table S21. The Coordinates of Atoms at the Transition State for the Reaction of **4** with Formaldehyde (RHF/6-31G*)

Total Energy (au): -443.19544

atom	x	y	z
B	.000000	.000000	.000000
N	.000000	.000000	1.499196
N	1.426525	.000000	-.392322
O	-.748891	1.245120	-.580405
C	-1.909853	1.480475	-.154004
C	-3.117569	-.045501	-.926659
C	-2.311618	-.989214	-.349151
C	-.961655	-1.257296	-.752646
H	-2.119582	1.353274	.894681

H	-2.482646	2.230001	-.674368
H	-2.952115	.238347	-1.951201
H	-4.108858	.124735	-.542175
H	-2.636352	-1.396072	.596655
C	1.390814	-.021636	1.941458
C	2.168997	.522297	.741990
H	1.550559	.579326	2.833405
H	1.728357	-1.033965	2.163553
H	3.203216	.187774	.748978
H	2.177759	1.614192	.774586
H	-.796286	-1.174254	-1.818606
H	-.560705	-2.184358	-.365933
H	1.669924	.429188	-1.261160
H	-.548818	-.686232	1.972691

Table S22. The Coordinates of Atoms in **4** (MP2/6-31G**)

Total Energy (au): -330.51115

atoms	x	y	z
B	.000000	.000000	.000000
N	1.423784	.000000	.000000
N	-.419762	1.364530	.000000
C	-.911721	-1.297754	.014837
C	-.308412	-2.395977	-.808523
C	.335786	-3.461515	-.314109
H	-1.016599	-1.633979	1.050791
H	-1.915906	-1.058906	-.343798
H	-.367196	-2.277539	-1.886913
H	.784798	-4.202651	-.960083
H	.418368	-3.622169	.753186
C	1.910777	1.357802	-.227233
C	.737339	2.220433	.259155
H	2.826856	1.576810	.324151
H	2.100578	1.546245	-1.290271
H	.685485	3.171058	-.274497
H	.848885	2.435670	1.328145
H	-1.326127	1.693586	.288172
H	1.992532	-.779038	-.287968

© 1998 American Chemical Society, J. Org. Chem., Omoto jo981190n Supporting Info Page 16

Table S23. The Coordinates of Atoms in the Complex for the Reaction of **4** with Formaldehyde (MP2/6-31G**)

Total Energy (au): -444.70270

atom	x	y	z
B	.000000	.000000	.000000
O	.000000	.000000	3.027155
N	1.421821	.000000	-.161254
N	-.418090	1.363509	.071427
C	-.942808	-1.274957	.044996
C	-.215159	-2.548721	.345268
C	-.412727	-3.314858	1.427129
H	-1.735755	-1.120083	.780675
H	-1.437634	-1.356139	-.929348
H	.537236	-2.859944	-.375327
H	.154866	-4.219890	1.592997
H	-1.162039	-3.058349	2.165022
C	1.871204	1.372993	-.394281
C	.768289	2.193594	.280815
H	2.852466	1.573975	.039160
H	1.914333	1.607794	-1.463976
H	.673366	3.186894	-.161314
H	.987858	2.304806	1.348373
H	-1.252426	1.641846	.563634
H	1.957792	-.747290	-.571454
C	.875676	-.853887	3.071108
H	.926890	-1.586255	3.891778
H	1.646551	-.927638	2.296132

Table S24. The Coordinates of Atoms at the Transition State for the Reaction of **4** with Formaldehyde (MP2/6-31G**)

Total Energy (au): -444.67715

atom	x	y	z
B	.000000	.000000	.000000
N	.000000	.000000	1.491287
N	1.420112	.000000	-.405587
O	-.750468	1.336845	-.559009

