Supporting Information

For

Bicyclic Proline Analgoues as Organocatalysts for Stereoselective Aldol Reactions: An *In-Silico* Density Functional Theory Study

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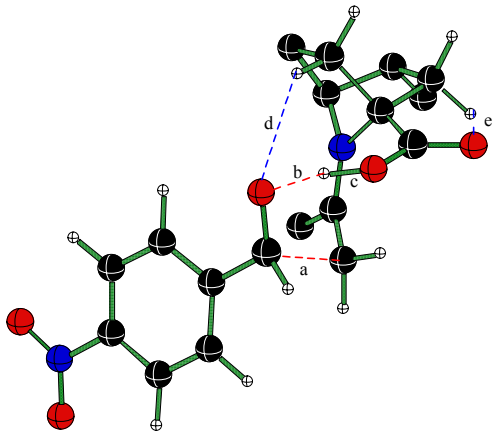


Fig. S1 The s-*re* TS of catalyst **1** **[**Atom colors: Black = C, Red = O, Blue = N]

Table S1 The Key Geometric Parameters for the Transition States Computed at the B3LYP/6-31G* level. Forming C-C (a) , alkoxideO…H (b) , and O=C-O…H (c) bond distances (in Ǻ)

Catalysts	Mode of approach	C…C bond (a in Å)	alkoxideO..H (b in Å)	H…O-C=O (c in Å)
1	s-*re*	1.92	1.45	1.05
	s-*si*	1.95	1.47	1.04
	a-*re*	1.74	1.32	1.14
	a-*si*	1.74	1.33	1.13
2	s-*re*	1.95	1.48	1.04
	s-*si*	1.97	1.49	1.03
	a-*re*	1.74	1.30	1.15
	a-*si*	1.77	1.31	1.15
3	s-*re*	2.02	1.54	1.02
	s-*si*	2.05	1.55	1.02
	a-*re*	1.76	1.26	1.20
	a-*si*	1.78	1.27	1.19
4	s-*re*	1.92	1.43	1.05
	s-*si*	1.94	1.45	1.04
	a-*re*	1.76	1.50	1.14

	a-*si*	1.89	1.23	1.20

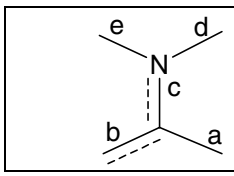
Table S1 (contd..)

Catalysts	Mode of approach	C…C bond (a in Å)	alkoxideO..H (b in Å)	H…O-C=O (c in Å)
5	s-*re*	1.99	1.55	1.03
	s-*si*	2.00	1.51	1.03
	a-*re*	1.81	1.24	1.20
	a-*si*	1.83	1.25	1.20
6	s-*re*	1.90	1.42	1.06
	s-*si*	1.93	1.43	1.05
	a-*re*	1.80	1.27	1.17
	a-*si*	1.85	1.26	1.17
7	s-*re*	1.98	1.52	1.03
	s-*si*	1.99	1.52	1.03
	a-*re*	1.88	1.20	1.25
	a-*si*	1.91	1.20	1.24
8	s-*re*	1.97	1.31	1.12
	s-*si*	2.01	1.26	1.16
	a-*re*	1.76	1.36	1.10
	a-*si*	1.79	1.34	1.12
9	s-*re*	1.92	1.32	1.11
	s-*si*	1.91	1.37	1.08
	a-*re*	1.86	1.45	1.05
	a-*si*	1.82	1.42	1.06
10	s-*re*	1.91	1.35	1.09
	s-*si*	1.90	1.39	1.07
	a-*re*	1.87	1.47	1.05
	a-*si*	1.82	1.43	1.06
11	s-*re*	1.79	1.51	1.03
	s-*si*	1.90	1.53	1.03
	a-*re*	1.98	1.54	1.03
	a-*si*	1.91	1.54	1.03

Table S2 The Weak Bonding Interactions in the Transition State Geometry Obtained at the B3LYP/6-31G* (distances d and e as in Figure 1 in Å) of Catalysts **1 - 7**

Catalysts	Mode of approach	$O^{\delta-}....H^{\delta+}$ (d)	O-C=O…H (e)
1	s-*re*	2.75	2.34(CH_3-H)
	s-*si*	2.77	2.35
	a-*re*	2.59	2.47
	a-*si*	2.59	2.49
2	s-*re*	2.52	2.50
	s-*si*	2.52	2.50
	a-*re*	2.59	2.85
	a-*si*	2.60	2.87
3	s-*re*	2.38	2.90
	s-*si*	2.35	2.88
	a-*re*	2.40	3.40
	a-*si*	2.37	3.41
4	s-*re*	2.48	2.88
	s-*si*	2.52	2.88
	a-*re*	2.49	3.13
	a-*si*	2.50	3.13
5	s-*re*	2.31	3.25
	s-*si*	2.26	3.26
	a-*re*	2.35	3.68
	a-*si*	2.32	3.40
6	s-*re*	2.33	2.99
	s-*si*	2.29	3.08
	a-*re*	2.73	3.09
	a-*si*	2.48	3.19
7	s-*re*	2.22	3.27
	s-*si*	2.18	3.27
	a-*re*	2.40	3.67
	a-*si*	2.35	3.67

