Supporting Information

A Unified Mechanistic View on the Morita–Baylis–Hillman Reaction: Computational and Experimental Investigations

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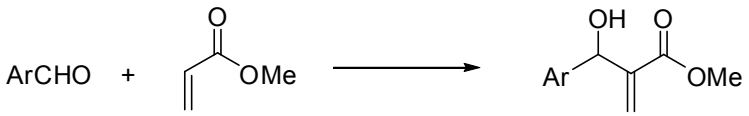
Contents:

Equilibrium Constant Measurement Details

a) Benzaldehyde



Initial concentrations:	C mol/L	C mol/L	0 mol/L
Equilibrium concentrations:	C - X mol/L	C - X mol/L	X mol/L

$$\frac{X}{C - X} = \frac{\%\ \text{MBH adduct}}{\%\ \text{PhCHO}} \qquad K_{eq} = \frac{X}{(C - X)^2}$$

PhCHO total volume = 5.4 mL C= 5/5.4 M
4-NO_2PhCHO total volume = 5.5 mL C=5/5.5 M

T (° C, K)	% PhCHO	% MBH adduct	% Conversion	x	K_{eq}	ΔG	time (h)[a]
21, 294	12.49	51.28	80.41	0.74455	22.64	-1.83	168
30, 303	17.79	43.41	70.93	0.65675	9.07	-1.33	168
40, 313	30.62	52.31	63.08	0.58403	5.00	-1.00	94
50, 323	29.60	33.11	52.80	0.48886	2.56	-0.60	94
60, 333	30.53	24.01	44.02	0.40761	1.52	-0.28	32
70, 343	38.64	16.52	29.95	0.27730	0.659	0.28	18
80, 353	43.23	10.79	19.97	0.18494	0.337	0.76	8
80, 353[b]	42.96	10.34	19.49	0.17962	0.3225	0.79	8
90, 363	44.66	8.67	16.26	0.15053	0.250	1.00	6
90, 363[b]	45.12	9.23	16.98	0.15724	0.266	0.96	6

[a] GC-FID, the reaction mixtures were sampled until full conversion was achieved. [b] Experiment performed under **microwave irradiation**.

b) 4-Nitrobenzaldehyde

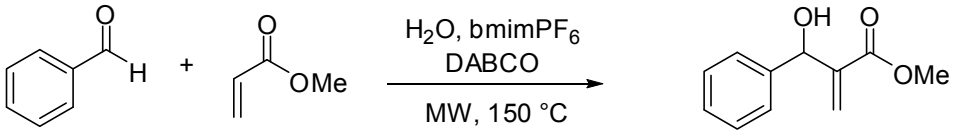
T (° C, K)	% NO2PhCHO[a]	% MBH Adduct[a]	% Conversion	x	K_{eq}	ΔG
19, 292	1.31	53.32	97.60	0.88730	1867.10	-4.38
30, 303	2.09	53.18	96.22	0.87472	740.17	-3.98
40, 313	4.54	51.21	91.86	0.83507	152.36	-3.13
50, 323	7.23	51.44	87.68	0.79707	63.51	-2.67
60, 333	8.60	46.51	84.39	0.76723	38.12	-2.41
70, 343	11.00	36.55	76.87	0.69879	15.80	-1.88
80, 353	13.29	25.96	66.14	0.60128	6.35	-1.30
90, 363	13.70	16.86	55.17	0.50155	3.02	-0.80

[a] GC-FID. In this case the reaction is fast in comparison with the benzaldehyde, but all the reactions were heated for 6 h to assure a correct equilibrium of the temperature .

Attempts to Reproduce Previously Published Experiments Describing Microwave-Assisted MBH Reactions

A publication by De Souza and coworkers[S1] describes microwave-assisted MBH reactions performed in a water/ionic liquid mixture. The article claims that equimolar amounts of benzaldehyde and methyl acrylate react with DABCO (2 equiv) in a water/bmimPF_6 mixture within 60 min at 100 or 150 °C to provide a 58% conversion to product **6a**. Since both bmimPF_6 as well as DABCO are rather unstable in superheated water these results appear to be rather unusual. Following the published experimental protocol as close as possible we have attempted to reproduce these transformations. In our hands, no trace of product **6a** was observable at either 100 °C or 150 °C by GC-FID analysis. Also, GC-FID monitoring revealed that DABCO had been completely decomposed under these conditions.

Based on the calculations and experiments described in this manuscript, we therefore strongly believe that previous reports on successful microwave-assisted MBH reactions are erroneous.[S2]



4a **2** **6a**

Experimental:[S1] To a solution of methyl acrylate (0.6 mmol), DABCO (2 equiv) and [bmim][PF_6] (0.1 mL) in water (5 mL) was added benzaldehyde (0.6 mmol). After microwave heating (Monowave 300, sealed vessel, internal temperature probe) for 60 min at either 100 °C or 150 °C the crude mixture was extracted with ethyl acetate (3 x 30 mL), and the organic phase dried with Na_2SO_4 and analyzed by GC-FID.

S1 De Souza, R. O. M. A.; De Souza, A. L. F.; Fernandez, T. L.; Silva, A. C.; Pereira, L. P.; Esteves, P. M.; Vasconcellos, M. L. A. A.; Antunes, O. A. C. *Lett. Org. Chem.* **2008**, *5*, 379-382.

S2 For a review on microwave-assisted MBH reactions, see: De Souza, R. O. M. A.; Miranda, L. S. M. *Mini Rev. Org. Chem.* **2010**, *7*, 212-220.

Complete Reference 16

Gaussian 09, Revision A.1, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

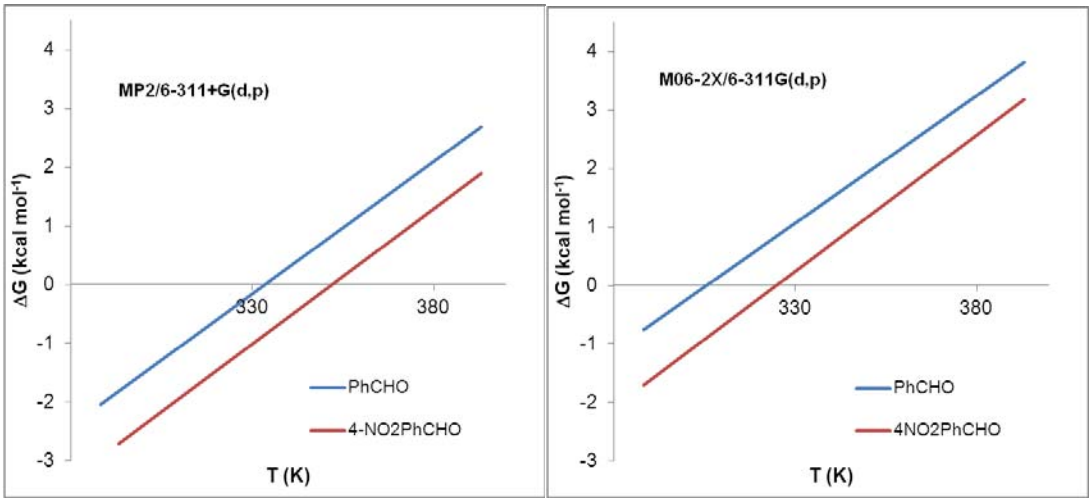


Figure S1. Free energy of reaction *vs* temperature for the MBH reactions of benzaldehyde (blue) and 4-nitrobenzaldehyde (red) with methyl acrylate calculated at the MP2/6-311+G(d,p) and M06-2X/6-311G(d,p) levels. Although the enthalpy of reaction is slightly overestimated by the DFT method, the deviation is only ~1 kcal mol^{-1}, and most importantly, this displacement is equally observed in the case of 4-nitrobenzaldehyde. Therefore, the effect of the nitro group in the thermodynamics is correctly modeled by the M06-2X approach.

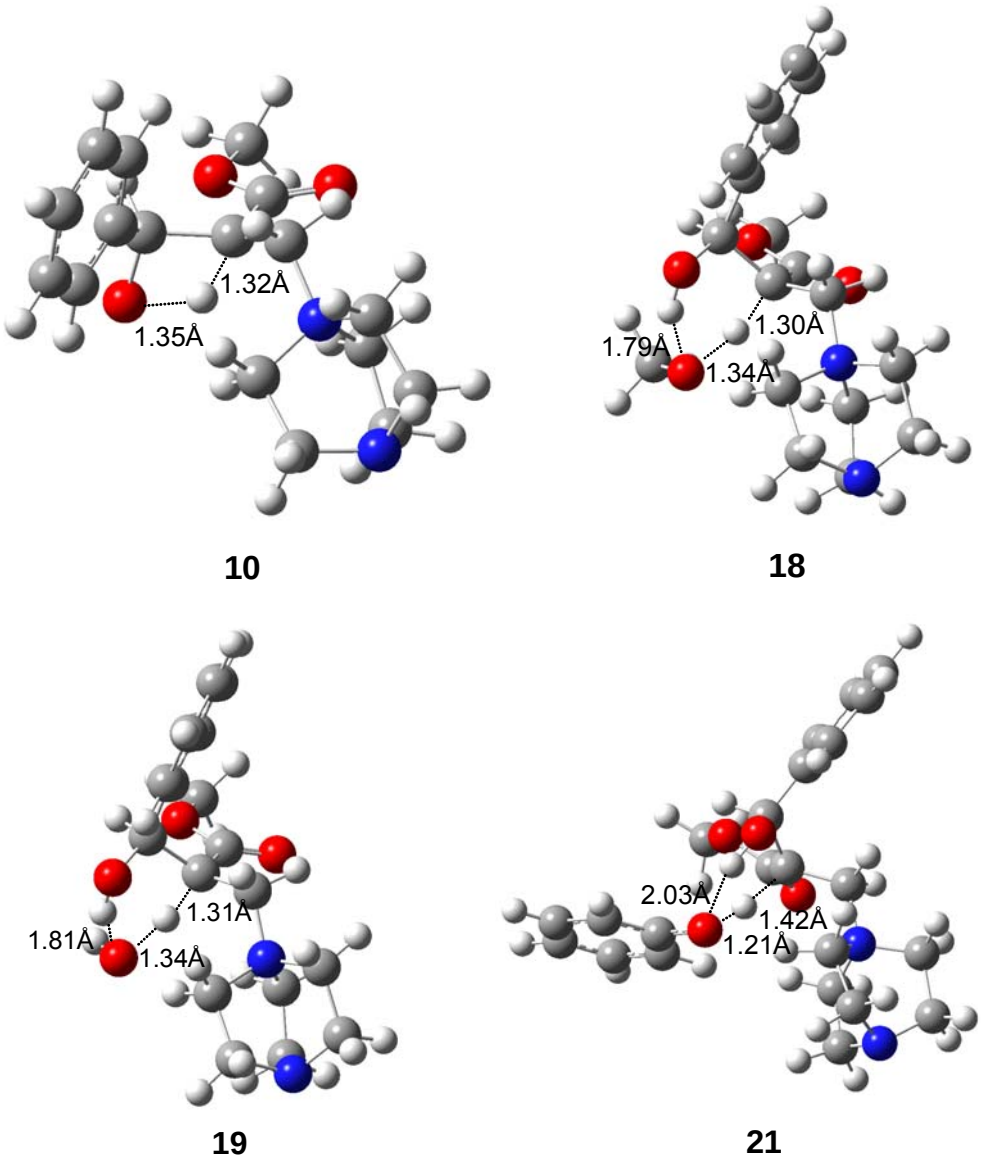
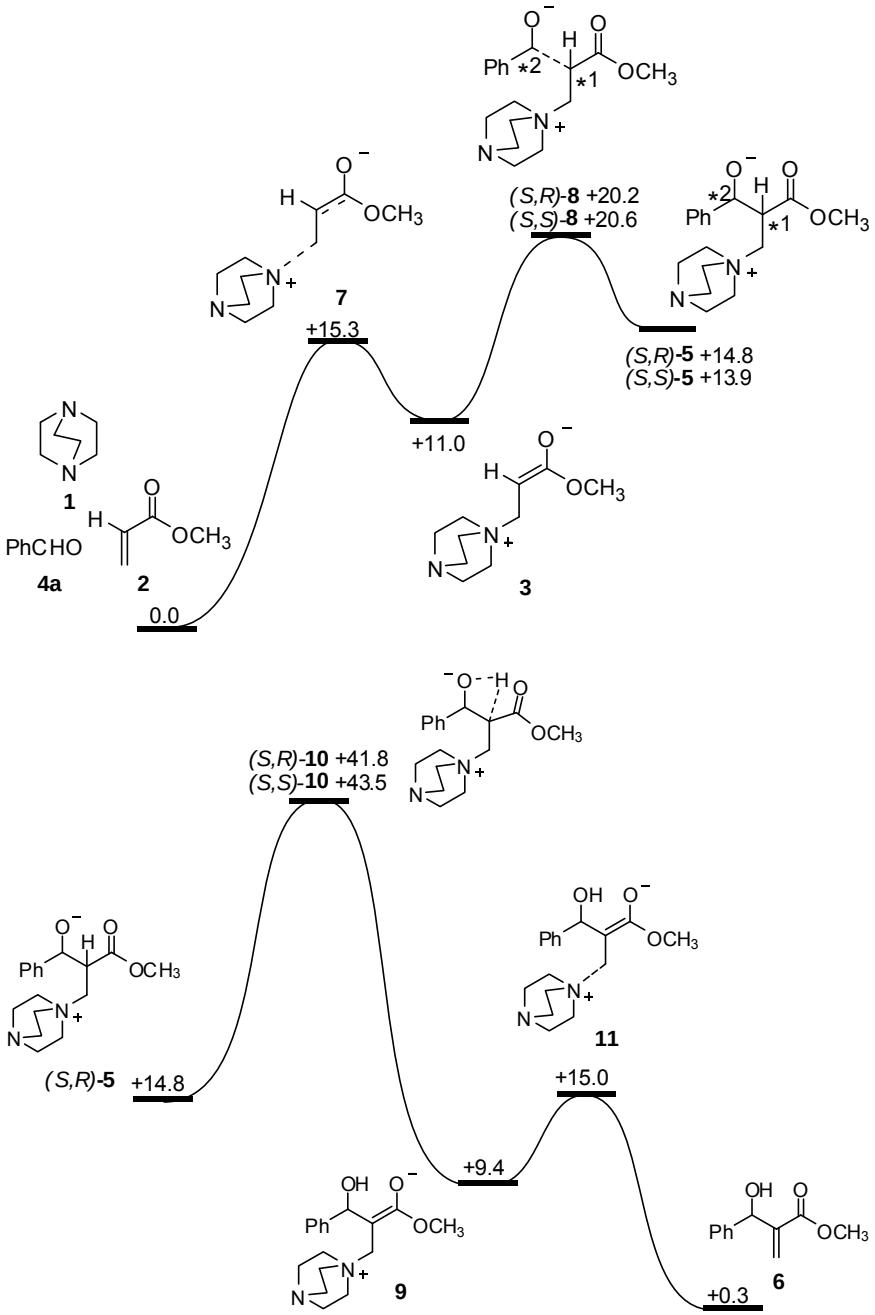
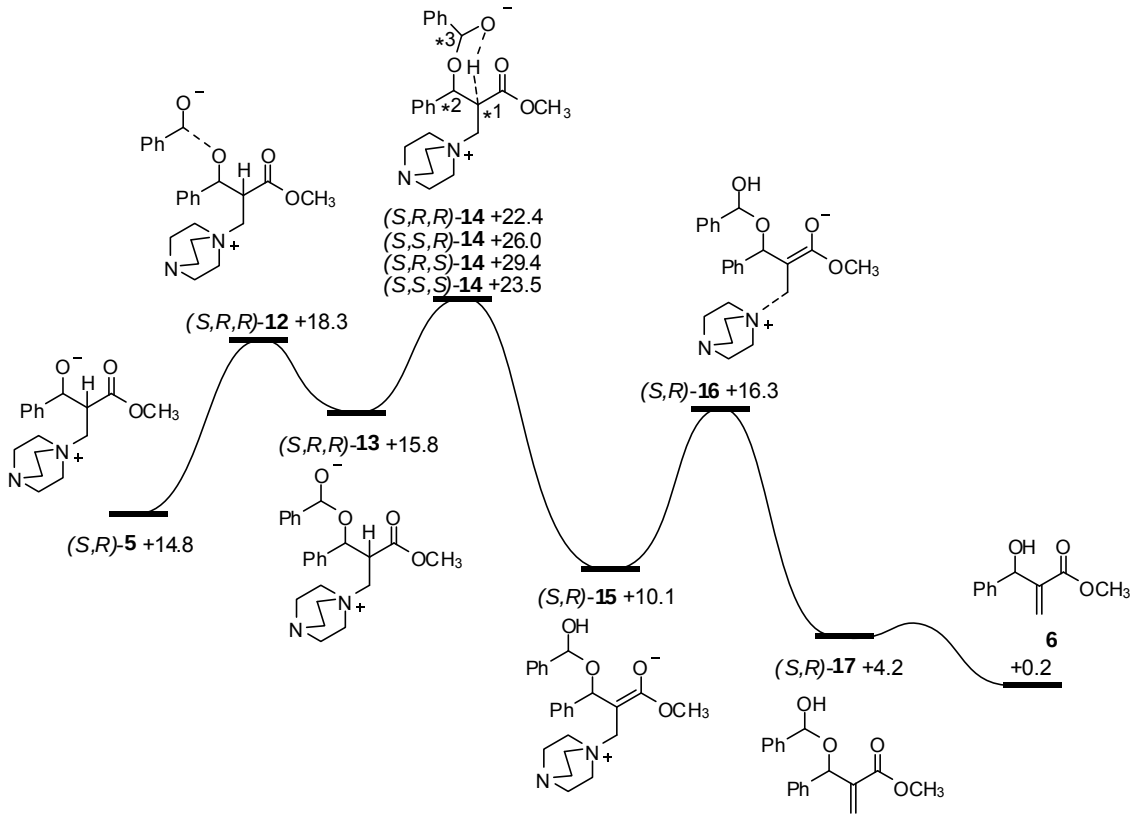


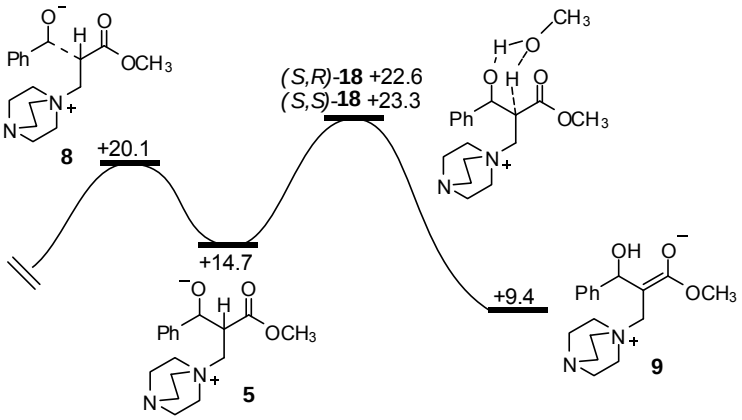
Figure S2. Optimized geometries for the key transition structures not included in the main manuscript.