C	-1.853023	1.602851	.008473
C	-3.220297	.013926	-.724578
C	-2.343858	-.921320	-.241666
C	-1.019368	-1.125139	-.777499
H	-1.969791	1.381149	1.066854
H	-2.492739	2.352386	-.450538
H	-3.116402	.378466	-1.738163
H	-4.172196	.187173	-.240184
H	-2.572162	-1.367756	.723552
C	1.404878	-.020876	1.920721
C	2.140928	.581774	.727348
H	1.571814	.554247	2.835432
H	1.769275	-1.040734	2.090700
H	3.201597	.318704	.728787
H	2.065354	1.677895	.771392
H	-.950933	-.960376	-1.851034
H	-.572861	-2.079341	-.506363
H	1.653865	.428268	-1.292324
H	-.548376	-.708901	1.958281

Table S25. The Coordinates of Atoms in **5** (RHF/6-31G*)

Total Energy (au): -292.17447

atom	x	y	z
B	.000000	.000000	.000000
O	1.362640	.000000	.000000
O	-.737029	1.144847	.000000
C	-.759724	-1.391360	-.040083
C	-.128576	-2.455142	.819237
C	-.719332	-3.072996	1.824101
H	-1.802078	-1.252114	.227970
H	-.751201	-1.725750	-1.080241
H	.893711	-2.702975	.583199
H	-.206481	-3.818198	2.406368
H	-1.737390	-2.860368	2.104717
H	1.784578	.846530	.019248
H	-.250352	1.956363	-.004779

Table S26. The Coordinates of Atoms in **5** (RHF/6-31G**)

Total Energy (au): -292.19747

atom	x	y	z
B	.000000	.000000	.000000
O	1.361163	.000000	.000000
O	-.737516	1.143232	.000000
C	-.763079	-1.388660	-.045285
C	-.088496	-2.490815	.726183
C	-.627754	-3.162374	1.725029
H	-1.787703	-1.257213	.288161
H	-.818840	-1.675222	-1.098724
H	.922182	-2.721992	.428482
H	-.083906	-3.934191	2.241229
H	-1.631628	-2.967928	2.065072
H	1.788335	.839174	.016981
H	-.261038	1.955837	-.005947

Table S27. The Coordinates of Atoms at the Transition State for the Reaction of **5** with Formaldehyde (RHF/6-31G*)

Total Energy (au): -406.00956

atom	x	y	z
B	.000000	.000000	.000000
O	.000000	.000000	1.434505
O	1.253412	.000000	-.638312
O	-.833435	1.224216	-.414512
C	-1.950417	1.388460	.143852
C	-3.184952	-.193757	-.572189
C	-2.266877	-1.086383	-.099686
C	-.954187	-1.276222	-.666106
H	-2.053790	1.198645	1.196806
H	-2.610541	2.120513	-.289599
H	-3.139390	.130226	-1.597324
H	-4.132744	-.074470	-.075343
H	-2.448618	-1.513513	.873315
H	.694813	-.549020	1.765451
H	1.811086	.680721	-.288237

H	-.922400	-1.177644	-1.742895
H	-.485029	-2.200502	-.350306

Table S28. The Coordinates of Atoms in **5** (MP2/6-31G**)

Total Energy (au): -293.05200

atoms	x	y	z
B	.000000	.000000	.000000
O	1.378389	.000000	.000000
O	-.777411	1.135344	.000000
C	-.719378	-1.403467	.039070
C	-.438175	-2.070128	1.356768
C	-1.352834	-2.296882	2.307489
H	-1.793644	-1.285403	-.102192
H	-.335599	-2.024955	-.774423
H	.593982	-2.351566	1.539049
H	-1.086589	-2.758481	3.247668
H	-2.391246	-2.027342	2.165824
H	1.778307	.876063	.019820
H	-.276865	1.958681	.010248

Table S29. The Coordinates of Atoms in the Complex for the Reaction of **5** with Formaldehyde (MP2/6-31G**)

Total Energy (au): -407.24521

atom	x	y	z
B	.000000	.000000	.000000
O	.000000	.000000	2.753179
O	1.382048	.000000	.018443
O	-.776700	1.126397	-.134741
C	-.747140	-1.394815	-.014202