Energy profiles taking into account all the stereoisomeric key transition states



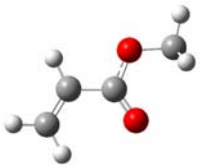


(Note: after the proton transfer the atom priority around C*[2] changes)



Cartesian coordinates, energy and imaginary frequency (transition structures) for all the calculated structures

s-cis-syn-Methyl Acrylate (MP2/6-311+G(d,p) in methanol)



MP2=-305.7252902

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.496720	-0.005007	0.000038
2	6	0	1.316962	-0.643483	-0.000012
3	1	0	3.428369	-0.562347	-0.000062
4	1	0	2.549123	1.080333	0.000021
5	1	0	1.249037	-1.726955	-0.000088
6	6	0	0.039653	0.110729	-0.000012
7	8	0	-0.071538	1.325515	-0.000015
8	8	0	-1.010868	-0.726848	0.000018
9	6	0	-2.304026	-0.085437	0.000005
10	1	0	-3.027585	-0.898475	-0.000043
11	1	0	-2.417809	0.528624	0.894874
12	1	0	-2.417744	0.528667	-0.894843

s-cis-syn-Methyl Acrylate (M062X/6-311G(d,p) in methanol)

E(RM062X) = -306.428018903

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.476650	-0.000494	0.000267
2	6	0	-1.318441	-0.649162	-0.000198
3	1	0	-3.419955	-0.533971	0.000192
4	1	0	-2.505435	1.084511	0.000571
5	1	0	-1.249076	-1.730405	-0.000598
6	6	0	-0.041878	0.103698	-0.000144
7	8	0	0.058992	1.310080	-0.000186
8	8	0	1.010491	-0.714916	0.000030
9	6	0	2.298320	-0.080995	0.000154
10	1	0	3.024523	-0.889537	-0.000006
11	1	0	2.412992	0.535108	-0.892411
12	1	0	2.412975	0.534696	0.893017

s-cis-syn-Methyl Acrylate (M062X/6-311G(d,p) in THF)

E(RM062X) = -306.427974755

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.477193	-0.003961	-0.000145
2	6	0	1.317347	-0.648748	0.000069

3	1	0	3.420250	-0.537660	-0.000045
4	1	0	2.503468	1.080795	-0.000196
5	1	0	1.247364	-1.729928	0.000266
6	6	0	0.040074	0.110813	0.000076
7	8	0	-0.058023	1.311617	0.000090
8	8	0	-1.010993	-0.716182	0.000027
9	6	0	-2.295364	-0.083939	-0.000101
10	1	0	-3.023779	-0.890967	-0.000659
11	1	0	-2.415612	0.534236	0.890559
12	1	0	-2.415059	0.535054	-0.890260

s-trans- syn-Methyl Acrylate (MP2/6-311+G(d,p) in Methanol)

MP2=-305.7244371

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.176645	-0.762659	0.032250
2	6	0	-1.487954	0.387364	-0.034088
3	1	0	-3.262747	-0.750305	0.020941
4	1	0	-1.679086	-1.725011	0.099893
5	1	0	-1.991551	1.348089	-0.091436
6	6	0	-0.009136	0.474913	-0.010968
7	8	0	0.593324	1.537752	0.033040
8	8	0	0.600988	-0.717230	-0.042421
9	6	0	2.042840	-0.668429	0.009638
10	1	0	2.363286	-1.708280	-0.013582
11	1	0	2.432095	-0.128429	-0.854980
12	1	0	2.368877	-0.187379	0.933226

s-trans- syn-Methyl Acrylate (M062X/6-311G(d,p) in Methanol)

E(RM062X) = -306.427109942

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.156685	-0.767387	0.000000
2	6	0	1.491493	0.382267	0.000000
3	1	0	3.240884	-0.779133	0.000001
4	1	0	1.642513	-1.722083	0.000000
5	1	0	1.994862	1.342247	0.000001
6	6	0	0.013921	0.475919	-0.000001
7	8	0	-0.581351	1.530909	0.000000
8	8	0	-0.602345	-0.705118	0.000000
9	6	0	-2.037472	-0.664151	0.000000
10	1	0	-2.359825	-1.701971	0.000000
11	1	0	-2.398312	-0.152635	0.892945
12	1	0	-2.398312	-0.152636	-0.892944

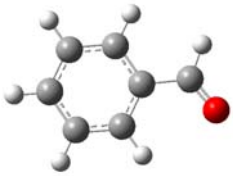
s-trans- syn-Methyl Acrylate (M062X/6-311G(d,p) in THF)

E(RM062X) = -306.427117984

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.155347	-0.767122	0.000000
2	6	0	1.490927	0.382615	0.000000
3	1	0	3.239409	-0.782724	0.000000
4	1	0	1.636741	-1.718976	0.000000
5	1	0	1.996986	1.341051	0.000000
6	6	0	0.009838	0.481622	0.000000
7	8	0	-0.582901	1.531349	0.000000
8	8	0	-0.600278	-0.707561	0.000000
9	6	0	-2.031763	-0.666717	0.000000
10	1	0	-2.357443	-1.703756	0.000000
11	1	0	-2.398177	-0.154145	0.890243
12	1	0	-2.398177	-0.154145	-0.890243

PhCHO (MP2/6-311+G(d,p) in Methanol)



MP2=-344.6750638

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.337567	-1.329835	0.005594
2	6	0	0.041507	-1.113426	-0.005984
3	6	0	0.535439	0.202590	0.010836
4	6	0	-0.348256	1.293666	-0.004248
5	6	0	-1.729302	1.070018	0.006262
6	6	0	-2.223405	-0.240599	-0.007154
7	1	0	-1.727322	-2.344546	-0.003204
8	1	0	0.736864	-1.949072	-0.001419
9	1	0	0.048274	2.307305	0.001759
10	1	0	-2.417414	1.911342	-0.001253
11	1	0	-3.296498	-0.415765	-0.002832
12	6	0	1.989309	0.471992	-0.003204
13	8	0	2.852206	-0.397005	0.001380
14	1	0	2.272097	1.540342	-0.016709

PhCHO (M062X/6-311G(d,p) in Methanol)

E(RM062X) = -345.521792396

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.321999	-1.326892	-0.000003
2	6	0	-0.045859	-1.100583	-0.000049
3	6	0	-0.529925	0.210513	-0.000058
4	6	0	0.353898	1.289410	-0.000014
5	6	0	1.725469	1.059844	0.000032
6	6	0	2.205969	-0.246490	0.000037
7	1	0	1.705345	-2.340466	0.000002

8	1	0	-0.749392	-1.925695	-0.000084
9	1	0	-0.036195	2.302411	-0.000017
10	1	0	2.417041	1.893978	0.000063
11	1	0	3.275020	-0.427073	0.000071
12	6	0	-1.983777	0.471268	-0.000129
13	8	0	-2.828082	-0.397736	0.000116
14	1	0	-2.273812	1.536310	0.000140

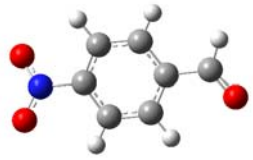
PhCHO (M062X/6-311G(d,p) in THF)

E(RM062X) = -345.522686787

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.324055	-1.325758	0.000003
2	6	0	-0.044070	-1.099540	-0.000031
3	6	0	-0.529511	0.210116	-0.000036
4	6	0	0.354404	1.288029	-0.000005
5	6	0	1.726296	1.059802	0.000016
6	6	0	2.207929	-0.245832	0.000022
7	1	0	1.707455	-2.339229	0.000009
8	1	0	-0.749745	-1.922502	-0.000052
9	1	0	-0.035547	2.301180	-0.000009
10	1	0	2.417161	1.894410	0.000031
11	1	0	3.276869	-0.425990	0.000043
12	6	0	-1.989257	0.467701	-0.000097
13	8	0	-2.830232	-0.396517	0.000073
14	1	0	-2.273408	1.537158	0.000159

4-NO_2PhCHO (MP2/6-311+G(d,p) in Methanol)



MP2=-548.7795154

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.296336	-1.163253	0.128987
2	6	0	-1.093073	-1.057176	0.124058
3	6	0	-1.700882	0.202452	-0.021856
4	6	0	-0.918369	1.360422	-0.159968
5	6	0	0.474780	1.275465	-0.143627
6	6	0	1.044868	0.009941	-0.003549
7	1	0	0.791562	-2.121976	0.245474
8	1	0	-1.708575	-1.945373	0.238011
9	1	0	-1.402288	2.327246	-0.280345
10	1	0	1.100602	2.155586	-0.250298
11	6	0	-3.176143	0.341224	-0.038200
12	8	0	-3.952197	-0.597046	0.080285
13	1	0	-3.552397	1.371602	-0.165977
14	7	0	2.506852	-0.094750	0.008302
15	8	0	3.146727	0.860306	0.452885
16	8	0	3.012724	-1.130547	-0.428176

4-NO_2PhCHO (M062X/6-311G(d,p) in Methanol)

E(RM062X) = -550.002738007

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.283757	-1.159378	-0.019687
2	6	0	-1.095821	-1.048180	-0.018212
3	6	0	-1.690979	0.214567	0.003173
4	6	0	-0.914920	1.371536	0.020607
5	6	0	0.469989	1.278150	0.016147
6	6	0	1.032339	0.011575	-0.002862
7	1	0	0.774029	-2.123123	-0.034958
8	1	0	-1.718942	-1.934478	-0.032349
9	1	0	-1.393986	2.344307	0.038674
10	1	0	1.097496	2.158815	0.028150
11	6	0	-3.170654	0.340303	0.007865
12	8	0	-3.917400	-0.609203	-0.010175
13	1	0	-3.559488	1.371992	0.029725
14	7	0	2.503041	-0.100074	-0.001003
15	8	0	3.152860	0.922390	-0.054160
16	8	0	2.989207	-1.209241	0.056285

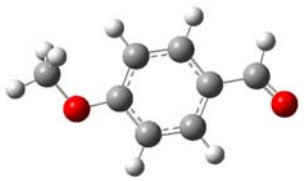
4-NO_2PhCHO (M062X/6-311G(d,p) in THF)

E(RM062X) = -550.006348649

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.283988	-1.158688	-0.000147
2	6	0	-1.095903	-1.047210	-0.000145
3	6	0	-1.692301	0.214754	0.000011
4	6	0	-0.914534	1.370419	0.000140
5	6	0	0.470593	1.276475	0.000117
6	6	0	1.034826	0.010900	-0.000014
7	1	0	0.775950	-2.121563	-0.000266
8	1	0	-1.721810	-1.931500	-0.000262
9	1	0	-1.392729	2.343858	0.000261
10	1	0	1.101175	2.154788	0.000196
11	6	0	-3.175770	0.337893	0.000062
12	8	0	-3.921114	-0.607270	-0.000058
13	1	0	-3.560001	1.374000	0.000227
14	7	0	2.509292	-0.100247	-0.000003
15	8	0	3.152405	0.926894	-0.000386
16	8	0	2.989582	-1.212762	0.000409

4-MeOPhCHO (MP2/6-311+G(d,p) in Methanol)

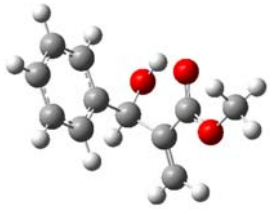


MP2=-458.9383011

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.380880	1.358835	-0.002655
2	6	0	-0.984531	1.108895	-0.001915
3	6	0	-1.455131	-0.219006	0.012699
4	6	0	-0.538062	-1.278126	-0.022661
5	6	0	0.839817	-1.036496	-0.026962
6	6	0	1.299429	0.289691	-0.033225
7	1	0	0.765471	2.375601	-0.004739
8	1	0	-1.691866	1.934242	0.018406
9	1	0	-0.900950	-2.304493	-0.022942
10	1	0	1.529444	-1.872715	-0.051451
11	6	0	-2.893920	-0.526456	0.006433
12	8	0	-3.785373	0.316202	0.024778
13	1	0	-3.146147	-1.602779	-0.013701
14	6	0	3.574838	-0.409277	0.061930
15	1	0	4.544369	0.085752	0.108204
16	1	0	3.410692	-0.989699	0.974547
17	1	0	3.536106	-1.062612	-0.814734
18	8	0	2.611993	0.647341	-0.044211

BH Adduct (MP2/6-311+G(d,p) in Methanol)



MP2=-650.428668

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.931278	1.329391	1.661475
2	6	0	-1.239756	0.926121	0.580716
3	1	0	-1.580861	2.173470	2.250350
4	1	0	-2.846642	0.833644	1.970588
5	6	0	-1.689616	-0.205954	-0.275671
6	8	0	-2.560278	-1.022355	0.322409
7	8	0	-1.284270	-0.363716	-1.420152
8	6	0	-3.054126	-2.103505	-0.501218
9	1	0	-3.761350	-2.637981	0.130257
10	1	0	-3.553918	-1.703965	-1.385027
11	1	0	-2.230412	-2.757033	-0.793051
12	6	0	0.038134	1.599086	0.128815
13	1	0	0.265293	2.398391	0.842095
14	8	0	-0.137407	2.253897	-1.127485
15	1	0	-0.409154	1.569085	-1.756587
16	6	0	3.267975	-1.298775	0.203799
17	6	0	2.451546	-1.107129	1.327054
18	6	0	1.413509	-0.169031	1.287512
19	6	0	1.182299	0.593282	0.129014
20	6	0	2.010178	0.407473	-0.986973
21	6	0	3.047040	-0.535752	-0.949229
22	1	0	4.070514	-2.032020	0.229607
23	1	0	2.618367	-1.689420	2.230424
24	1	0	0.781550	-0.026405	2.162521
25	1	0	1.848019	0.992983	-1.887454
26	1	0	3.678806	-0.674587	-1.823652

BH Adduct (M062X/6-311G(d,p) in Methanol)

E(RM062X) = -651.974484795

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.749372	1.507400	1.564003
2	6	0	-1.185800	0.971979	0.484906
3	1	0	-1.323661	2.391332	2.027640
4	1	0	-2.641981	1.084994	2.010223
5	6	0	-1.758695	-0.229805	-0.184365
6	8	0	-2.765475	-0.790533	0.470926
7	8	0	-1.339369	-0.652577	-1.243330
8	6	0	-3.366416	-1.935531	-0.156786
9	1	0	-4.165663	-2.248021	0.509517
10	1	0	-3.767963	-1.658232	-1.131638
11	1	0	-2.628784	-2.730439	-0.268485
12	6	0	0.073237	1.525609	-0.155495
13	1	0	0.331144	2.445929	0.374383
14	8	0	-0.150927	1.907698	-1.500769
15	1	0	-0.458633	1.123081	-1.974334
16	6	0	3.379874	-1.214071	0.342385
17	6	0	2.673266	-0.747211	1.448592
18	6	0	1.606851	0.127087	1.275595
19	6	0	1.236087	0.550386	-0.002686
20	6	0	1.949790	0.086752	-1.104751
21	6	0	3.015311	-0.794219	-0.932039
22	1	0	4.208263	-1.900560	0.474851
23	1	0	2.953073	-1.065408	2.446616
24	1	0	1.056846	0.486829	2.140239
25	1	0	1.677946	0.414406	-2.101040
26	1	0	3.560773	-1.150877	-1.798745

Nitro-substituted BH adduct (MP2/6-311+G(d,p) in Methanol)

MP2=-854.5352155

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.197343	-0.589445	1.738050
2	6	0	2.400094	-0.565895	0.655877
3	1	0	3.149402	-1.422719	2.434832
4	1	0	3.905776	0.207853	1.941730
5	6	0	2.445558	0.535434	-0.345616
6	8	0	2.943359	1.676999	0.132912
7	8	0	2.048645	0.390651	-1.494796
8	6	0	3.048840	2.753141	-0.828163
9	1	0	3.474372	3.586522	-0.272430
10	1	0	3.708450	2.460283	-1.646629
11	1	0	2.059490	3.011195	-1.209316

12	6	0	1.409057	-1.666406	0.344733
13	1	0	1.433339	-2.385863	1.170438
14	8	0	1.792257	-2.403559	-0.814324
15	1	0	1.858693	-1.763881	-1.539526
16	6	0	-2.538042	0.010881	0.105760
17	6	0	-1.731328	0.336157	1.196355
18	6	0	-0.455884	-0.229277	1.256111
19	6	0	0.004926	-1.085818	0.241183
20	6	0	-0.840649	-1.392381	-0.834057
21	6	0	-2.126589	-0.847831	-0.911498
22	1	0	-2.093613	0.997949	1.976858
23	1	0	0.184558	-0.001392	2.105727
24	1	0	-0.496819	-2.051873	-1.624925
25	1	0	-2.782803	-1.072147	-1.746659
26	7	0	-3.874988	0.601338	0.026359
27	8	0	-4.754753	-0.034523	-0.558295
28	8	0	-4.048993	1.704601	0.548625

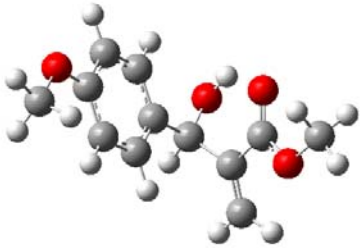
Nitro-substituted BH adduct (M062X/6-311G(d,p) in Methanol)

E(RM062X) = -856.459778144

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.909386	-0.808049	1.847675
2	6	0	2.306883	-0.661626	0.671380
3	1	0	2.699475	-1.672349	2.469506
4	1	0	3.618848	-0.078014	2.219544
5	6	0	2.573139	0.504856	-0.215922
6	8	0	3.379818	1.416262	0.305763
7	8	0	2.090569	0.600821	-1.326768
8	6	0	3.691846	2.539975	-0.535496
9	1	0	4.350181	3.170600	0.055613
10	1	0	4.196669	2.198812	-1.439621
11	1	0	2.780244	3.078039	-0.795765
12	6	0	1.295004	-1.653196	0.128488
13	1	0	1.255744	-2.496716	0.822142
14	8	0	1.697983	-2.190974	-1.115082
15	1	0	1.820919	-1.450039	-1.724562
16	6	0	-2.625569	0.059738	0.063696
17	6	0	-1.910542	0.053801	1.254592
18	6	0	-0.640350	-0.497565	1.252001
19	6	0	-0.097586	-1.035503	0.081541
20	6	0	-0.843729	-1.018203	-1.095411
21	6	0	-2.117303	-0.466568	-1.113777
22	1	0	-2.340706	0.471077	2.155091
23	1	0	-0.064365	-0.511179	2.171042
24	1	0	-0.434938	-1.439523	-2.004561
25	1	0	-2.704452	-0.446135	-2.021961
26	7	0	-3.971083	0.643507	0.052642
27	8	0	-4.589037	0.646146	-0.993029
28	8	0	-4.407723	1.098359	1.090671

Methoxy-substituted BH adduct (MP2/6-311+G(d,p) in Methanol)

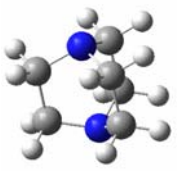


MP2=-764.6896381

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.813187	-0.480583	1.907583
2	6	0	2.118955	-0.521089	0.756465
3	1	0	2.711884	-1.282045	2.635355
4	1	0	3.487645	0.338259	2.139405
5	6	0	2.244144	0.535473	-0.285421
6	8	0	2.708577	1.699012	0.177427
7	8	0	1.938019	0.342334	-1.454985
8	6	0	2.885300	2.729189	-0.822403
9	1	0	3.270096	3.588853	-0.276991
10	1	0	3.601961	2.400040	-1.576475
11	1	0	1.926875	2.967437	-1.286505
12	6	0	1.167990	-1.646311	0.410854
13	1	0	1.150661	-2.343420	1.255444
14	8	0	1.647612	-2.410169	-0.696652
15	1	0	1.732161	-1.791004	-1.437104
16	6	0	-2.808474	0.005870	-0.164105
17	6	0	-2.068534	0.317702	0.986407
18	6	0	-0.787655	-0.229634	1.147432
19	6	0	-0.231002	-1.087943	0.188546
20	6	0	-0.990762	-1.401961	-0.949631
21	6	0	-2.264940	-0.859005	-1.126945
22	1	0	-2.462131	0.977015	1.752486
23	1	0	-0.221167	0.022265	2.042466
24	1	0	-0.589524	-2.069211	-1.707298
25	1	0	-2.851551	-1.096170	-2.011581
26	6	0	-4.623978	1.385299	0.529185
27	1	0	-5.599677	1.665478	0.131966
28	1	0	-4.749826	0.889966	1.497033
29	1	0	-4.002772	2.279140	0.643094
30	8	0	-4.060459	0.490242	-0.434428

DABCO (M062X/6-311G(d,p) in Methanol)



E(RM062X) = -345.279703304

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.777664	-0.340245	1.335523
2	6	0	-0.776781	-0.334097	1.337561
3	1	0	1.168286	-1.322501	1.613297

4	1	0	1.176170	0.389174	2.045188
5	1	0	-1.174355	-1.313077	1.617011
6	1	0	-1.167735	0.398851	2.047789
7	6	0	0.772232	-0.992052	-0.961422
8	1	0	1.166938	-0.744841	-1.950133
9	1	0	1.163856	-1.973707	-0.682756
10	6	0	-0.781971	-0.986896	-0.959004
11	1	0	-1.178109	-0.737862	-1.946687
12	1	0	-1.179210	-1.965696	-0.678255
13	6	0	-0.772838	1.329343	-0.375790
14	1	0	-1.167868	1.581342	-1.363143
15	1	0	-1.163232	2.062036	0.335094
16	6	0	0.781668	1.323906	-0.377015
17	1	0	1.176896	1.574085	-1.364752
18	1	0	1.178347	2.053152	0.333946
19	7	0	-1.289412	0.004635	0.001211
20	7	0	1.289436	-0.004737	-0.002028

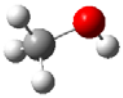
DABCO (M062X/6-311G(d,p) in THF)

E(RM062X) = -345.274828709

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.777386	-0.980123	-0.971819
2	6	0	0.779605	-0.979210	-0.970981
3	1	0	-1.173149	-1.962619	-0.701585
4	1	0	-1.173437	-0.719274	-1.956633
5	1	0	1.176240	-1.961360	-0.700762
6	1	0	1.176396	-0.717458	-1.955256
7	6	0	-0.779318	-0.351793	1.333412
8	1	0	-1.176416	0.372791	2.048972
9	1	0	-1.175622	-1.335365	1.598923
10	6	0	0.777799	-0.351423	1.334382
11	1	0	1.173671	0.373026	2.050759
12	1	0	1.174215	-1.334931	1.599959
13	6	0	0.778440	1.331641	-0.361807
14	1	0	1.173984	2.053225	0.357644
15	1	0	1.175593	1.590011	-1.346844
16	6	0	-0.779132	1.330884	-0.363129
17	1	0	-1.176601	2.052343	0.355384
18	1	0	-1.174868	1.588519	-1.348929
19	7	0	1.283559	0.000656	0.000732
20	7	0	-1.283566	-0.000479	-0.001015

Methanol (M062X/6-311G(d,p) in Methanol)



E(RM062X) = -115.707108497

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.666267	-0.019329	0.000008
2	1	0	1.092919	0.984182	-0.001134
3	1	0	1.018644	-0.549315	-0.890711
4	1	0	1.018841	-0.547477	0.891746
5	8	0	-0.749527	0.123507	0.000012

6	1	0	-1.131790	-0.759474	-0.000044

Water (M062X/6-311G(d,p) in Methanol)

E(RM062X) = -76.4257583834

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.118984
2	1	0	0.000000	0.756424	-0.475936
3	1	0	0.000000	-0.756424	-0.475936

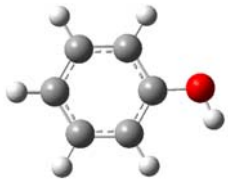
Water (M062X/6-311G(d,p) in THF)

E(RM062X) = -76.4189183790

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.118911
2	1	0	0.000000	0.755464	-0.475643
3	1	0	0.000000	-0.755464	-0.475643

Phenol (M062X/6-311G(d,p) in Methanol)

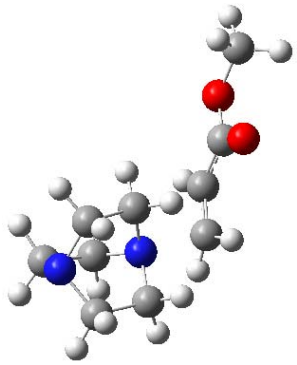


E(RM062X) = -307.431594589

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.203212	0.233614	0.000000
2	6	0	-1.185166	-1.157772	0.000000
3	6	0	0.021362	-1.851040	0.000000
4	6	0	1.218479	-1.137637	0.000000
5	6	0	1.214448	0.251586	0.000000
6	6	0	0.000000	0.936472	0.000000
7	1	0	-2.141163	0.779694	0.000000
8	1	0	-2.124046	-1.700094	0.000000
9	1	0	0.029919	-2.934334	0.000000
10	1	0	2.165303	-1.665994	0.000000
11	1	0	2.137559	0.820066	0.000000
12	8	0	0.048132	2.299037	0.000000
13	1	0	-0.848097	2.657025	0.000000

TS 5 (M062X/6-311G(d,p) in Methanol)

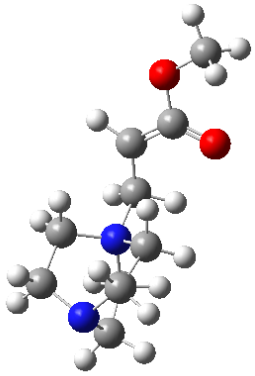


Imaginary Frecuency: -169.6640 cm^{-1}
E(RM062X) = -651.705576759

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.773478	1.222346	0.455331
2	1	0	1.947332	1.508731	1.484300
3	6	0	2.665983	0.254211	-0.132251
4	8	0	3.669830	-0.095073	0.706508
5	8	0	2.591828	-0.227245	-1.256269
6	6	0	4.616490	-1.035468	0.193579
7	1	0	5.326829	-1.211805	0.998103
8	1	0	4.122024	-1.968479	-0.081188
9	1	0	5.131539	-0.626596	-0.677271
10	6	0	0.728603	1.715468	-0.272174
11	1	0	0.165822	2.567915	0.093318
12	1	0	0.698526	1.548837	-1.344770
13	7	0	-1.016684	0.535501	-0.097188
14	6	0	-1.481971	0.602854	1.291314
15	6	0	-0.668664	-0.850759	-0.431623
16	6	0	-2.074175	1.008803	-0.996468
17	6	0	-2.654515	-0.399437	1.480238
18	1	0	-0.635754	0.370718	1.944360
19	1	0	-1.797503	1.631067	1.487233
20	1	0	-0.213563	-0.860479	-1.424564
21	1	0	0.078422	-1.188860	0.292277
22	6	0	-1.957948	-1.716810	-0.380151
23	6	0	-3.364990	0.181899	-0.726052
24	1	0	-1.720985	0.881710	-2.022931
25	1	0	-2.231667	2.075128	-0.814782
26	1	0	-2.354629	-1.238015	2.112696
27	1	0	-3.508372	0.090482	1.952479
28	7	0	-3.075168	-0.940948	0.179067
29	1	0	-2.242581	-2.045037	-1.382285
30	1	0	-1.804509	-2.606170	0.234537
31	1	0	-3.772552	-0.213748	-1.658521
32	1	0	-4.132417	0.802636	-0.258508

Intermediate 6 (*E* isomer) (M062X/6-311G(d,p) in Methanol)

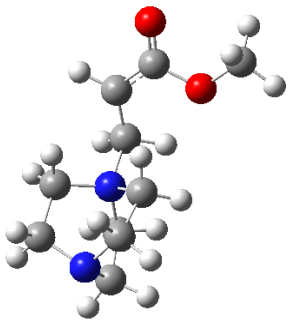


E(RM062X) = -651.718118909

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.548336	-1.074249	0.350764
2	1	0	-1.707869	-1.587622	1.288880
3	6	0	-2.522534	-0.215969	-0.131749
4	8	0	-3.627892	-0.107762	0.703849
5	8	0	-2.518556	0.442660	-1.197482
6	6	0	-4.664386	0.756297	0.256440
7	1	0	-5.438991	0.715446	1.021711
8	1	0	-4.310490	1.784761	0.151683
9	1	0	-5.078016	0.423850	-0.698578
10	6	0	-0.370355	-1.370302	-0.471292
11	1	0	-0.000317	-2.391093	-0.349380
12	1	0	-0.551805	-1.179174	-1.531645
13	7	0	0.894795	-0.513429	-0.170755
14	6	0	1.309819	-0.668186	1.259824
15	6	0	0.638300	0.938149	-0.438616
16	6	0	2.023973	-0.967215	-1.043862
17	6	0	2.694895	-0.007113	1.437984
18	1	0	0.536013	-0.191404	1.860573
19	1	0	1.327929	-1.735823	1.481921
20	1	0	0.491368	1.034331	-1.515334
21	1	0	-0.284369	1.204622	0.073954
22	6	0	1.852990	1.746863	0.069296
23	6	0	3.192915	0.030077	-0.889801
24	1	0	1.649504	-1.012071	-2.066547
25	1	0	2.288896	-1.973143	-0.715246
26	1	0	2.707068	0.578719	2.357767
27	1	0	3.476024	-0.766021	1.508019
28	7	0	3.005394	0.867488	0.300684
29	1	0	2.119365	2.508717	-0.664325
30	1	0	1.615007	2.247542	1.009268
31	1	0	3.253387	0.685369	-1.760155
32	1	0	4.133864	-0.514721	-0.806945

Intermediate 6 (*Z* isomer) (M062X/6-311G(d,p) in Methanol)

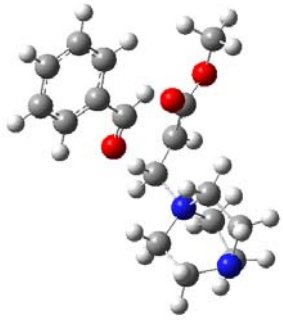


E(RM062X) = -651.715862456

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.549410	-1.350633	0.155881
2	1	0	1.529274	-2.354090	-0.249026
3	6	0	2.649156	-0.572330	-0.174940
4	8	0	2.637756	0.703771	0.384298
5	8	0	3.622550	-0.887791	-0.892481
6	6	0	3.773134	1.513417	0.109141
7	1	0	3.604189	2.454513	0.631649
8	1	0	4.692045	1.052045	0.477710
9	1	0	3.877150	1.705683	-0.961071
10	6	0	0.495591	-0.921348	1.081768
11	1	0	0.094910	-1.743055	1.680880
12	1	0	0.816589	-0.119459	1.748635
13	7	0	-0.790984	-0.338552	0.419074
14	6	0	-1.384964	-1.323378	-0.539824
15	6	0	-0.492629	0.928794	-0.319648
16	6	0	-1.804331	-0.041729	1.481240
17	6	0	-2.777465	-0.806753	-0.964721
18	1	0	-0.692595	-1.400748	-1.377158
19	1	0	-1.437273	-2.285638	-0.029529
20	1	0	-0.215082	1.668037	0.433552
21	1	0	0.362695	0.734530	-0.964897
22	6	0	-1.754758	1.336518	-1.111794
23	6	0	-2.976587	0.732102	0.838548
24	1	0	-1.305201	0.534488	2.260356
25	1	0	-2.116159	-1.003116	1.891825
26	1	0	-2.905608	-0.937604	-2.039896
27	1	0	-3.564947	-1.366743	-0.457637
28	7	0	-2.934878	0.612164	-0.624014
29	1	0	-1.921355	2.409645	-1.011057
30	1	0	-1.631918	1.110112	-2.172401
31	1	0	-2.923466	1.791314	1.095304
32	1	0	-3.924010	0.339006	1.208899

_(S,R)_-TS 7 (M062X/6-311G(d,p) in Methanol)