C	.088974	-2.565872	.394928
C	-.199230	-3.393700	1.409069
H	-1.641075	-1.324317	.608009
H	-1.104976	-1.541924	-1.040117
H	.998211	-2.733017	-.173935
H	.444205	-4.224880	1.662366
H	-1.097937	-3.266814	1.999285
H	1.767180	.882819	-.003097
H	-.286496	1.953481	-.085224
C	.840629	-.857444	2.991479
C	.772631	-1.499825	3.881648
C	1.701605	-1.021708	2.335032

Table S30. The Coordinates of Atoms at the Transition State for the Reaction of **5** with Formaldehyde (MP2/6-31G**)

Total Energy (au): -407.23104

atoms	x	y	z
B	.000000	.000000	.000000
O	.000000	.000000	1.443342
O	1.244327	.000000	-.673723
O	-.823602	1.333043	-.373451
C	-1.873423	1.539051	.295582
C	-3.310645	-.145609	-.479943
C	-2.331531	-1.000807	-.071082
C	-1.032787	-1.115780	-.716073
H	-1.939864	1.211164	1.326940
H	-2.580469	2.273603	-.080870
H	-3.283258	.283865	-1.473235
H	-4.231969	-.037714	.076959
H	-2.446900	-1.472302	.900620
H	.659406	-.626197	1.755793
H	1.860091	.572850	-.202965
H	-1.065914	-.923159	-1.786701
H	-.559383	-2.080448	-.532382

Table S31. The Coordinates of Atoms in **6** (RHF/6-31G*)

Total Energy (au): -520.55404

atoms	x	y	z
B	.000000	.000000	.000000
O	1.376486	.000000	.000000
O	-.481613	1.288746	.000000
C	-.898637	-1.291290	-.035745
C	-.321019	-2.449519	.737399
C	-.902115	-3.042292	1.761819
H	-1.896162	-1.051702	.319030
H	-1.008079	-1.577476	-1.083917
H	.648675	-2.792912	.414783
H	-.432211	-3.860707	2.277573
H	-1.868277	-2.735447	2.125648
C	1.751045	1.310511	.000264
C	.614908	2.098483	-.000645
C	3.010432	1.850221	.001025
C	3.093304	3.243106	.000485
C	.679248	3.467141	-.000822
C	1.954805	4.032790	-.000485
H	3.885809	1.228488	.002351
H	4.061063	3.710575	.000977
H	-.209775	4.069215	-.001123
H	2.053609	5.102988	-.000699

Table S32. The Coordinates of Atoms in **6** (RHF/6-31G**)

Total Energy (au): -520.57013

atom	x	y	z
B	.000000	.000000	.000000
O	1.376391	.000000	.000000
O	-.481492	1.289048	.000000
C	-.900845	-1.288073	-.039754
C	-.294869	-2.477138	.659572
C	-.839293	-3.117861	1.674705
H	-1.880945	-1.058379	.367034
H	-1.057989	-1.530359	-1.093330

© 1998 American Chemical Society, J. Org. Chem., Omoto jo981190n Supporting Info Page 22

H	.664245	-2.803059	.288789
H	-.349200	-3.957626	2.134914
H	-1.793082	-2.829644	2.084595
C	1.751105	1.310491	-.000378
C	.615096	2.098594	-.001236
C	3.010528	1.849742	-.000044
C	3.093248	3.242418	-.001025
C	.679499	3.467122	-.001791
C	1.955111	4.032105	-.001943
H	3.885832	1.227524	.001299
H	4.061204	3.710220	-.000909
H	-.209724	4.069297	-.002033
H	2.054502	5.102575	-.002514

Table S33. The Coordinates of Atoms at the Transition State for the Reaction of **6** with Formaldehyde (RHF/6-31G*)