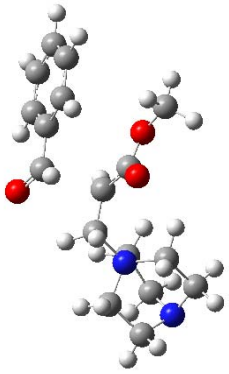
Imaginary Frequency: -222.6747 cm^{-1}

E(RM062X) = -997.248609001

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.239672	-1.330434	2.535017
2	1	0	2.101466	0.510428	2.331185
3	6	0	-0.545249	-0.532784	0.321566
4	1	0	-0.103003	-0.852190	-0.624480
5	1	0	-0.528136	-1.368044	1.030663
6	6	0	0.173794	0.630643	0.874967
7	1	0	-0.137227	1.032445	1.830761
8	6	0	0.813981	1.525943	-0.020968
9	8	0	1.347961	2.611265	0.614284
10	8	0	0.991462	1.370937	-1.231601
11	6	0	2.057768	3.533281	-0.212917
12	1	0	2.443273	4.298739	0.457897
13	1	0	2.883348	3.041849	-0.730630
14	1	0	1.389904	3.986051	-0.948652
15	6	0	1.802672	-0.439395	1.860531
16	6	0	4.177423	-1.449433	-1.567202
17	6	0	4.307511	-0.196044	-0.973437
18	6	0	3.536417	0.130464	0.136999
19	6	0	2.627178	-0.790484	0.660781
20	6	0	2.512867	-2.051336	0.072887
21	6	0	3.279162	-2.376286	-1.041202
22	1	0	4.776571	-1.705210	-2.433977
23	1	0	5.011184	0.525127	-1.374638
24	1	0	3.633759	1.107392	0.602724
25	1	0	1.822179	-2.771671	0.498230
26	1	0	3.181544	-3.355200	-1.497815
27	7	0	-2.029731	-0.338476	0.014169
28	6	0	-2.243429	0.655017	-1.089816
29	6	0	-2.773490	0.135480	1.229025
30	6	0	-2.612341	-1.655941	-0.415324
31	6	0	-3.758971	0.933492	-1.200079
32	1	0	-1.679769	1.551668	-0.839458
33	1	0	-1.827977	0.207952	-1.993898
34	1	0	-2.461968	-0.487483	2.067902
35	1	0	-2.458394	1.162758	1.408077
36	6	0	-4.286449	0.030842	0.939918
37	6	0	-4.044517	-1.412256	-0.935313
38	1	0	-2.591063	-2.303373	0.461864
39	1	0	-1.955353	-2.066842	-1.181744
40	1	0	-4.001692	1.899903	-0.755195
41	1	0	-4.050144	0.957848	-2.250625
42	7	0	-4.534103	-0.098770	-0.501683
43	1	0	-4.713167	-0.841164	1.438130
44	1	0	-4.791310	0.920858	1.316663
45	1	0	-4.709094	-2.190410	-0.558772
46	1	0	-4.066813	-1.442074	-2.025705

***(S,S)*-TS 7 (M062X/6-311G(d,p) in Methanol)**

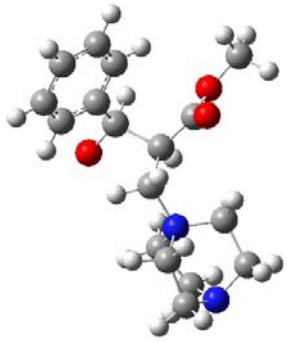


Imaginary Frequency: -205.1311 cm-1
E(RM062X) = -997.247217620

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.191360	-2.491306	-1.133153
2	6	0	5.129597	-0.233733	1.054685
3	6	0	4.369391	-1.338688	1.437891
4	6	0	3.241457	-1.694321	0.709454
5	6	0	2.855235	-0.940033	-0.399369
6	6	0	3.623576	0.156517	-0.787357
7	6	0	4.757529	0.510854	-0.061555
8	1	0	6.011147	0.041946	1.622649
9	1	0	4.660568	-1.922101	2.304507
10	1	0	2.646391	-2.555485	0.994390
11	1	0	3.323965	0.737167	-1.656190
12	1	0	5.349979	1.366760	-0.366238
13	6	0	-0.988943	-0.590073	-0.824401
14	1	0	-1.042685	-0.167401	-1.830344
15	1	0	-0.956327	-1.680997	-0.896705
16	6	0	0.180969	-0.070529	-0.089040
17	1	0	0.383357	-0.451401	0.904679
18	6	0	0.652548	1.233275	-0.384508
19	8	0	1.467311	1.743620	0.582705
20	8	0	0.451486	1.871953	-1.424140
21	6	0	2.094718	2.989610	0.282662
22	1	0	2.763759	3.195638	1.116423
23	1	0	2.665690	2.932604	-0.645423
24	1	0	1.351755	3.785883	0.199426
25	6	0	1.640861	-1.327954	-1.183080
26	1	0	1.473354	-0.705250	-2.079313
27	7	0	-2.360602	-0.300580	-0.208098
28	6	0	-2.690135	1.163294	-0.245263
29	6	0	-2.418545	-0.764037	1.217677
30	6	0	-3.405846	-1.043968	-0.990952
31	6	0	-3.995461	1.384260	0.552709
32	1	0	-1.850428	1.702462	0.190074
33	1	0	-2.786827	1.432965	-1.297875
34	1	0	-2.008179	-1.773609	1.250978
35	1	0	-1.776524	-0.096019	1.790312
36	6	0	-3.889714	-0.706635	1.685392
37	6	0	-4.798368	-0.585345	-0.510485
38	1	0	-3.229298	-2.104609	-0.808586
39	1	0	-3.236132	-0.827911	-2.045583
40	1	0	-3.776912	1.826556	1.526004
41	1	0	-4.646885	2.066767	0.005799
42	7	0	-4.695685	0.114390	0.774288
43	1	0	-4.321757	-1.708228	1.714322
44	1	0	-3.936892	-0.285617	2.690069
45	1	0	-5.452806	-1.450937	-0.402003
46	1	0	-5.248782	0.095056	-1.234743

***(S,R)*-Intermediate 8 (M062X/6-311G(d,p) in Methanol)**



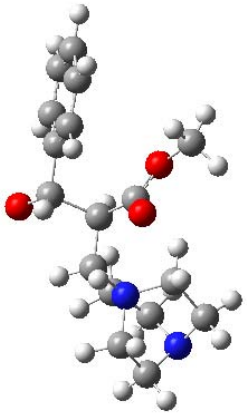
E(RM062X) = -997.260947212

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.907296	0.650617	2.107355
2	6	0	4.468898	-1.660831	-1.195171
3	6	0	4.401590	-0.301528	-0.894381
4	6	0	3.435817	0.169627	-0.011218
5	6	0	2.518986	-0.702818	0.584895
6	6	0	2.610893	-2.062589	0.293310
7	6	0	3.572776	-2.539820	-0.595042
8	1	0	5.221243	-2.031435	-1.882497
9	1	0	5.107906	0.389791	-1.341460
10	1	0	3.407642	1.228951	0.234264
11	1	0	1.929660	-2.745491	0.787408
12	1	0	3.627284	-3.601359	-0.812024
13	6	0	-0.421581	-0.516556	-0.141349
14	1	0	-0.093518	-0.479953	-1.180728
15	1	0	-0.223634	-1.504218	0.276617
16	6	0	0.286316	0.532129	0.694348
17	1	0	-0.353852	0.947403	1.473558
18	6	0	0.791090	1.682282	-0.125539
19	8	0	1.168937	2.701430	0.650556
20	8	0	0.895744	1.712359	-1.332588
21	6	0	1.744782	3.830787	-0.022047
22	1	0	2.006033	4.536985	0.761644
23	1	0	2.635525	3.528106	-0.574151
24	1	0	1.018853	4.272167	-0.705737
25	6	0	1.442136	-0.190499	1.553408
26	8	0	0.887938	-1.131984	2.337368
27	7	0	-1.922504	-0.395737	-0.167472
28	6	0	-2.371385	0.987161	-0.555589
29	6	0	-2.517339	-0.755823	1.168761
30	6	0	-2.469607	-1.363682	-1.184530
31	6	0	-3.891936	0.943465	-0.822292
32	1	0	-2.122933	1.648710	0.274324
33	1	0	-1.800020	1.276127	-1.437823
34	1	0	-2.332758	-1.822641	1.301898
35	1	0	-1.983485	-0.211094	1.944606
36	6	0	-4.019687	-0.410977	1.131498
37	6	0	-4.003261	-1.423482	-1.022702
38	1	0	-1.991449	-2.326120	-1.003821
39	1	0	-2.164685	-0.985581	-2.160608
40	1	0	-4.362992	1.821462	-0.379781
41	1	0	-4.091914	0.951662	-1.894777
42	7	0	-4.487109	-0.270995	-0.253557
43	1	0	-4.583622	-1.199635	1.630321
44	1	0	-4.210306	0.528505	1.652487

45	1	0	-4.298328	-2.333228	-0.497838
46	1	0	-4.472533	-1.428124	-2.006893

_(S,S)_-Intermediate 8 (M062X/6-311G(d,p) in Methanol)



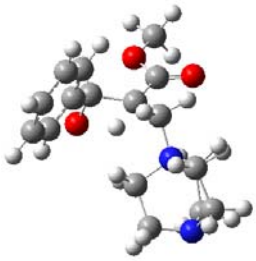
E(RM062X) = -997.261281618

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.027331	-2.640033	-0.479194
2	6	0	5.164369	-0.006845	0.760076
3	6	0	4.401910	-0.938798	1.461399
4	6	0	3.196809	-1.394299	0.935759
5	6	0	2.729885	-0.920540	-0.290202
6	6	0	3.509240	-0.001808	-0.995261
7	6	0	4.717268	0.456168	-0.474660
8	1	0	6.105183	0.346985	1.167057
9	1	0	4.750619	-1.312650	2.418333
10	1	0	2.603999	-2.131241	1.466521
11	1	0	3.164989	0.361389	-1.959845
12	1	0	5.311758	1.169546	-1.035443
13	6	0	-1.013870	-0.672327	-1.007645
14	1	0	-1.027919	-0.148109	-1.964931
15	1	0	-1.062065	-1.748537	-1.175290
16	6	0	0.263667	-0.352721	-0.258020
17	1	0	0.200388	-0.564213	0.810252
18	6	0	0.712003	1.061966	-0.459345
19	8	0	1.247136	1.587883	0.643972
20	8	0	0.664029	1.660951	-1.513320
21	6	0	1.848679	2.883005	0.500642
22	1	0	2.270364	3.120124	1.474041
23	1	0	2.633635	2.850113	-0.256663
24	1	0	1.094626	3.620098	0.221262
25	6	0	1.368251	-1.384132	-0.817012
26	1	0	1.380543	-1.188842	-1.914112
27	7	0	-2.297816	-0.309678	-0.308804
28	6	0	-2.288582	1.105077	0.204355
29	6	0	-2.573632	-1.248175	0.836476
30	6	0	-3.431711	-0.441044	-1.292774
31	6	0	-3.722718	1.464925	0.654677
32	1	0	-1.579504	1.139570	1.032462
33	1	0	-1.938642	1.742132	-0.608327
34	1	0	-2.761752	-2.223414	0.386262
35	1	0	-1.679323	-1.306481	1.453408
36	6	0	-3.790716	-0.709628	1.617024
37	6	0	-4.762262	-0.323873	-0.521513
38	1	0	-3.317820	-1.405320	-1.787403

39	1	0	-3.297881	0.357848	-2.022566
40	1	0	-3.680481	1.997523	1.604884
41	1	0	-4.201756	2.113321	-0.080346
42	7	0	-4.540018	0.256887	0.807112
43	1	0	-4.441633	-1.540270	1.891133
44	1	0	-3.468979	-0.210790	2.532397
45	1	0	-5.219179	-1.306219	-0.393802
46	1	0	-5.453836	0.304855	-1.082951

_(S,R)_-TS 10 (M062X/6-311G(d,p) in Methanol)



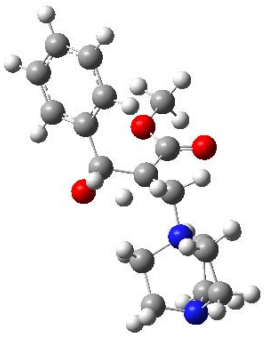
Imaginary Frequency: -1649.4670 cm^{-1}
E(RM062X) = -997.210730538

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.343312	0.740508	2.036367
2	1	0	2.613512	1.404465	0.519869
3	6	0	-0.250790	0.278343	-0.979580
4	1	0	-0.572310	0.832133	-1.863036
5	1	0	0.330262	-0.586858	-1.302328
6	6	0	0.512731	1.159039	-0.030400
7	1	0	0.289172	1.101666	1.266544
8	6	0	0.411933	2.580281	-0.352639
9	8	0	1.317722	3.350036	0.281517
10	8	0	-0.447946	3.083952	-1.063627
11	6	0	1.183210	4.762351	0.095201
12	1	0	1.974820	5.213922	0.688659
13	1	0	1.307741	5.024175	-0.956376
14	1	0	0.208489	5.104667	0.445610
15	6	0	1.801522	0.686457	0.696382
16	6	0	3.335677	-3.152896	-0.554509
17	6	0	3.407165	-2.051819	-1.408028
18	6	0	2.908886	-0.821093	-0.998947
19	6	0	2.324078	-0.668637	0.263085
20	6	0	2.265743	-1.770210	1.111718
21	6	0	2.766587	-3.007336	0.705725
22	1	0	3.724539	-4.113931	-0.871892
23	1	0	3.854823	-2.155699	-2.390535
24	1	0	2.966247	0.036092	-1.665258
25	1	0	1.827478	-1.648019	2.094979
26	1	0	2.715017	-3.856241	1.379039
27	7	0	-1.534147	-0.313325	-0.415690
28	6	0	-2.186605	-1.156247	-1.478156
29	6	0	-1.257862	-1.198181	0.767732
30	6	0	-2.501242	0.763453	-0.011947
31	6	0	-3.587247	-1.575965	-0.980488
32	1	0	-1.527418	-2.009511	-1.641334
33	1	0	-2.232568	-0.557357	-2.386915
34	6	0	-2.559011	-1.947797	1.131286
35	1	0	-0.905128	-0.555908	1.573039
36	1	0	-0.455371	-1.876341	0.477006
37	6	0	-3.696139	0.099286	0.705241
38	1	0	-1.970369	1.458103	0.635907

39	1	0	-2.791578	1.275198	-0.930520
40	7	0	-3.717137	-1.346935	0.461746
41	1	0	-3.750454	-2.632414	-1.195685
42	1	0	-4.361545	-1.000275	-1.489731
43	1	0	-2.709157	-1.915707	2.210668
44	1	0	-2.494549	-2.993420	0.826153
45	1	0	-3.632190	0.262494	1.782154
46	1	0	-4.626999	0.540448	0.347474

_(S,S)_-TS 10 (M062X/6-311G(d,p) in Methanol)



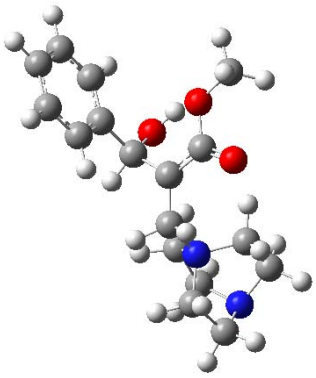
Imaginary Frequency: -1686.9330 cm^{-1}
E(RM062X) = -997.209222930

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.837755	-0.807695	-1.884171
2	6	0	-5.257431	-1.012783	0.629865
3	6	0	-4.893413	-1.091006	-0.710254
4	6	0	-3.549042	-1.052517	-1.076343
5	6	0	-2.554685	-0.939137	-0.108561
6	6	0	-2.926873	-0.864649	1.236289
7	6	0	-4.266789	-0.899748	1.604723
8	1	0	-6.303152	-1.038179	0.915502
9	1	0	-5.657332	-1.179534	-1.475450
10	1	0	-3.258927	-1.102193	-2.119015
11	1	0	-2.158308	-0.768993	1.999225
12	1	0	-4.541216	-0.835223	2.652194
13	6	0	0.864127	-0.086909	1.041512
14	1	0	0.941971	0.691314	1.801983
15	1	0	0.694214	-1.045740	1.535049
16	6	0	-0.208173	0.220807	0.035891
17	1	0	-0.024959	0.079748	-1.270012
18	6	0	-0.754433	1.568453	0.149386
19	8	0	-1.885942	1.757025	-0.552847
20	8	0	-0.221788	2.497490	0.744430
21	6	0	-2.435924	3.077179	-0.525041
22	1	0	-3.343133	3.029722	-1.123398
23	1	0	-2.676999	3.369124	0.498075
24	1	0	-1.737288	3.795297	-0.956901
25	6	0	-1.087658	-0.931164	-0.494975
26	1	0	-0.658972	-1.864349	-0.091462
27	7	0	2.264282	-0.197752	0.461398
28	6	0	3.225924	-0.529746	1.569229
29	6	0	2.343416	-1.294026	-0.564729
30	6	0	2.695656	1.096448	-0.166396
31	6	0	4.663755	-0.423834	1.017860
32	1	0	2.977331	-1.539021	1.899085
33	1	0	3.042557	0.172321	2.381880
34	6	0	3.829948	-1.512531	-0.926977
35	1	0	1.745961	-0.981206	-1.419715

36	1	0	1.889765	-2.180117	-0.119473
37	6	0	4.039932	0.858084	-0.887921
38	1	0	1.909747	1.408649	-0.851769
39	1	0	2.774770	1.819544	0.646777
40	7	0	4.656104	-0.399034	-0.448396
41	1	0	5.252254	-1.274132	1.363641
42	1	0	5.141568	0.490423	1.372588
43	1	0	3.933253	-1.598164	-2.009066
44	1	0	4.202146	-2.432842	-0.474220
45	1	0	3.888093	0.802446	-1.966935
46	1	0	4.717820	1.686519	-0.680234

Intermediate 9 (M062X/6-311G(d,p) in Methanol)



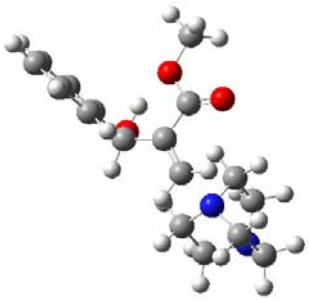
E(RM062X) = -997.266347162

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.290487	0.224518	-0.327392
2	6	0	0.609665	1.572070	-0.460259
3	8	0	1.650249	1.966191	0.372958
4	8	0	0.079379	2.432747	-1.194161
5	6	0	2.087740	3.313600	0.235149
6	1	0	2.907528	3.436482	0.941616
7	1	0	2.445214	3.509114	-0.778115
8	1	0	1.287705	4.016640	0.475290
9	6	0	-0.807159	-0.312798	-1.145264
10	1	0	-0.975009	0.281719	-2.045226
11	1	0	-0.660243	-1.358938	-1.427795
12	6	0	1.070473	-0.663524	0.605894
13	1	0	0.627640	-1.664110	0.560074
14	6	0	5.222551	-1.245576	-0.512486
15	6	0	4.902231	-0.874919	0.788247
16	6	0	3.572045	-0.680314	1.158391
17	6	0	2.544369	-0.837814	0.230042
18	6	0	2.876338	-1.210157	-1.075719
19	6	0	4.200254	-1.416430	-1.444880
20	1	0	6.256436	-1.400472	-0.799726
21	1	0	5.688031	-0.737971	1.523429
22	1	0	3.332273	-0.402464	2.177509
23	1	0	2.086538	-1.334321	-1.810412
24	1	0	4.437095	-1.706611	-2.462902
25	8	0	0.947086	-0.284690	1.987342
26	1	0	1.183392	0.651741	2.022493
27	7	0	-2.211949	-0.338285	-0.471193
28	6	0	-3.202856	-0.942091	-1.418732
29	6	0	-2.183821	-1.166211	0.776724
30	6	0	-2.671550	1.044537	-0.120292
31	6	0	-4.617301	-0.778141	-0.820747
32	1	0	-2.920950	-1.988902	-1.540360

33	1	0	-3.095876	-0.429119	-2.374508
34	6	0	-3.635390	-1.353097	1.272443
35	1	0	-1.555376	-0.634955	1.491467
36	1	0	-1.712922	-2.116742	0.523979
37	6	0	-3.974014	0.930269	0.704375
38	1	0	-1.867585	1.522394	0.437050
39	1	0	-2.818140	1.570954	-1.064401
40	7	0	-4.543511	-0.417630	0.599804
41	1	0	-5.173845	-1.709595	-0.929988
42	1	0	-5.162596	0.009698	-1.342800
43	1	0	-3.680812	-1.185876	2.348988
44	1	0	-3.979117	-2.368639	1.069636
45	1	0	-3.777837	1.135151	1.758047
46	1	0	-4.701405	1.658719	0.344308

TS 11 (M062X/6-311G(d,p) in Methanol)



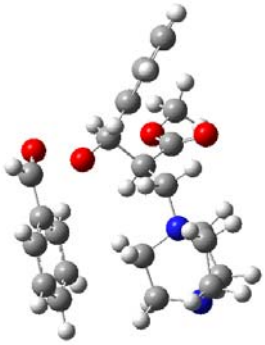
Imaginary Frequency: -162.9545 cm^{-1}
E(RM062X) = -997.254119584

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.441801	0.171848	0.597843
2	6	0	-0.701001	1.589499	0.451143
3	8	0	-1.626895	1.846903	-0.504675
4	8	0	-0.177603	2.501438	1.075879
5	6	0	-1.985938	3.219874	-0.687724
6	1	0	-2.744179	3.224562	-1.467578
7	1	0	-2.394496	3.631673	0.235896
8	1	0	-1.119937	3.804830	-1.000261
9	6	0	0.539636	-0.216379	1.469757
10	1	0	0.923703	0.499074	2.190044
11	1	0	0.640674	-1.263888	1.736079
12	6	0	-1.143773	-0.812647	-0.306501
13	1	0	-0.748589	-1.805100	-0.067476
14	6	0	-5.422888	-1.043799	0.325413
15	6	0	-4.913777	-0.976603	-0.966768
16	6	0	-3.538821	-0.895298	-1.178302
17	6	0	-2.655988	-0.868938	-0.099975
18	6	0	-3.174569	-0.937120	1.195382
19	6	0	-4.545764	-1.027289	1.407701
20	1	0	-6.492473	-1.107451	0.490100
21	1	0	-5.586757	-0.988434	-1.817121
22	1	0	-3.152172	-0.850416	-2.189075
23	1	0	-2.496969	-0.917629	2.042888
24	1	0	-4.931073	-1.081307	2.419923
25	8	0	-0.812247	-0.617757	-1.684076
26	1	0	-1.095335	0.276718	-1.916150
27	7	0	2.416106	-0.304288	0.535546
28	6	0	3.515114	-0.338245	1.509136
29	6	0	2.453938	-1.517669	-0.293038
30	6	0	2.556103	0.875043	-0.325554

31	6	0	4.863090	-0.246949	0.736388
32	1	0	3.433861	-1.271523	2.072193
33	1	0	3.391430	0.496192	2.203514
34	6	0	3.870441	-1.657340	-0.912017
35	1	0	1.682083	-1.415127	-1.060107
36	1	0	2.204181	-2.375624	0.335997
37	6	0	3.832441	0.708592	-1.195191
38	1	0	1.652688	0.956854	-0.937812
39	1	0	2.616405	1.754041	0.320838
40	7	0	4.638796	-0.420513	-0.706307
41	1	0	5.559607	-1.013705	1.081342
42	1	0	5.331116	0.728332	0.888909
43	1	0	3.806934	-1.861127	-1.982789
44	1	0	4.419223	-2.477351	-0.443463
45	1	0	3.573271	0.509149	-2.237438
46	1	0	4.437794	1.616716	-1.166313

_(S,R,R)_-TS 12 (M062X/6-311G(d,p) in Methanol)



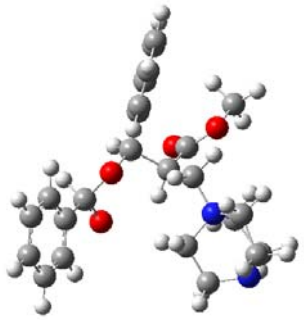
Imaginary Frequency: -92.8637 cm^{-1}
E(RM062X) = -1342.79971535

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.803400	1.723656	0.563247
2	6	0	-0.293656	-1.168212	-0.536239
3	1	0	-0.980478	-2.015431	-0.520732
4	1	0	-0.288842	-0.715765	-1.528164
5	6	0	-0.694401	-0.120553	0.485052
6	1	0	0.161432	0.433796	0.875744
7	6	0	-1.426605	-0.702017	1.660404
8	8	0	-1.541888	0.189986	2.646436
9	8	0	-1.905612	-1.812848	1.727995
10	6	0	-2.308257	-0.221614	3.788222
11	1	0	-2.341089	0.642528	4.446469
12	1	0	-3.315977	-0.507585	3.484730
13	1	0	-1.819792	-1.059387	4.287161
14	6	0	-1.546934	1.018099	-0.252383
15	8	0	-0.795390	1.585685	-1.218160
16	6	0	0.060028	3.474449	-0.297662
17	1	0	-0.220983	3.868679	-1.282789
18	8	0	-0.623990	3.693646	0.693292
19	6	0	4.076754	2.028628	-0.021919
20	6	0	3.309045	2.172548	1.133366
21	6	0	1.999349	2.631878	1.044695
22	6	0	1.451810	2.945343	-0.199860
23	6	0	2.220414	2.797633	-1.353046
24	6	0	3.530972	2.338850	-1.265810
25	1	0	5.099690	1.675409	0.047667
26	1	0	3.735197	1.931856	2.101038
27	1	0	1.393764	2.756823	1.936098

28	1	0	1.785232	3.041229	-2.317670
29	1	0	4.127274	2.225979	-2.164329
30	6	0	-5.272400	-0.718205	-1.642696
31	6	0	-4.229797	-0.484367	-2.534325
32	6	0	-3.039616	0.085862	-2.087992
33	6	0	-2.868974	0.421266	-0.745224
34	6	0	-3.928633	0.196920	0.139062
35	6	0	-5.119835	-0.370125	-0.302230
36	1	0	-6.201039	-1.156728	-1.990691
37	1	0	-4.345524	-0.739615	-3.582227
38	1	0	-2.234574	0.292221	-2.784440
39	1	0	-3.826851	0.485851	1.182591
40	1	0	-5.932235	-0.531892	0.397801
41	7	0	1.087131	-1.740602	-0.360007
42	6	0	1.321275	-2.245320	1.037818
43	6	0	2.139510	-0.716142	-0.696179
44	6	0	1.253047	-2.900491	-1.307499
45	6	0	2.640503	-3.048631	1.043726
46	1	0	1.369854	-1.370556	1.687279
47	1	0	0.461384	-2.855602	1.312195
48	1	0	2.045580	-0.525099	-1.766197
49	1	0	1.910388	0.196148	-0.150234
50	6	0	3.514789	-1.297725	-0.309133
51	6	0	2.740702	-3.308278	-1.319921
52	1	0	0.900257	-2.571787	-2.284589
53	1	0	0.603646	-3.693722	-0.936003
54	1	0	3.216336	-2.796004	1.934411
55	1	0	2.433553	-4.119630	1.062220
56	7	0	3.437606	-2.755581	-0.152953
57	1	0	4.244604	-1.049405	-1.081091
58	1	0	3.858346	-0.871600	0.635375
59	1	0	3.232459	-2.935937	-2.219754
60	1	0	2.819137	-4.395682	-1.312257

***(S,R,R)*-Intermediate 13 (M062X/6-311G(d,p) in Methanol)**



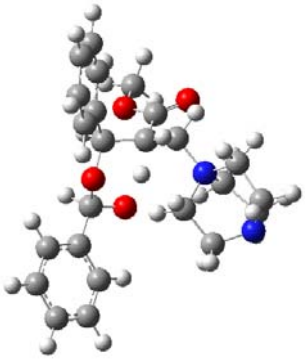
E(RM062X) = -1342.80627244

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.190244	-1.847469	-1.740511
2	6	0	-1.006188	0.536681	0.621473
3	1	0	-1.930454	0.319049	1.156084
4	1	0	-0.161515	0.181037	1.212115
5	6	0	-0.984032	-0.106151	-0.759506
6	1	0	-0.405304	0.481020	-1.472120
7	6	0	-2.329127	-0.339072	-1.404736
8	8	0	-3.356838	-0.327321	-0.561798
9	8	0	-2.450448	-0.566421	-2.587161
10	6	0	-4.641125	-0.635189	-1.127428
11	1	0	-5.347433	-0.571279	-0.304135
12	1	0	-4.890500	0.087649	-1.904403

13	1	0	-4.631209	-1.643059	-1.544489
14	6	0	-0.195001	-1.459030	-0.714317
15	8	0	1.111419	-1.204004	-0.281668
16	6	0	2.056761	-0.934616	-1.418544
17	1	0	2.060899	-1.908899	-1.959151
18	8	0	1.702266	0.086558	-2.169621
19	6	0	5.900579	-0.555558	0.549526
20	6	0	5.468016	0.415404	-0.347316
21	6	0	4.226444	0.288952	-0.968678
22	6	0	3.404860	-0.800959	-0.698602
23	6	0	3.848812	-1.776613	0.197699
24	6	0	5.086780	-1.655454	0.819938
25	1	0	6.866662	-0.460971	1.033093
26	1	0	6.098004	1.270611	-0.567768
27	1	0	3.883263	1.033841	-1.677372
28	1	0	3.217824	-2.635023	0.407870
29	1	0	5.420844	-2.418203	1.515145
30	6	0	-2.261027	-4.236298	1.860719
31	6	0	-1.162495	-3.531659	2.341756
32	6	0	-0.474038	-2.650098	1.511397
33	6	0	-0.879995	-2.464241	0.190147
34	6	0	-1.975003	-3.187369	-0.290989
35	6	0	-2.663767	-4.065155	0.538503
36	1	0	-2.795717	-4.922019	2.508124
37	1	0	-0.836429	-3.668335	3.366789
38	1	0	0.386966	-2.110331	1.888708
39	1	0	-2.283528	-3.071268	-1.326456
40	1	0	-3.509508	-4.621578	0.150021
41	7	0	-0.863535	2.033702	0.595771
42	6	0	-1.147822	2.573929	1.975009
43	6	0	-1.828603	2.680706	-0.362874
44	6	0	0.545877	2.432846	0.233288
45	6	0	-0.739532	4.062390	2.004212
46	1	0	-2.214575	2.427901	2.148496
47	1	0	-0.579264	1.970143	2.681999
48	1	0	-1.499539	2.425756	-1.370052
49	1	0	-2.811819	2.248738	-0.175579
50	6	0	-1.799134	4.205311	-0.118934
51	6	0	0.564478	3.958026	0.014432
52	1	0	0.853688	1.873924	-0.650201
53	1	0	1.166772	2.124678	1.076055
54	1	0	-1.495640	4.634839	2.542256
55	1	0	0.215401	4.188251	2.516343
56	7	0	-0.604565	4.587664	0.640839
57	1	0	-1.803310	4.723971	-1.077813
58	1	0	-2.679043	4.519273	0.444478
59	1	0	0.548528	4.193309	-1.050865
60	1	0	1.477387	4.373686	0.442012

_(S,R,R)_-TS 14 (M062X/6-311G(d,p) in Methanol)



Imaginary Frequency: -1322.5123 cm^{-1}
E(RM062X) = -1342.79095531

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.302805	-1.791329	1.374788
2	6	0	1.270481	1.115034	-0.524983
3	1	0	2.185434	1.710036	-0.542307
4	1	0	1.236601	0.512422	-1.435127
5	6	0	1.199692	0.254836	0.715937
6	1	0	0.045929	0.270437	1.362148
7	6	0	2.153890	0.660999	1.742882
8	8	0	2.330744	-0.260795	2.713807
9	8	0	2.706820	1.750355	1.812749
10	6	0	3.150092	0.136421	3.818023
11	1	0	3.185983	-0.724635	4.481435
12	1	0	4.155340	0.392046	3.480875
13	1	0	2.707615	0.989244	4.334777
14	6	0	1.053775	-1.260818	0.448954
15	8	0	-0.296475	-1.554476	0.115980
16	6	0	-1.164253	-1.410999	1.267104
17	1	0	-0.824111	-2.176725	1.989930
18	8	0	-1.089814	-0.154860	1.802737
19	6	0	-5.115260	-2.513598	-0.079279
20	6	0	-4.930004	-1.350101	0.659164
21	6	0	-3.653974	-0.989036	1.088631
22	6	0	-2.555760	-1.787336	0.781048
23	6	0	-2.747706	-2.959399	0.046413
24	6	0	-4.019418	-3.319781	-0.384379
25	1	0	-6.107447	-2.795806	-0.413164
26	1	0	-5.779212	-0.721527	0.904172
27	1	0	-3.504702	-0.086197	1.668297
28	1	0	-1.894884	-3.587963	-0.188694
29	1	0	-4.158665	-4.230932	-0.955690
30	6	0	3.733342	-2.646076	-2.634361
31	6	0	2.361371	-2.681855	-2.852287
32	6	0	1.478274	-2.248959	-1.863166
33	6	0	1.963831	-1.774762	-0.646528
34	6	0	3.345190	-1.737321	-0.434551
35	6	0	4.224130	-2.172238	-1.418125
36	1	0	4.417883	-2.986007	-3.403155
37	1	0	1.971371	-3.048244	-3.795672
38	1	0	0.410104	-2.279600	-2.040826
39	1	0	3.731028	-1.368626	0.512152
40	1	0	5.292707	-2.144738	-1.236415
41	7	0	0.151549	2.125831	-0.705021
42	6	0	-0.068574	2.954699	0.531783
43	6	0	-1.142741	1.450745	-1.069019
44	6	0	0.522661	3.055820	-1.828254
45	6	0	-1.003220	4.127885	0.164749
46	1	0	-0.513434	2.295688	1.276039
47	1	0	0.908328	3.288092	0.878521
48	1	0	-0.995766	1.018173	-2.060028
49	1	0	-1.311039	0.658767	-0.344638
50	6	0	-2.262290	2.511372	-1.042851
51	6	0	-0.711780	3.908144	-2.184917
52	1	0	0.857922	2.440768	-2.663322
53	1	0	1.356970	3.658392	-1.467278
54	1	0	-1.736827	4.269291	0.959029
55	1	0	-0.434870	5.053220	0.056774
56	7	0	-1.699654	3.866303	-1.100664
57	1	0	-2.932138	2.356488	-1.889292
58	1	0	-2.846783	2.425152	-0.124682
59	1	0	-1.185361	3.535252	-3.094269
60	1	0	-0.404743	4.940074	-2.358689

***(S,R,R)*-TS 14 (M062X/6-311G(d,p) in THF)**

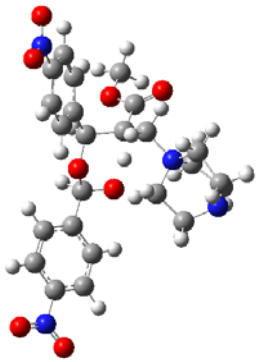
Imaginary Frequency: -1159.5176 cm^{-1}
E(RM062X) = -1342.77701528