Total Energy (au): -634.39422

atoms	x	y	z
B	.000000	.000000	.000000
O	.000000	.000000	1.451603
O	1.363369	.000000	-.424983
O	-.720910	1.239249	-.520995
C	-1.873576	1.473250	-.061220
C	-3.120279	-.074712	-.788063
C	-2.285902	-.976740	-.194990
C	-.940847	-1.254288	-.650711
H	-2.060046	1.350975	.991295
H	-2.462462	2.211080	-.577717
H	-2.980126	.186252	-1.822495
H	-4.095663	.116481	-.374619
H	-2.559531	-1.343529	.781316
C	1.295285	.134122	1.820036
C	2.111052	.132286	.691150
H	-.834306	-1.222917	-1.727521
H	-.540202	-2.176409	-.249401
C	1.815460	.247332	3.080246
C	3.471047	.243938	.794776
C	3.206957	.363254	3.197670
C	4.015186	.361493	2.080428
H	1.176632	.245513	3.944486
H	4.092394	.241454	-.081694
H	3.646248	.454214	4.175009

H	5.080872	.451774	2.192897

Table S34. The Coordinates of Atoms in **7** (RHF/6-31G*)

Total Energy (au): -388.25481

atoms	x	y	z
B	.000000	.000000	.000000
O	1.371667	.000000	.000000
N	-.483823	1.322132	.000000
C	-.809181	-1.365257	-.017377
C	-.347438	-2.310261	1.062864
C	-1.098680	-2.781892	2.039513
H	-1.880579	-1.208327	.061563
H	-.633539	-1.830314	-.988996
H	.691757	-2.593710	1.019500
H	-.699284	-3.444620	2.786856
H	-2.141319	-2.526761	2.131777
C	1.852201	1.322856	.099049
C	.630046	2.244360	-.087564
H	2.306824	1.457863	1.073598
H	2.612657	1.483776	-.654025
H	.644932	2.753386	-1.050543
H	.579739	3.011083	.681806
C	-1.818111	1.847030	-.071461
H	-2.011284	2.543330	.741442
H	-2.538894	1.043877	-.001757
H	-1.990410	2.375575	-1.007590

Table S35. The Coordinates of Atoms in **7** (RHF/6-31G**)

Total Energy (au): -388.27427

atom	x	y	z
B	.000000	.000000	.000000
O	1.371781	.000000	.000000
N	-.483301	1.322271	.000000
C	-.809467	-1.363947	-.022005
C	-.323705	-2.330861	1.026879
C	-1.054629	-2.828700	2.005431
H	-1.878579	-1.207142	.083837
H	-.655284	-1.807781	-1.007513
H	.716323	-2.608352	.958208
H	-.636848	-3.506809	2.728878
H	-2.096667	-2.579597	2.121660
C	1.852397	1.323052	.100323
C	.631056	2.244167	-.088442
H	2.305336	1.459636	1.076531
H	2.614905	1.486243	-.651462
H	.647461	2.752094	-1.052841
H	.581642	3.012840	.679960
C	-1.817867	1.846851	-.071108
H	-2.012001	2.543299	.742111
H	-2.539211	1.043744	-.001552
H	-1.991352	2.375830	-1.007372

Table S36. The Coordinates of Atoms at the Transition State for the Reaction of **7** with Formaldehyde (RHF/6-31G*)

Total Energy (au): -502.08082

atom	x	y	z
B	.000000	.000000	.000000
O	.000000	.000000	1.427449
N	1.414327	.000000	-.424042
O	-.788587	1.248397	-.517177
C	-1.912802	1.472137	.003841
C	-3.180915	-.102907	-.629470
C	-2.294275	-.998965	-.104206

C	-.986287	-1.256654	-.650596
H	-2.037926	1.351165	1.065710
H	-2.545757	2.195617	-.482197
H	-3.123264	.158385	-1.671835
H	-4.127259	.071674	-.146505
H	-2.489798	-1.369642	.888962
C	1.324881	.049515	1.891564
C	2.163244	.513868	.700424
H	1.394132	.718838	2.742487
H	1.634081	-.940882	2.215629
H	3.177936	.122144	.734982
H	2.236773	1.606355	.682770
H	-.951453	-1.210894	-1.731771
H	-.541676	-2.172251	-.284137
C	1.844716	.439312	-1.721783
H	2.866590	.121791	-1.918037
H	1.807848	1.525241	-1.841929
H	1.216162	.003146	-2.490764