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.462103	-1.629548	1.456025
2	6	0	1.129684	1.148700	-0.597527
3	1	0	1.991111	1.810761	-0.698451
4	1	0	1.083157	0.496834	-1.472901
5	6	0	1.207621	0.360735	0.689208
6	1	0	0.099667	0.347994	1.361462
7	6	0	2.219945	0.901225	1.603093
8	8	0	2.583445	0.034557	2.574844
9	8	0	2.667848	2.032501	1.571728
10	6	0	3.473015	0.551744	3.564247
11	1	0	3.666232	-0.270840	4.249467
12	1	0	4.405482	0.888107	3.108940
13	1	0	3.013321	1.384394	4.098869
14	6	0	1.156896	-1.174754	0.505335
15	8	0	-0.169038	-1.566961	0.209818
16	6	0	-1.049982	-1.382664	1.354807
17	1	0	-0.668466	-2.085029	2.124701
18	8	0	-1.063675	-0.103870	1.794442
19	6	0	-4.916347	-2.796948	0.046360
20	6	0	-4.804487	-1.587984	0.725259
21	6	0	-3.554422	-1.133907	1.142974
22	6	0	-2.410476	-1.881973	0.883258
23	6	0	-2.527817	-3.097670	0.206867
24	6	0	-3.773242	-3.552119	-0.212090
25	1	0	-5.887500	-3.151435	-0.280354
26	1	0	-5.691198	-0.998904	0.933077
27	1	0	-3.442236	-0.196081	1.674126
28	1	0	-1.634808	-3.678646	0.002440
29	1	0	-3.855741	-4.495562	-0.740564
30	6	0	3.827305	-2.539990	-2.597291
31	6	0	2.454725	-2.694642	-2.750703
32	6	0	1.581621	-2.270663	-1.749481
33	6	0	2.075664	-1.685058	-0.585896
34	6	0	3.457067	-1.530711	-0.438241
35	6	0	4.327158	-1.957296	-1.433646
36	1	0	4.505310	-2.873099	-3.374653
37	1	0	2.057308	-3.147807	-3.652215
38	1	0	0.511338	-2.393652	-1.862720
39	1	0	3.850139	-1.081894	0.469400
40	1	0	5.396826	-1.838404	-1.301468
41	7	0	-0.073626	2.068388	-0.751611
42	6	0	-0.321731	2.883856	0.490593
43	6	0	-1.322351	1.291076	-1.070654
44	6	0	0.191370	3.012231	-1.892257
45	6	0	-1.342994	3.989097	0.138856
46	1	0	-0.713018	2.193239	1.236375
47	1	0	0.640768	3.272878	0.821018
48	1	0	-1.172641	0.867196	-2.065175
49	1	0	-1.404307	0.495752	-0.334741
50	6	0	-2.517122	2.267371	-1.013327
51	6	0	-1.116755	3.767030	-2.216629
52	1	0	0.549669	2.416069	-2.731640
53	1	0	0.987330	3.680759	-1.561372
54	1	0	-2.060854	4.092595	0.953369
55	1	0	-0.844880	4.950242	-0.001546
56	7	0	-2.055727	3.657406	-1.098915
57	1	0	-3.203594	2.058897	-1.834912
58	1	0	-3.061623	2.146585	-0.074513
59	1	0	-1.591774	3.350011	-3.106330

60	1	0	-0.896361	4.818092	-2.407396

Nitro-substituted *(S,R,R)*-TS 14 (M062X/6-311G(d,p) in THF)



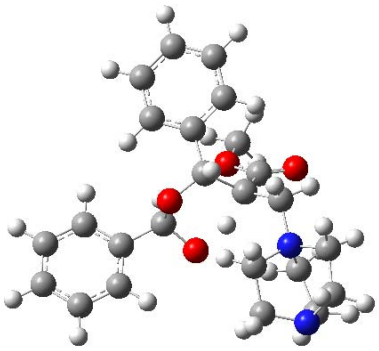
Imaginary Frequency: -1200.778 cm-1
E(RM062X) = -1751.75401536

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.194085	-0.482135	2.306499
2	6	0	1.363713	1.496070	-0.539821
3	1	0	2.291701	2.045852	-0.705390
4	1	0	1.371356	0.601013	-1.165695
5	6	0	1.189673	1.161148	0.923886
6	1	0	-0.022505	1.366665	1.376841
7	6	0	2.087375	1.944721	1.780498
8	8	0	2.226932	1.428392	3.021310
9	8	0	2.623809	2.991348	1.470208
10	6	0	3.006440	2.205466	3.931712
11	1	0	3.013864	1.648393	4.865913
12	1	0	4.024453	2.328581	3.559276
13	1	0	2.557489	3.188077	4.082917
14	6	0	1.073233	-0.350730	1.224354
15	8	0	-0.206561	-0.812384	0.839417
16	6	0	-1.239456	-0.271890	1.707069
17	1	0	-1.035865	-0.704024	2.708119
18	8	0	-1.246670	1.079415	1.724444
19	6	0	-4.901297	-1.966570	0.288591
20	6	0	-4.866696	-0.618038	0.610089
21	6	0	-3.669268	-0.079738	1.064785
22	6	0	-2.537090	-0.879912	1.190940
23	6	0	-2.605327	-2.236469	0.865303
24	6	0	-3.789933	-2.791978	0.408306
25	1	0	-5.757484	-0.013092	0.506805
26	1	0	-3.593459	0.967926	1.327608
27	1	0	-1.720606	-2.854304	0.963220
28	1	0	-3.861404	-3.839044	0.147125
29	6	0	4.106071	-2.612342	-0.758664
30	6	0	2.788156	-2.801146	-1.142316
31	6	0	1.796167	-2.080736	-0.487786
32	6	0	2.125591	-1.184013	0.527874
33	6	0	3.466503	-1.016939	0.890756
34	6	0	4.466776	-1.731927	0.254368
35	1	0	2.548154	-3.496825	-1.934998
36	1	0	0.757795	-2.213930	-0.762147
37	1	0	3.726640	-0.327163	1.687017
38	1	0	5.505826	-1.617582	0.531233
39	7	0	0.285623	2.372947	-1.161298
40	6	0	-0.050120	3.554603	-0.290120
41	6	0	-0.975147	1.591420	-1.418740
42	6	0	0.790992	2.886853	-2.481309

43	6	0	-0.911327	4.531168	-1.122439
44	1	0	-0.595035	3.159551	0.566301
45	1	0	0.890888	3.987378	0.047066
46	1	0	-0.729526	0.864363	-2.194654
47	1	0	-1.231108	1.078551	-0.495200
48	6	0	-2.070094	2.587045	-1.860969
49	6	0	-0.383120	3.558312	-3.226816
50	1	0	1.201354	2.036530	-3.026417
51	1	0	1.595620	3.586858	-2.253216
52	1	0	-1.722089	4.917086	-0.503522
53	1	0	-0.314676	5.376746	-1.469594
54	7	0	-1.473594	3.854143	-2.295156
55	1	0	-2.650010	2.157130	-2.678680
56	1	0	-2.750404	2.797437	-1.033264
57	1	0	-0.768974	2.901978	-4.008661
58	1	0	-0.040069	4.482398	-3.693734
59	7	0	-6.164100	-2.548245	-0.195100
60	8	0	-6.183647	-3.735734	-0.445936
61	8	0	-7.119725	-1.810090	-0.318275
62	7	0	5.161969	-3.370495	-1.447505
63	8	0	6.303990	-3.233524	-1.059829
64	8	0	4.836099	-4.091065	-2.368173

***(S,S,R)*-TS 14 (M062X/6-311G(d,p) in Methanol)**



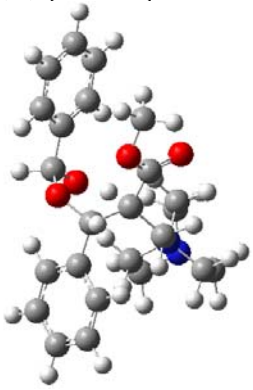
Imaginary Frequency: -1234.7988 cm^{-1}
E(RM062X) = -1342.78484184

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.119578	-3.314574	-1.057907
2	6	0	-4.300268	-1.940137	-0.961795
3	6	0	-3.199263	-1.084987	-0.921080
4	6	0	-1.906303	-1.597563	-0.959638
5	6	0	-1.730579	-2.980388	-1.070693
6	6	0	-2.826382	-3.832937	-1.120526
7	1	0	-4.975779	-3.978754	-1.088279
8	1	0	-5.301833	-1.526341	-0.919389
9	1	0	-3.347329	-0.013792	-0.859111
10	1	0	-0.725524	-3.393227	-1.111784
11	1	0	-2.672635	-4.903081	-1.205343
12	6	0	1.733971	-1.532234	-0.600627
13	1	0	2.102649	-2.476747	-0.198862
14	1	0	1.634469	-1.630128	-1.683401
15	6	0	0.438312	-1.118318	0.055954
16	1	0	0.465385	0.004247	0.702515
17	6	0	0.074120	-2.006956	1.166387
18	8	0	-1.118434	-1.696840	1.702751
19	8	0	0.766412	-2.891332	1.647242
20	6	0	-1.601184	-2.565279	2.730995
21	1	0	-2.587952	-2.189862	2.993021

22	1	0	-1.676791	-3.588380	2.357983
23	1	0	-0.944609	-2.536914	3.601484
24	6	0	-0.679556	-0.694157	-0.940106
25	1	0	-0.236263	-0.767201	-1.938206
26	8	0	-1.031346	0.685854	-0.845833
27	6	0	-1.144763	1.211885	0.509080
28	1	0	-1.885220	0.582299	1.029303
29	8	0	0.072025	1.196658	1.123381
30	6	0	-2.803500	5.151025	-0.061712
31	6	0	-1.422529	4.972427	-0.028216
32	6	0	-0.887021	3.703501	0.172716
33	6	0	-1.726071	2.603261	0.335780
34	6	0	-3.107232	2.788067	0.306610
35	6	0	-3.646437	4.056186	0.108623
36	1	0	-3.221174	6.140220	-0.213001
37	1	0	-0.762496	5.823506	-0.154711
38	1	0	0.187047	3.560349	0.212643
39	1	0	-3.763944	1.934547	0.447724
40	1	0	-4.722152	4.191516	0.092548
41	7	0	2.878864	-0.555989	-0.411842
42	6	0	3.148511	-0.293536	1.045694
43	6	0	2.592212	0.750315	-1.098583
44	6	0	4.125631	-1.138046	-1.019462
45	6	0	4.482665	0.476537	1.156394
46	1	0	2.314080	0.293183	1.425309
47	1	0	3.175141	-1.260099	1.549182
48	1	0	2.596639	0.539191	-2.169080
49	1	0	1.599227	1.076536	-0.793808
50	6	0	3.688812	1.755721	-0.688238
51	6	0	5.210046	-0.040656	-1.046292
52	1	0	3.867799	-1.491224	-2.017833
53	1	0	4.404274	-1.989133	-0.397027
54	1	0	4.380607	1.272451	1.894755
55	1	0	5.286600	-0.186824	1.478821
56	7	0	4.857267	1.055990	-0.138691
57	1	0	3.988689	2.342980	-1.556801
58	1	0	3.311517	2.440783	0.073393
59	1	0	5.318249	0.368317	-2.051918
60	1	0	6.167461	-0.468094	-0.746859

_(S,R,S)_-TS 14 (M062X/6-311G(d,p) in Methanol)



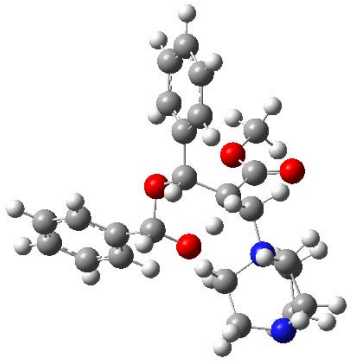
Imaginary Frequency: -1308.0401 cm^{-1}
E(RM062X) = -1342.78115326

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.375339	3.627691	-0.335870
2	6	0	-2.477923	3.274517	-1.339689
3	6	0	-1.280648	2.639797	-1.021416

4	6	0	-0.968916	2.336957	0.304244
5	6	0	-1.856189	2.731760	1.307821
6	6	0	-3.056142	3.362432	0.993285
7	1	0	-4.307253	4.122614	-0.584826
8	1	0	-2.708965	3.496163	-2.376005
9	1	0	-0.591315	2.364492	-1.810378
10	1	0	-1.604579	2.541519	2.347496
11	1	0	-3.734926	3.656834	1.785991
12	6	0	-1.182340	-0.457549	1.437572
13	1	0	-1.862373	0.319878	1.784258
14	1	0	-1.000159	-1.142777	2.265450
15	6	0	0.127049	0.082389	0.906654
16	1	0	0.303017	-0.186160	-0.374599
17	6	0	0.311390	1.610702	0.679222
18	1	0	0.682462	2.075142	1.598480
19	8	0	1.330195	1.888017	-0.287462
20	6	0	1.591407	0.958215	-1.387509
21	1	0	1.717614	1.625178	-2.254707
22	8	0	0.577789	0.075404	-1.594477
23	6	0	5.456484	-0.897063	-0.763900
24	6	0	4.348675	-1.680438	-1.065835
25	6	0	3.099464	-1.086500	-1.252167
26	6	0	2.947352	0.291245	-1.132500
27	6	0	4.064498	1.073310	-0.826824
28	6	0	5.310153	0.485014	-0.642571
29	1	0	6.428639	-1.356488	-0.623070
30	1	0	4.453590	-2.755978	-1.160737
31	1	0	2.236790	-1.693467	-1.502458
32	1	0	3.952233	2.148725	-0.729542
33	1	0	6.169951	1.102080	-0.404545
34	6	0	1.252146	-0.563400	1.590776
35	8	0	2.291967	0.247971	1.842337
36	8	0	1.291154	-1.747728	1.901708
37	6	0	3.471151	-0.372221	2.362512
38	1	0	4.211278	0.420721	2.444046
39	1	0	3.822417	-1.151150	1.683557
40	1	0	3.274941	-0.803379	3.345486
41	7	0	-2.026583	-1.279472	0.469182
42	6	0	-3.240455	-1.783946	1.202559
43	6	0	-2.508375	-0.450724	-0.690349
44	6	0	-1.271437	-2.472758	-0.047682
45	6	0	-3.975896	-2.795033	0.296146
46	1	0	-3.848038	-0.907655	1.432386
47	1	0	-2.899089	-2.238510	2.131989
48	1	0	-1.632784	-0.201777	-1.287999
49	1	0	-2.933990	0.462574	-0.273440
50	6	0	-3.552501	-1.272028	-1.479275
51	6	0	-2.118569	-3.139228	-1.151657
52	1	0	-0.307391	-2.132314	-0.420818
53	1	0	-1.110946	-3.127287	0.810088
54	1	0	-5.049328	-2.607457	0.336278
55	1	0	-3.793675	-3.815139	0.637733
56	7	0	-3.512380	-2.685272	-1.090581
57	1	0	-3.350764	-1.186103	-2.547442
58	1	0	-4.558599	-0.894431	-1.289861
59	1	0	-1.723388	-2.888075	-2.137309
60	1	0	-2.081706	-4.222727	-1.033829

_(S,S,S)_-TS 14 (M062X/6-311G(d,p) in Methanol)



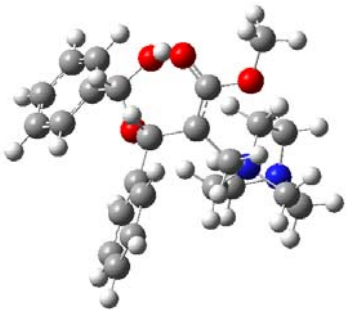
Imaginary Frequency: -1308.2792 cm^{-1}
E(RM062X) = -1342.78831055

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.245922	0.565231	-1.716338
2	6	0	-1.910067	1.030698	-0.376322
3	1	0	-1.827309	1.261747	-1.439698
4	1	0	-2.407872	1.864050	0.122047
5	6	0	-0.570744	0.727150	0.248797
6	1	0	-0.332024	-0.540206	0.558309
7	6	0	0.636994	0.831660	-0.723330
8	8	0	1.668497	-0.087876	-0.397736
9	6	0	1.202985	-1.453980	-0.374860
10	1	0	0.736580	-1.626987	-1.365720
11	8	0	0.310807	-1.657092	0.640079
12	6	0	4.764960	-3.875033	-0.134192
13	6	0	3.753780	-4.034700	0.807169
14	6	0	2.600100	-3.255110	0.736536
15	6	0	2.451676	-2.313131	-0.275905
16	6	0	3.468542	-2.157205	-1.220349
17	6	0	4.619782	-2.932142	-1.151003
18	1	0	5.662397	-4.481130	-0.078971
19	1	0	3.861757	-4.766489	1.600296
20	1	0	1.809955	-3.372752	1.468127
21	1	0	3.354542	-1.420905	-2.009804
22	1	0	5.404416	-2.803411	-1.888449
23	6	0	-0.406808	1.372666	1.551835
24	8	0	0.857032	1.311403	2.006140
25	8	0	-1.297285	1.862765	2.232438
26	6	0	1.115513	1.951378	3.258204
27	1	0	2.182717	1.834092	3.433736
28	1	0	0.549734	1.473695	4.059334
29	1	0	0.858336	3.010666	3.207359
30	6	0	2.274162	4.823166	-0.966619
31	6	0	2.992834	3.818384	-0.326828
32	6	0	2.480765	2.525462	-0.251010
33	6	0	1.242134	2.220832	-0.815136
34	6	0	0.528204	3.233656	-1.460509
35	6	0	1.038481	4.525518	-1.535285
36	1	0	2.674387	5.828842	-1.027168
37	1	0	3.957315	4.038720	0.117529
38	1	0	3.041903	1.747945	0.251765
39	1	0	-0.429843	3.011027	-1.920160
40	1	0	0.474372	5.298630	-2.045188
41	7	0	-2.920062	-0.105203	-0.325024
42	6	0	-4.208839	0.364491	-0.942873
43	6	0	-2.437523	-1.300640	-1.103361
44	6	0	-3.205701	-0.531357	1.087591
45	6	0	-5.292801	-0.702232	-0.682896
46	1	0	-4.006685	0.506624	-2.005252
47	1	0	-4.456704	1.324352	-0.491151

48	1	0	-1.606357	-1.726568	-0.542329
49	1	0	-2.083410	-0.935424	-2.067714
50	6	0	-3.615640	-2.289970	-1.247580
51	6	0	-4.076840	-1.805523	1.037019
52	1	0	-2.254594	-0.709093	1.585906
53	1	0	-3.712591	0.307667	1.565584
54	1	0	-5.886234	-0.846464	-1.586256
55	1	0	-5.960142	-0.382029	0.118599
56	7	0	-4.680801	-1.975666	-0.289443
57	1	0	-3.258943	-3.305763	-1.074430
58	1	0	-4.037196	-2.242356	-2.252935
59	1	0	-3.472811	-2.688238	1.253109
60	1	0	-4.863671	-1.737217	1.789214

***(S,R)*-Intermediate 15 (M062X/6-311G(d,p) in Methanol)**



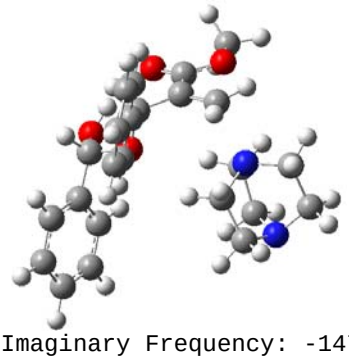
E(RM062X) = -1342.81448472

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.462755	1.509576	2.014763
2	6	0	-2.232867	0.370894	0.196909
3	1	0	-3.203631	0.165340	0.648334
4	1	0	-2.306682	1.289940	-0.390603
5	6	0	-1.159688	0.420093	1.212923
6	1	0	0.848750	-1.066718	2.473113
7	6	0	0.101670	1.217036	1.021805
8	8	0	1.191398	0.498741	0.384931
9	6	0	2.061271	-0.180696	1.258322
10	1	0	2.321298	0.498762	2.083084
11	8	0	1.492357	-1.346118	1.783875
12	6	0	5.629981	-1.103015	-0.974995
13	6	0	5.040546	-2.078837	-0.179445
14	6	0	3.883137	-1.792663	0.542160
15	6	0	3.306164	-0.527733	0.468314
16	6	0	3.903057	0.451280	-0.328972
17	6	0	5.059116	0.166138	-1.045835
18	1	0	6.530312	-1.327463	-1.535853
19	1	0	5.480225	-3.068028	-0.116905
20	1	0	3.429292	-2.553310	1.164502
21	1	0	3.459901	1.439757	-0.384798
22	1	0	5.514544	0.933675	-1.661541
23	6	0	-0.652662	4.873152	-1.161058
24	6	0	0.190410	3.912850	-1.705604
25	6	0	0.456352	2.731116	-1.012473
26	6	0	-0.125465	2.494798	0.231193
27	6	0	-0.970817	3.468189	0.773238
28	6	0	-1.231579	4.647305	0.087532
29	1	0	-0.857961	5.791223	-1.699861
30	1	0	0.648457	4.078356	-2.674798
31	1	0	1.119160	1.992174	-1.445667
32	1	0	-1.431348	3.290619	1.740728
33	1	0	-1.887445	5.391676	0.525484

34	6	0	-1.305556	-0.245577	2.423559
35	8	0	-2.513348	-0.876220	2.619345
36	8	0	-0.442473	-0.333728	3.340811
37	6	0	-2.684868	-1.545154	3.865332
38	1	0	-3.683338	-1.978499	3.831522
39	1	0	-1.944342	-2.336371	3.996109
40	1	0	-2.617101	-0.846224	4.701215
41	7	0	-2.099081	-0.726384	-0.889721
42	6	0	-1.806107	-2.070666	-0.291340
43	6	0	-1.005684	-0.388886	-1.860021
44	6	0	-3.390049	-0.817898	-1.646773
45	6	0	-1.945332	-3.134122	-1.403694
46	1	0	-0.796859	-2.016920	0.117379
47	1	0	-2.512542	-2.225928	0.522616
48	1	0	-1.329948	0.508254	-2.390249
49	1	0	-0.111432	-0.168140	-1.280344
50	6	0	-0.802550	-1.592516	-2.805741
51	6	0	-3.175289	-1.726246	-2.876937
52	1	0	-3.679107	0.196171	-1.923448
53	1	0	-4.127898	-1.225335	-0.954538
54	1	0	-1.119943	-3.843963	-1.337489
55	1	0	-2.879755	-3.686060	-1.289141
56	7	0	-1.943627	-2.511589	-2.733158
57	1	0	-0.686429	-1.236842	-3.830155
58	1	0	0.097935	-2.145692	-2.532896
59	1	0	-3.094965	-1.128421	-3.786272
60	1	0	-4.025568	-2.400235	-2.986221

***(S,R)*-TS 16 (M062X/6-311G(d,p) in Methanol)**



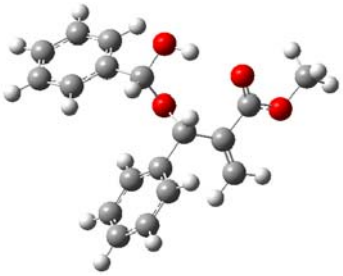
Imaginary Frequency: -147.3279 cm^{-1}
E(RM062X) = -1342.79661098

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.682535	2.132565	1.647027
2	6	0	-2.032213	1.456439	-0.175134
3	1	0	-3.102311	1.436376	-0.009720
4	1	0	-1.702822	1.819854	-1.142771
5	6	0	-1.175141	1.457357	0.884002
6	1	0	0.851369	0.309976	3.128850
7	6	0	0.319364	1.601246	0.758824
8	8	0	0.900059	0.284997	0.760078
9	6	0	2.025324	0.116301	1.598391
10	1	0	2.597028	1.053243	1.621380
11	8	0	1.614503	-0.245548	2.891707
12	6	0	4.337742	-3.031123	-0.189039
13	6	0	3.217297	-3.339140	0.580266
14	6	0	2.481362	-2.323112	1.180095
15	6	0	2.862803	-0.992294	1.011521
16	6	0	3.982634	-0.686339	0.242583
17	6	0	4.720586	-1.703946	-0.356507

18	1	0	4.910958	-3.824934	-0.654591
19	1	0	2.918833	-4.372868	0.713627
20	1	0	1.613068	-2.558881	1.785402
21	1	0	4.277609	0.350704	0.115043
22	1	0	5.594390	-1.459731	-0.950066
23	6	0	1.581173	3.890279	-2.677094
24	6	0	1.965194	2.560854	-2.556202
25	6	0	1.562894	1.808358	-1.451827
26	6	0	0.769589	2.381603	-0.461521
27	6	0	0.393316	3.722424	-0.584877
28	6	0	0.793700	4.471428	-1.683422
29	1	0	1.892570	4.473919	-3.536103
30	1	0	2.581484	2.101303	-3.321064
31	1	0	1.871765	0.773690	-1.361106
32	1	0	-0.219549	4.178038	0.187074
33	1	0	0.494081	5.510295	-1.765267
34	6	0	-1.631785	1.102795	2.218022
35	8	0	-2.951615	0.880327	2.319345
36	8	0	-0.902661	1.008017	3.201107
37	6	0	-3.428135	0.479239	3.608825
38	1	0	-4.494158	0.304054	3.484829
39	1	0	-2.929855	-0.436835	3.928663
40	1	0	-3.259469	1.267942	4.342942
41	7	0	-2.208747	-0.538342	-1.042154
42	6	0	-3.442908	-0.699888	-1.819498
43	6	0	-1.049442	-0.784714	-1.910518
44	6	0	-2.203109	-1.501318	0.063856
45	6	0	-3.577964	-2.193565	-2.232972
46	1	0	-3.379488	-0.044123	-2.691675
47	1	0	-4.288217	-0.376311	-1.206793
48	6	0	-1.222027	-2.163892	-2.603863
49	1	0	-0.156523	-0.758698	-1.281865
50	1	0	-0.980928	0.026820	-2.640008
51	6	0	-2.083421	-2.934080	-0.520287
52	1	0	-1.367277	-1.260822	0.727998
53	1	0	-3.134145	-1.372220	0.621949
54	7	0	-2.320492	-2.913236	-1.974009
55	1	0	-3.823640	-2.280665	-3.293375
56	1	0	-4.370141	-2.684252	-1.662557
57	1	0	-0.303527	-2.750017	-2.530084
58	1	0	-1.459985	-2.041428	-3.663148
59	1	0	-1.084913	-3.343986	-0.349699
60	1	0	-2.807349	-3.603787	-0.051376

_(S,R)_-Intermediate 17 (M062X/6-311G(d,p) in Methanol)



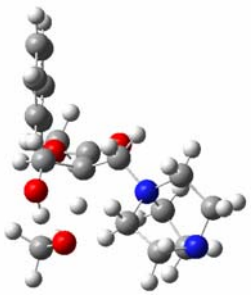
E(RM062X) = -997.513020428

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.219403	0.233343	1.447450
2	6	0	-2.837176	0.693383	-1.331106
3	1	0	-3.702417	0.309213	-1.857796
4	1	0	-2.493916	1.690558	-1.584092

5	6	0	-2.224697	-0.028753	-0.397531
6	1	0	-0.449319	-2.000587	1.687575
7	6	0	-1.006312	0.407302	0.385657
8	8	0	0.056778	-0.453529	-0.028285
9	6	0	0.938776	-0.837013	1.013275
10	1	0	0.954928	-0.041412	1.769446
11	8	0	0.512669	-2.049303	1.575741
12	6	0	4.810315	-1.269819	-0.791351
13	6	0	3.902935	-2.325507	-0.833491
14	6	0	2.655755	-2.199374	-0.230503
15	6	0	2.312527	-1.014340	0.417556
16	6	0	3.219802	0.041625	0.457377
17	6	0	4.468082	-0.085350	-0.145126
18	1	0	5.783129	-1.372123	-1.259124
19	1	0	4.167537	-3.248258	-1.337299
20	1	0	1.946931	-3.018728	-0.257721
21	1	0	2.948458	0.962577	0.964554
22	1	0	5.173469	0.736888	-0.106085
23	6	0	-0.039018	4.564560	-0.167324
24	6	0	0.633765	3.593446	-0.901807
25	6	0	0.332685	2.245056	-0.722934
26	6	0	-0.640997	1.862527	0.196787
27	6	0	-1.311997	2.838906	0.933876
28	6	0	-1.014733	4.184588	0.751700
29	1	0	0.197137	5.613372	-0.306901
30	1	0	1.396234	3.884015	-1.615819
31	1	0	0.857396	1.486780	-1.292644
32	1	0	-2.069136	2.540101	1.652800
33	1	0	-1.538571	4.937189	1.330129
34	6	0	-2.711474	-1.388719	-0.020387
35	8	0	-3.635021	-1.875186	-0.836312
36	8	0	-2.309797	-1.993618	0.952817
37	6	0	-4.163354	-3.167243	-0.493816
38	1	0	-4.890939	-3.397052	-1.267392
39	1	0	-3.363631	-3.908075	-0.487631
40	1	0	-4.644226	-3.126358	0.483753

_(S,R)_-TS 18 (M062X/6-311G(d,p) in Methanol)



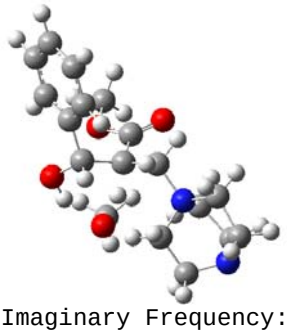
Imaginary Frequency: -1189.0478 cm^{-1}
E(RM062X) = -1112.97035197

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.075356	1.199703	1.253901
2	6	0	-0.237028	-0.555429	-0.638694
3	1	0	-0.109380	-0.534525	-1.722295
4	1	0	0.178899	-1.490467	-0.258324
5	6	0	0.416308	0.647015	0.011346
6	1	0	-0.348366	1.279577	0.847977
7	6	0	0.740969	1.694094	-0.963806
8	8	0	1.632017	2.600479	-0.514531
9	8	0	0.222447	1.820261	-2.062618

10	6	0	1.871232	3.726027	-1.366114
11	1	0	2.610580	4.333313	-0.849159
12	1	0	2.261133	3.400147	-2.331115
13	1	0	0.952053	4.295050	-1.513799
14	6	0	1.512116	0.286709	1.036682
15	8	0	0.904384	-0.183637	2.233430
16	1	0	0.221897	0.492352	2.443741
17	8	0	-0.898644	1.805705	1.952519
18	1	0	0.673566	3.109774	2.405079
19	6	0	4.291025	-2.636688	-0.505172
20	6	0	3.489927	-2.955478	0.584596
21	6	0	2.595045	-2.017564	1.100410
22	6	0	2.492755	-0.751445	0.528309
23	6	0	3.304524	-0.436447	-0.566374
24	6	0	4.196245	-1.369687	-1.079608
25	1	0	4.986470	-3.366068	-0.905027
26	1	0	3.559401	-3.937378	1.040019
27	1	0	1.975853	-2.270455	1.952314
28	1	0	3.240854	0.550972	-1.014703
29	1	0	4.819419	-1.109101	-1.927975
30	6	0	-0.387108	3.104069	2.103931
31	1	0	-0.461978	3.691481	1.174049
32	1	0	-0.938034	3.660415	2.875434
33	7	0	-1.734192	-0.701356	-0.431617
34	6	0	-2.483060	0.512685	-0.906363
35	6	0	-2.073946	-0.951531	1.014850
36	6	0	-2.212210	-1.887049	-1.228208
37	6	0	-3.963873	0.355092	-0.500069
38	1	0	-2.030463	1.387067	-0.443418
39	1	0	-2.340473	0.557965	-1.986478
40	1	0	-1.406343	-1.736038	1.370452
41	1	0	-1.870455	-0.027124	1.550599
42	6	0	-3.561193	-1.359958	1.100598
43	6	0	-3.755135	-1.907287	-1.203318
44	1	0	-1.773124	-2.768795	-0.759959
45	1	0	-1.820056	-1.783641	-2.238850
46	1	0	-4.187832	0.984726	0.362668
47	1	0	-4.603785	0.666012	-1.326698
48	7	0	-4.267764	-1.035210	-0.142864
49	1	0	-3.656849	-2.432667	1.276466
50	1	0	-4.034514	-0.835318	1.931369
51	1	0	-4.104754	-2.926677	-1.036853
52	1	0	-4.156561	-1.559581	-2.156437

_(S,S)_-TS 18 (M062X/6-311G(d,p) in Methanol)



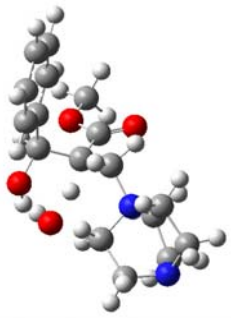
Imaginary Frequency: -1227.1338 cm^{-1}
E(RM062X) = -1112.96841762

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.556306	-0.952844	0.433211
2	1	0	0.425592	-1.130641	1.501889

3	1	0	0.328207	-1.876842	-0.100203
4	6	0	-0.281254	0.205767	-0.060634
5	1	0	0.383861	1.112523	-0.744191
6	6	0	-0.808204	1.014814	1.045950
7	8	0	-1.756572	1.882152	0.653611
8	8	0	-0.415215	0.997719	2.204040
9	6	0	-2.289749	2.744250	1.661201
10	1	0	-3.057247	3.335626	1.166398
11	1	0	-2.730090	2.161592	2.471769
12	1	0	-1.511813	3.398078	2.059555
13	6	0	-1.284455	-0.186698	-1.182398
14	8	0	-1.602082	0.909451	-2.025699
15	1	0	-0.778905	1.447170	-2.091069
16	8	0	0.771662	2.035667	-1.590625
17	1	0	-0.365573	3.722454	-1.107929
18	1	0	-0.764996	-0.953672	-1.773471
19	6	0	0.623799	3.269978	-0.936936
20	1	0	0.745034	3.174222	0.156515
21	1	0	1.377233	3.994186	-1.276299
22	6	0	-4.902589	-2.008708	0.333857
23	6	0	-4.889042	-0.654776	0.011070
24	6	0	-3.734003	-0.060586	-0.489798
25	6	0	-2.571333	-0.812470	-0.672648
26	6	0	-2.601717	-2.175735	-0.366658
27	6	0	-3.753915	-2.769717	0.139189
28	1	0	-5.804129	-2.468505	0.722709
29	1	0	-5.784505	-0.057577	0.145027
30	1	0	-3.733880	0.990787	-0.746923
31	1	0	-1.721095	-2.785297	-0.543113
32	1	0	-3.757500	-3.829756	0.367979
33	7	0	2.053821	-0.784866	0.248373
34	6	0	2.560886	0.478095	0.891698
35	6	0	2.417004	-0.773781	-1.211136
36	6	0	2.758092	-1.947221	0.893083
37	6	0	4.104702	0.429570	0.894020
38	1	0	2.180340	1.308121	0.298164
39	1	0	2.140880	0.522343	1.895508
40	1	0	2.207726	-1.777363	-1.584158
41	1	0	1.776250	-0.051016	-1.711554
42	6	0	3.907501	-0.395749	-1.329214
43	6	0	4.244312	-1.906754	0.478361
44	1	0	2.258710	-2.857040	0.560994
45	1	0	2.619942	-1.832541	1.968787
46	1	0	4.498246	1.407202	0.614325
47	1	0	4.480143	0.181803	1.888237
48	7	0	4.597602	-0.582884	-0.047255
49	1	0	4.381378	-1.013003	-2.093165
50	1	0	4.010082	0.650754	-1.622081
51	1	0	4.445608	-2.647797	-0.296836
52	1	0	4.870143	-2.136093	1.341385