Table S37. The Coordinates of Atoms in **8** (RHF/6-31G*)

Total Energy (au): -935.42657

atom	x	y	z
B	.000000	.000000	.000000
O	1.355525	.000000	.000000
N	-.447579	1.385680	.000000
C	-.860556	-1.321869	-.048619
C	-.041954	-2.579834	.081041
C	-.223503	-3.506848	1.000929
H	-1.635839	-1.286758	.707681
H	-1.395151	-1.330059	-1.001059
H	.749886	-2.709770	-.639075
H	.395691	-4.385353	1.044326
H	-.995641	-3.425240	1.747352
C	1.882983	1.304946	-.096518
C	.716290	2.268003	.172895
H	2.683217	1.418997	.620791
H	2.290629	1.440632	-1.090936
H	.703826	3.095043	-.525749
H	.732607	2.673332	1.174558
S	-1.957273	2.005269	.122656
O	-1.877749	3.185040	.928010
O	-2.848451	.945424	.473992

C	-2.356426	2.513937	-1.526465
H	-3.341098	2.960286	-1.492656
H	-2.362569	1.648307	-2.172876
H	-1.635349	3.244215	-1.865173

Table S38. The Coordinates of Atoms in **8** (RHF/6-31G**)

Total Energy (au): -935.44672

atom	x	y	z
B	.000000	.000000	.000000
O	1.355648	.000000	.000000
N	-.447379	1.385754	.000000
C	-.859873	-1.320669	-.049283
C	-.044484	-2.578213	.097018
C	-.241413	-3.502177	1.016281
H	-1.645508	-1.277723	.695842
H	-1.380272	-1.332045	-1.009918
H	.759396	-2.711118	-.609984
H	.377468	-4.380635	1.070662
H	-1.025913	-3.416494	1.749760
C	1.883136	1.305233	-.096879
C	.716946	2.267977	.172862
H	2.684132	1.421431	.620557
H	2.290853	1.442372	-1.092141
H	.705986	3.095781	-.525829
H	.733506	2.673610	1.175136
S	-1.956752	2.005412	.126388
O	-1.875218	3.184035	.933489
O	-2.847443	.945321	.478939
C	-2.360758	2.516118	-1.519505
H	-3.345370	2.962366	-1.479668
H	-2.369076	1.650358	-2.165992
H	-1.640010	3.246958	-1.858234

Table S39. The Coordinates of Atoms at the Transition State for the Reaction of **8** with Formaldehyde (RHF/6-31G*)

Total Energy (au): -1049.26745

atoms	x	y	z
B	.000000	.000000	.000000
O	.000000	.000000	1.428307
N	1.480394	.000000	-.365153
O	-.706206	1.246683	-.519134
C	-1.862872	1.485159	-.073600
C	-3.106908	-.042560	-.834485
C	-2.294049	-.948956	-.219850
C	-.945046	-1.246988	-.656615
H	-2.064710	1.355451	.975310
H	-2.436984	2.233931	-.591215
H	-2.936983	.217547	-1.864510
H	-4.088541	.161357	-.442071
H	-2.591689	-1.308446	.752184
C	1.301629	.000875	1.942243
C	2.211315	.477041	.810189
H	1.358437	.649103	2.809075
H	1.574293	-1.004267	2.253158
H	3.204334	.046946	.879111
H	2.309569	1.556239	.796329
H	-.829161	-1.230072	-1.730488
H	-.569471	-2.171076	-.233762
S	2.108481	.250040	-1.835770
C	3.254994	-1.085994	-2.047888
O	2.882284	1.459289	-1.849024
O	1.066026	.065410	-2.804065
H	3.716585	-.962002	-3.018204
H	2.716654	-2.021480	-2.005387
H	4.012485	-1.044792	-1.278025

© 1998 American Chemical Society, J. Org. Chem., Omoto jo981190n Supporting Info Page 28

Table S40. The Coordinates of Atoms in **9** (RHF/6-31G*)

Total Energy (au): -1231.98403

atoms	x	y	z
B	.000000	.000000	.000000
O	1.352623	.000000	.000000
N	-.440328	1.398463	.000000
C	-.839909	-1.331354	.007185
C	-.658231	-2.037363	1.333644
C	-1.582049	-2.130922	2.270228
H	-1.890062	-1.159115	-.181983
H	-.457299	-1.966336	-.790538
H	.315423	-2.466934	1.506940
H	-1.386260	-2.636110	3.199451
H	-2.562995	-1.706473	2.145547
C	1.883093	1.298131	.170445
C	.740118	2.275631	-.137314
H	2.227277	1.400308	1.191687
H	2.724289	1.427703	-.494798
H	.801124	2.668999	-1.143444
H	.693574	3.098183	.558417
S	-1.930686	2.012991	.079855
O	-1.853386	3.363859	.516528
O	-2.811003	1.074056	.680324
C	-2.431670	2.094587	-1.667470
F	-3.637065	2.586256	-1.756751
F	-2.411347	.894318	-2.195920
F	-1.600524	2.860314	-2.335922

Table S41. The Coordinates of Atoms in **9** (RHF/6-31G**)

Total Energy (au): -1231.99905

atom	x	y	z
B	.000000	.000000	.000000
O	1.352708	.000000	.000000
N	-.439766	1.398677	.000000
C	-.840864	-1.329597	.004810
C	-.647442	-2.048629	1.321923

C	-1.564654	-2.155438	2.263085
H	-1.892236	-1.152128	-.172638
H	-.465164	-1.956016	-.803293
H	.329090	-2.477103	1.484866
H	-1.359429	-2.670190	3.185324
H	-2.547780	-1.732326	2.147750
C	1.883031	1.298380	.171562
C	.741261	2.275221	-.139259
H	2.224728	1.402119	1.194506
H	2.726559	1.429690	-.491765
H	.803289	2.665560	-1.147270
H	.694970	3.100458	.554229
S	-1.929179	2.014385	.083454
O	-1.850029	3.364009	.523814
O	-2.810157	1.074900	.682245
C	-2.431878	2.101571	-1.663056
F	-3.635655	2.597532	-1.750379
F	-2.416008	.902429	-2.194140
F	-1.598561	2.865965	-2.330470

Table S42. The Coordinates of Atoms at the Transition State for the Reaction of **9** with Formaldehyde (RHF/6-31G*)

Total Energy (au): -1345.82981

atom	x	y	z
B	.000000	.000000	.000000
O	.000000	.000000	1.425340
N	1.491352	.000000	-.354382
O	-.680783	1.253892	-.522937
C	-1.839864	1.502076	-.086503
C	-3.095673	-.014584	-.870679
C	-2.295115	-.923554	-.246312
C	-.941862	-1.233505	-.671073
H	-2.053088	1.368932	.959489
H	-2.402756	2.256536	-.607751
H	-2.911147	.248073	-1.897569
H	-4.079277	.198109	-.488332
H	-2.605205	-1.282093	.722046
C	1.296207	-.074183	1.950207
C	2.240662	.397990	.845281
H	1.370757	.542741	2.837551
H	1.521856	-1.099692	2.228865
H	3.209173	-.078025	.896329

H	2.381048	1.471841	.864504
H	-.824598	-1.221311	-1.745464
H	-.583146	-2.166270	-.253527
S	2.162753	.054419	-1.795443
C	2.867672	-1.611627	-1.980312
O	3.292828	.924104	-1.800765
O	1.160763	.129549	-2.806552
F	3.485182	-1.711300	-3.129903
F	1.919163	-2.518850	-1.928016
F	3.726975	-1.855465	-1.014416

Table S43. The Coordinates of Atoms in **10** (RHF/6-31G*)