***(S,R)*-TS 19 (M062X/6-311G(d,p) in Methanol)**



Imaginary Frequency: -1223.5807 cm^{-1}

E(RM062X) = -1073.68623806

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.051996	1.029728	1.597203
2	6	0	-0.272477	-0.334413	-0.576811
3	1	0	-0.125970	-0.153459	-1.642819
4	1	0	0.108407	-1.329560	-0.337838
5	6	0	0.401477	0.729640	0.262242
6	1	0	-0.329177	1.230821	1.221011
7	6	0	0.746371	1.920438	-0.518221
8	8	0	1.591462	2.754229	0.121623
9	8	0	0.278306	2.221219	-1.605802
10	6	0	1.898783	3.978439	-0.553076
11	1	0	2.573864	4.517300	0.107629
12	1	0	2.388013	3.777683	-1.507345
13	1	0	0.992804	4.561942	-0.721421
14	6	0	1.498526	0.174781	1.195838
15	8	0	0.886501	-0.534798	2.264380
16	1	0	0.221249	0.097901	2.616707
17	8	0	-0.849130	1.537282	2.415437
18	6	0	4.297551	-2.356610	-0.901354
19	6	0	3.430972	-2.911813	0.032539
20	6	0	2.530601	-2.103428	0.725992
21	6	0	2.487507	-0.730687	0.490237
22	6	0	3.366024	-0.178196	-0.447898
23	6	0	4.263432	-0.982958	-1.138293
24	1	0	4.997305	-2.985273	-1.440195
25	1	0	3.452186	-3.978677	0.226169
26	1	0	1.860131	-2.540227	1.456076
27	1	0	3.352294	0.892555	-0.631129
28	1	0	4.940742	-0.539729	-1.859994
29	7	0	-1.776377	-0.461914	-0.410222
30	6	0	-2.482316	0.835074	-0.689447
31	6	0	-2.141260	-0.922297	0.976790
32	6	0	-2.280096	-1.491512	-1.386006
33	6	0	-3.971712	0.661950	-0.320298
34	1	0	-2.004878	1.609185	-0.091960
35	1	0	-2.330469	1.046978	-1.748212
36	1	0	-1.498483	-1.769249	1.214283
37	1	0	-1.921172	-0.095767	1.648846
38	6	0	-3.638798	-1.300378	0.983287
39	6	0	-3.822895	-1.461458	-1.380746
40	1	0	-1.878532	-2.449850	-1.054537
41	1	0	-1.867701	-1.246772	-2.364160
42	1	0	-4.183737	1.149241	0.633016
43	1	0	-4.593382	1.125168	-1.087162
44	7	0	-4.322039	-0.756882	-0.195989
45	1	0	-3.762653	-2.384467	0.978513
46	1	0	-4.107686	-0.907195	1.885849
47	1	0	-4.208700	-2.481205	-1.387115
48	1	0	-4.197461	-0.948004	-2.267751
49	1	0	-0.367342	2.319618	2.706064

***(S,R)*-TS 19 (M062X/6-311G(d,p) in THF)**

Imaginary Frequency: -950.8626 cm^{-1}

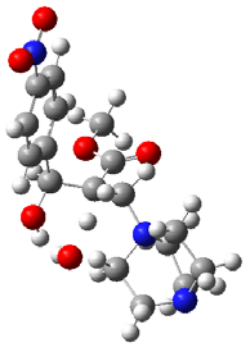
E(RM062X) = -1073.66905107

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.046419	0.993440	1.637626

2	6	0	-0.261909	-0.259580	-0.613023
3	1	0	-0.141439	0.003269	-1.664849
4	1	0	0.138954	-1.262002	-0.449203
5	6	0	0.414273	0.762548	0.272537
6	1	0	-0.334875	1.203133	1.207123
7	6	0	0.776531	1.974258	-0.480415
8	8	0	1.658939	2.759971	0.175614
9	8	0	0.299397	2.316440	-1.544375
10	6	0	1.982211	3.995546	-0.461738
11	1	0	2.678527	4.499909	0.204708
12	1	0	2.453089	3.820629	-1.430567
13	1	0	1.088492	4.604752	-0.603252
14	6	0	1.484927	0.156216	1.207016
15	8	0	0.844381	-0.577925	2.230576
16	1	0	0.157898	0.046302	2.576180
17	8	0	-0.969168	1.340553	2.414404
18	6	0	4.263114	-2.379207	-0.917623
19	6	0	3.437207	-2.920508	0.060258
20	6	0	2.546491	-2.106662	0.759473
21	6	0	2.470609	-0.742472	0.486135
22	6	0	3.308246	-0.204459	-0.496106
23	6	0	4.197280	-1.013799	-1.192089
24	1	0	4.955632	-3.011598	-1.461254
25	1	0	3.484419	-3.980798	0.283725
26	1	0	1.904898	-2.520026	1.527497
27	1	0	3.267357	0.859693	-0.710008
28	1	0	4.842766	-0.580659	-1.948070
29	7	0	-1.763562	-0.422610	-0.430907
30	6	0	-2.484161	0.890708	-0.562051
31	6	0	-2.102362	-1.021074	0.911560
32	6	0	-2.268191	-1.354074	-1.498743
33	6	0	-3.973077	0.657194	-0.212992
34	1	0	-2.017015	1.586555	0.131054
35	1	0	-2.328259	1.228170	-1.586975
36	1	0	-1.439145	-1.872913	1.057429
37	1	0	-1.886578	-0.254392	1.655450
38	6	0	-3.597249	-1.416051	0.899580
39	6	0	-3.812119	-1.355620	-1.466369
40	1	0	-1.843200	-2.333862	-1.275342
41	1	0	-1.878207	-1.003598	-2.453413
42	1	0	-4.191502	1.053126	0.780532
43	1	0	-4.607413	1.172507	-0.935591
44	7	0	-4.297409	-0.771623	-0.215801
45	1	0	-3.716806	-2.496274	0.795874
46	1	0	-4.060079	-1.109728	1.838733
47	1	0	-4.182242	-2.377458	-1.558886
48	1	0	-4.212434	-0.770396	-2.296100
49	1	0	-0.711768	2.171761	2.822323

Nitro substituted *(S,R)*-TS 19 (M062X/6-311G(d,p) in THF)

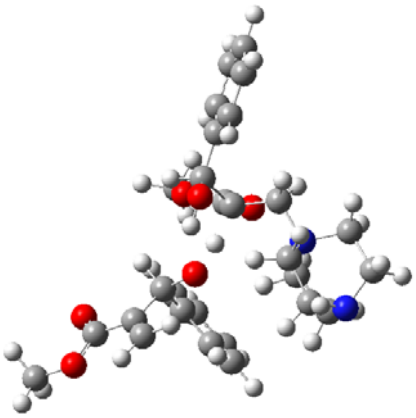


Imaginary Frequency: -980.7381 cm^{-1}
E(RM062X) = -1278.15796903

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.694197	1.942648	1.746040
2	6	0	-0.818212	-0.254667	-0.460063
3	1	0	-0.607115	-0.124789	-1.522140
4	1	0	-0.196830	-1.063945	-0.070217
5	6	0	-0.590756	1.038250	0.292857
6	1	0	-1.543270	1.339341	1.085396
7	6	0	-0.494233	2.189230	-0.621851
8	8	0	0.026171	3.289188	-0.035160
9	8	0	-0.896081	2.215976	-1.767473
10	6	0	0.064250	4.463401	-0.848199
11	1	0	0.532071	5.232624	-0.237859
12	1	0	0.652308	4.289213	-1.750393
13	1	0	-0.943901	4.770203	-1.130666
14	6	0	0.477909	0.923496	1.403925
15	8	0	-0.031740	0.144887	2.462050
16	1	0	-0.914034	0.560363	2.653755
17	8	0	-2.317688	1.409132	2.216975
18	6	0	4.131031	-0.762189	-0.047153
19	6	0	3.414117	-1.460925	0.911069
20	6	0	2.233024	-0.908495	1.391997
21	6	0	1.778480	0.322013	0.916849
22	6	0	2.532235	1.003561	-0.046066
23	6	0	3.711499	0.469867	-0.535886
24	1	0	3.777890	-2.413984	1.271349
25	1	0	1.656935	-1.424949	2.148386
26	1	0	2.195755	1.969019	-0.408158
27	1	0	4.301003	0.990562	-1.278054
28	7	0	-2.231833	-0.815069	-0.419048
29	6	0	-3.249574	0.211977	-0.832563
30	6	0	-2.591872	-1.319920	0.956735
31	6	0	-2.306921	-1.971586	-1.377968
32	6	0	-4.656035	-0.391276	-0.613461
33	1	0	-3.092815	1.092587	-0.213892
34	1	0	-3.041344	0.452210	-1.875358
35	1	0	-1.758495	-1.931520	1.300513
36	1	0	-2.688859	-0.439545	1.591983
37	6	0	-3.912754	-2.117095	0.848678
38	6	0	-3.781552	-2.416350	-1.504431
39	1	0	-1.665158	-2.752488	-0.967481
40	1	0	-1.896907	-1.635783	-2.329739
41	1	0	-5.116682	0.043957	0.275195
42	1	0	-5.290000	-0.169090	-1.472813
43	7	0	-4.583932	-1.842217	-0.424334
44	1	0	-3.727593	-3.191139	0.909059
45	1	0	-4.572621	-1.837400	1.670918
46	1	0	-3.844362	-3.504462	-1.464510
47	1	0	-4.199173	-2.083025	-2.456104
48	7	0	5.380792	-1.340567	-0.561406
49	8	0	5.985530	-0.720995	-1.412557
50	8	0	5.742643	-2.408042	-0.110489
51	1	0	-2.380681	2.317431	2.524729

***(S,R)*-TS 20 (M062X/6-311G(d,p) in Methanol)**



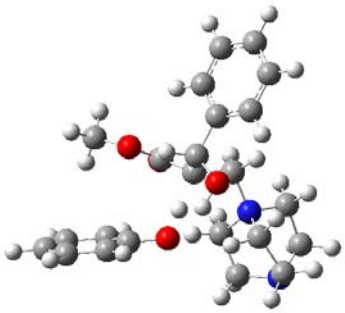
Imaginary Frequency: -1307.8302 cm^{-1}
E(RM062X) = -1649.24621223

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.008799	-2.450446	-0.447383
2	6	0	2.334446	0.683743	0.178619
3	1	0	2.837379	0.819617	1.138235
4	1	0	3.091816	0.487218	-0.583418
5	6	0	1.314408	-0.436618	0.233589
6	1	0	0.126765	-0.144327	-0.346651
7	6	0	0.967944	-0.793036	1.609841
8	8	0	0.387298	-2.008060	1.733911
9	8	0	1.123805	-0.082478	2.592591
10	6	0	0.104851	-2.435482	3.070472
11	1	0	-0.403052	-3.392606	2.972556
12	1	0	1.034807	-2.560880	3.628547
13	1	0	-0.533227	-1.718565	3.586833
14	6	0	1.663294	-1.612210	-0.704139
15	8	0	1.430641	-1.236481	-2.057888
16	1	0	0.504433	-0.933352	-2.081605
17	8	0	-0.872319	-0.052893	-1.144686
18	6	0	-1.987863	-0.655512	-0.567452
19	1	0	-1.763913	-1.682826	-0.236841
20	6	0	-3.064674	1.645169	2.934619
21	6	0	-2.769786	0.291891	3.060142
22	6	0	-2.462242	-0.463362	1.929094
23	6	0	-2.435595	0.126873	0.668985
24	6	0	-2.748774	1.483104	0.548625
25	6	0	-3.062053	2.238889	1.672553
26	1	0	-3.303856	2.234661	3.812671
27	1	0	-2.780068	-0.178503	4.037482
28	1	0	-2.245685	-1.522660	2.022539
29	1	0	-2.736884	1.945831	-0.434870
30	1	0	-3.305089	3.290761	1.567763
31	6	0	-3.111887	-0.159068	-2.755778
32	6	0	-3.133845	-0.745613	-1.561535
33	1	0	-3.945989	-0.233519	-3.442850
34	1	0	-2.239644	0.404118	-3.066590
35	6	0	-4.302802	-1.554139	-1.115691
36	8	0	-5.356624	-1.476005	-1.927466
37	8	0	-4.301563	-2.231466	-0.110415
38	6	0	-6.497156	-2.263379	-1.555028
39	1	0	-7.242868	-2.079543	-2.323947
40	1	0	-6.232606	-3.320857	-1.527718
41	1	0	-6.870800	-1.948425	-0.580273
42	6	0	5.753687	-2.933005	-0.257275
43	6	0	5.331503	-2.387422	-1.463458
44	6	0	4.011426	-1.966948	-1.622883
45	6	0	3.099851	-2.085380	-0.575126
46	6	0	3.532150	-2.637074	0.635663

47	6	0	4.846411	-3.058270	0.793789
48	1	0	6.779504	-3.261366	-0.134541
49	1	0	6.029442	-2.287582	-2.287465
50	1	0	3.687224	-1.547951	-2.567396
51	1	0	2.830806	-2.747371	1.457413
52	1	0	5.164862	-3.486935	1.737592
53	7	0	1.806033	2.062401	-0.175401
54	6	0	2.896120	3.072509	0.054679
55	6	0	0.626605	2.447819	0.675344
56	6	0	1.415794	2.135577	-1.626049
57	6	0	2.441499	4.422365	-0.540429
58	1	0	3.050001	3.121853	1.133162
59	1	0	3.800168	2.692175	-0.420732
60	1	0	-0.199028	1.810183	0.365945
61	1	0	0.886812	2.227894	1.709430
62	6	0	0.327189	3.943670	0.438245
63	6	0	0.701358	3.480679	-1.863265
64	1	0	0.772866	1.288179	-1.845262
65	1	0	2.343945	2.046355	-2.192953
66	1	0	2.697313	5.229159	0.146989
67	1	0	2.943471	4.611631	-1.490528
68	7	0	0.993821	4.423689	-0.777623
69	1	0	-0.750147	4.087637	0.340000
70	1	0	0.675916	4.544856	1.279545
71	1	0	-0.379756	3.333769	-1.905179
72	1	0	1.026237	3.903646	-2.814588

_(S,R)_-TS 21 (M062X/6-311G(d,p) in Methanol)



Imaginary Frequency: -1274.3006 cm-1
E(RM062X) = -1304.70615293

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.166815	-2.172164	-0.890916
2	6	0	1.415004	0.531589	0.589506
3	1	0	1.654948	0.487591	1.653384
4	1	0	2.317186	0.297988	0.018731
5	6	0	0.288474	-0.411847	0.240734
6	1	0	-0.814301	0.163957	-0.445966
7	6	0	-0.414545	-0.900978	1.413297
8	8	0	-1.128683	-2.031088	1.198172
9	8	0	-0.451631	-0.344421	2.505874
10	6	0	-1.948540	-2.475582	2.281065
11	1	0	-2.516407	-3.318555	1.892613
12	1	0	-1.331606	-2.795974	3.122675
13	1	0	-2.625745	-1.684956	2.606271
14	6	0	0.639693	-1.433590	-0.849412
15	8	0	0.741493	-0.789182	-2.118246
16	1	0	-0.111878	-0.354018	-2.264124
17	8	0	-1.663654	0.466260	-1.245611
18	6	0	4.329086	-3.544498	-0.046629

19	6	0	4.180952	-2.838052	-1.233577
20	6	0	2.993485	-2.159170	-1.507159
21	6	0	1.940911	-2.176295	-0.593496
22	6	0	2.098051	-2.890941	0.599230
23	6	0	3.279106	-3.570209	0.869979
24	1	0	5.251949	-4.072475	0.165142
25	1	0	4.990390	-2.811407	-1.955021
26	1	0	2.886855	-1.616053	-2.437530
27	1	0	1.287116	-2.924002	1.320417
28	1	0	3.381645	-4.120605	1.798645
29	6	0	-2.863290	-0.045032	-0.931567
30	6	0	-3.631816	-0.690432	-1.912355
31	6	0	-3.381354	0.046022	0.370947
32	6	0	-4.873215	-1.230122	-1.598293
33	1	0	-3.234140	-0.758090	-2.919590
34	6	0	-4.619143	-0.508794	0.678034
35	1	0	-2.800395	0.550318	1.138577
36	6	0	-5.375436	-1.150166	-0.300509
37	1	0	-5.449854	-1.724368	-2.373169
38	1	0	-4.997846	-0.433281	1.692137
39	1	0	-6.341416	-1.576577	-0.057219
40	7	0	1.182502	2.012220	0.318824
41	6	0	-0.018123	2.530328	1.059097
42	6	0	1.005536	2.286845	-1.149691
43	6	0	2.390510	2.777152	0.790454
44	6	0	-0.278381	3.982980	0.601896
45	1	0	-0.856917	1.876945	0.828095
46	1	0	0.218567	2.455584	2.121113
47	1	0	1.807671	1.768838	-1.673532
48	1	0	0.047702	1.859608	-1.438010
49	6	0	1.046725	3.815209	-1.367930
50	6	0	2.077029	4.287355	0.721305
51	1	0	3.212739	2.488953	0.134563
52	1	0	2.609545	2.450419	1.806379
53	1	0	-1.131209	4.018197	-0.078014
54	1	0	-0.507117	4.603594	1.469065
55	7	0	0.887381	4.532533	-0.098899
56	1	0	1.998189	4.114583	-1.810386
57	1	0	0.246490	4.106575	-2.049111
58	1	0	2.928606	4.817704	0.293923
59	1	0	1.892353	4.685197	1.720311