Total Energy (au): -744.29603

atoms	x	y	z
B	.000000	.000000	.000000
O	1.365626	.000000	.000000
O	-.502865	1.265693	.000000
C	-.879882	-1.305831	-.026777
C	-.330532	-2.411931	.838254
C	-.956340	-2.952650	1.865334
H	-1.899953	-1.066885	.255936
H	-.918130	-1.646331	-1.063507
H	.657754	-2.759888	.584411
H	-.504826	-3.734474	2.449760
H	-1.942906	-2.638518	2.162016
C	1.833333	1.327265	.001335
C	.553169	2.188939	-.007606
H	2.434656	1.500320	.881737
C	2.715620	1.548184	-1.217283
H	.498439	2.795191	-.902072
C	.485544	3.144723	1.167939
O	3.776333	.762466	-1.193705
O	2.497930	2.330927	-2.082871
H	4.294975	.926039	-1.976065
O	-.746934	3.471376	1.501019
O	1.451783	3.594295	1.694209
H	-.707555	4.104429	2.212135

Table S44. The Coordinates of Atoms in **10** (RHF/6-31G**)

Total Energy (au): -744.32144

atom	x	y	z
B	.000000	.000000	.000000
O	1.365156	.000000	.000000
O	-.502988	1.266136	.000000
C	-.882712	-1.302348	-.033399
C	-.300407	-2.445962	.756379
C	-.888659	-3.039621	1.775875
H	-1.888023	-1.070919	.304032
H	-.970119	-1.596282	-1.081827
H	.680017	-2.777050	.452023
H	-.413521	-3.847443	2.304000
H	-1.865469	-2.743681	2.120981
C	1.832661	1.326811	-.004829
C	.553841	2.189372	.000590
H	2.443609	1.504772	.869655
C	2.705402	1.557645	-1.227777
H	.499078	2.810383	-.884862
C	.486050	3.126540	1.191543
O	3.720736	.716959	-1.266683
O	2.519419	2.400717	-2.043206
H	4.238106	.896919	-2.040991
O	-.744178	3.482585	1.497967
O	1.450072	3.538374	1.751835
H	-.710193	4.097406	2.219543

Table S45. The Coordinates of Atoms at the Transition State for the Reaction of **10** with Formaldehyde (RHF/6-31G*)

Total Energy (au): -858.13799

atom	x	y	z
B	.000000	.000000	.000000
O	.000000	.000000	1.437751
O	1.353819	.000000	-.423988
O	-.736382	1.241508	-.507629
C	-1.883225	1.461921	-.025693

C	-3.124442	-.092826	-.741840
C	-2.268405	-.994669	-.179175
C	-.930784	-1.252105	-.666491
H	-2.049319	1.329250	1.028713
H	-2.487551	2.198904	-.525491
H	-3.010619	.180852	-1.776246
H	-4.092735	.082103	-.305046
H	-2.513885	-1.376587	.798587
C	1.307339	.019210	1.893498
C	2.150256	.377308	.654094
H	1.433402	.752495	2.678412
C	1.761055	-1.309180	2.477312
H	3.093289	-.151922	.624053
C	2.461726	1.868202	.581672
H	-.844545	-1.201953	-1.744366
H	-.513973	-2.174273	-.283153
O	.822842	-2.239951	2.549306
O	2.874770	-1.490012	2.856294
H	1.219371	-3.011950	2.942128
O	3.124657	2.171912	-.523215
O	2.173221	2.679112	1.402048
H	3.280718	3.111156	-.527693

Table S46. The Coordinates of Atoms in **11** (RHF/6-31G*)

Total Energy (au): -340.19210

atom	x	y	z
B	.000000	.000000	.000000
F	1.312765	.000000	.000000
F	-.584280	1.175927	.000000
C	-.840363	-1.330792	-.044195
C	-.110419	-2.545034	.466867
C	-.507008	-3.297912	1.473633
H	-1.776329	-1.186810	.487548
H	-1.117805	-1.484512	-1.090443
H	.809151	-2.790344	-.039479
H	.064153	-4.149799	1.796487
H	-1.416061	-3.095281	2.014456

Table S47. The Coordinates of Atoms in **11** (RHF/6-31G**)

Total Energy (au): -340.20101

atom	x	y	z
B	.000000	.000000	.000000
F	1.312718	.000000	.000000
F	-.584193	1.176215	.000000
C	-.842651	-1.327463	-.045291
C	-.105961	-2.554464	.421392
C	-.482965	-3.329328	1.418474
H	-1.764260	-1.188459	.512649
H	-1.147256	-1.456161	-1.087586
H	.801949	-2.791631	-.110547
H	.093394	-4.190156	1.707535
H	-1.379652	-3.135321	1.983317

Table S48. The Coordinates of Atoms at the Transition State for The Reaction of **11** with Formaldehyde (RHF/6-31G*)

Total Energy (au): -454.04878

atom	x	y	z
B	.000000	.000000	.000000
F	.000000	.000000	1.376283
F	1.234000	.000000	-.548300
O	-.745945	1.235560	-.471687
C	-1.866919	1.472526	.056422
C	-3.160643	-.084815	-.600917
C	-2.292843	-.985678	-.057047
C	-.975640	-1.263931	-.588329
H	-1.995107	1.345228	1.116392
H	-2.486196	2.209420	-.424120
H	-3.078580	.179337	-1.640838
H	-4.110888	.106138	-.132448
H	-2.511492	-1.351305	.933487
H	-.933407	-1.242535	-1.669623
H	-.553171	-2.185293	-.205969

Table S49. The Coordinates of Atoms in **11** (MP2/6-31G**)

Total Energy (au): -341.02657

atom	x	y	z
B	.000000	.000000	.000000
F	1.334307	.000000	.000000
F	-.597577	1.192096	.000000
C	-.815118	-1.339500	-.033946
C	-.121260	-2.466709	.675059
C	-.628720	-3.120642	1.725511
H	-1.814288	-1.178815	.372346
H	-.952613	-1.594426	-1.091949
H	.861016	-2.738606	.304909
H	-.082118	-3.916311	2.210284
H	-1.603678	-2.875926	2.126196

Table S50. The Coordinates of Atoms in the Complex for the Reaction of **11** with Formaldehyde (MP2/6-31G**)

Total Energy (au): -455.22605

atom	x	y	z
B	.000000	.000000	.000000
O	.000000	.000000	1.770888
F	1.349390	.000000	-.281326
F	-.643418	1.165295	-.277524
C	-.776553	-1.380681	-.253758
C	.021565	-2.557403	.194654
C	-.197192	-3.252590	1.324439
H	-1.749284	-1.357995	.239910
H	-.963282	-1.441764	-1.329591
H	.883997	-2.816530	-.412231
H	.438254	-4.077772	1.614744
H	-1.055107	-3.045504	1.952291
C	.904667	-.650002	2.307758
H	.835002	-.877832	3.370873
H	1.780243	-.961331	1.744968

Table S51. The Coordinates of Atoms at the Transition State for the Reaction of **11** with Formaldehyde (MP2/6-31G**)

Total Energy (au): -455.22498

atom	x	y	z
B	.000000	.000000	.000000
F	.000000	.000000	1.388719
F	1.242706	.000000	-.569424
O	-.716423	1.347188	-.461241
C	-1.758911	1.648779	.182965
C	-3.286329	-.004853	-.498947
C	-2.359625	-.878159	-.014446
C	-1.059634	-1.109570	-.635032
H	-1.851123	1.387787	1.231243
H	-2.421897	2.395680	-.242613
H	-3.221656	.354269	-1.518198
H	-4.207258	.190320	.034106
H	-2.513235	-1.279618	.983056
H	-1.081704	-1.002190	-1.717821
H	-.643738	-2.081949	-.371139

Table S52. The Coordinates of Atoms in Formaldehyde (RHF/6-31G*)

Total Energy (au): -113.86633

atoms	x	y	z
C	.000000	.000000	.000000
O	.000000	.000000	1.184333
H	.923971	.000000	-.581569
H	-.923950	.000000	-.581617

Table S53. The Coordinates of Atoms in Formaldehyde (MP2/6-31G**)

Total Energy (au): -114.18350

atom	x	y	z
C	.000000	.000000	.000000
O	.000000	.000000	1.220381
H	.930707	.000000	-.586870
H	-.930740	.000000	-.586804