Table S3 Dihedral angles (º) θ_1, θ_2, θ_3, and θ_4 of Transition State Geometries of Catalysts **1-11** Computed at the B3LYP/6-31G* level



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θ_2 = <bce
θ_3 = <bcd
θ_4 = <ace

Catalysts	Mode of approach	θ_1	θ_2	θ_3	θ_4
1	s-*re*	-5.17	29.18	-173.57	-162.42
	s-*si*	-4.74	26.71	-173.68	-164.35
	a-*re*	-21.17	-42.21	143.79	152.82
	a-*si*	-21.35	-40.31	145.02	153.31
2	s-*re*	-5.02	20.27	-174.62	-170.12
	s-*si*	-2.38	16.99	-172.63	-172.76
	a-*re*	-21.38	-45.76	143.21	149.66
	a-*si*	-21.39	-43.87	144.98	149.76
3	s-*re*	-18.16	22.51	169.27	-164.92
	s-*si*	-12.31	15.17	173.56	-170.70
	a-*re*	-18.74	-61.43	143.98	135.85
	a-*si*	-19.88	-60.46	144.50	135.15
4	s-*re*	-9.48	13.41	177.27	-173.34
	s-*si*	-0.61	0.32	-176.54	176.26
	a-*re*	-20.07	-60.12	143.27	136.55
	a-*si*	-19.17	-56.45	147.65	136.73
5	s-*re*	-10.09	15.64	176.31	-170.75
	s-*si*	-0.61	0.32	-176.34	176.26
	a-*re*	-20.07	-60.12	143.27	136.55
	a-*si*	-21.79	-59.91	143.50	134.79
6	s-*re*	-11.69	9.78	173.74	-175.65
	s-*si*	-4.56	-2.28	178.94	174.22
	a-*re*	-21.04	-64.20	144.35	130.40
	a-*si*	-24.21	-63.36	143.72	128.70

Table S3 (contd..)

Catalysts	Mode of approach	θ_1	θ_2	θ_3	θ_4
7	s-*re*	9.78	-11.69	173.74	-175.65
	s-*si*	-4.56	-2.28	178.94	174.22
	a-*re*	-21.04	-64.20	144.35	130.40
	a-*si*	-24.21	-63.36	143.72	128.70
8	s-*re*	-7.54	6.58	173.74	-174.70
	s-*si*	-7.72	8.30	176.70	-175.52
	a-*re*	-15.65	-30.75	149.79	163.81
	a-*si*	-14.48	-28.37	152.50	164.65
9	s-*re*	-5.08	24.45	-171.26	-169.36
	s-*si*	-5.13	25.16	-171.62	-168.35
	a-*re*	-4.86	-22.88	161.01	171.25
	a-*si*	-4.56	-22.05	162.78	171.00
10	s-*re*	-4.69	29.46	-171.66	-163.57
	s-*si*	-6.53	29.06	-173.54	-163.57
	a-*re*	-5.19	-24.94	160.00	169.87
	a-*si*	-5.12	-24.30	160.51	170.08
11	s-*re*	-5.56	13.38	-176.36	-175.81
	s-*si*	-5.91	11.59	-177.73	-176.59
	a-*re*	5.94	2.72	-178.65	-172.68
	a-*si*	10.69	-4.02	-174.81	-178.52

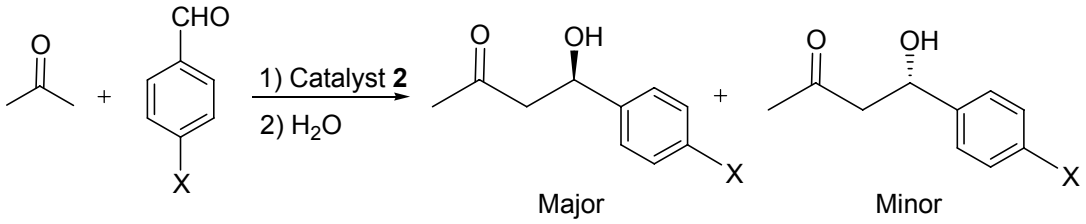
Table S4 Synthetic Availability/Application of Proposed Catalysts

Catalysts	Availability/ Application	References
8	Synthesis	(a) O. O. Grygorenko, O. S. Artamonov, G. V. Palarmarchuk, R. I. Zubatyuk, O. V. Shishkin and I. V. Komarov, *Tetrahedron. Asymmetry* 2006, **17**, 252.
9	Synthesis, Application as ligand for copper in catalytic asymmetric allylic oxidation of olefins[a], application as ligand and in ligand synthesis[b] , synthesis of 2-azanorbornyl methanols for enantioselective addition of diethyl zinc to aryl halide[c]	(a) M. J. Sodergen and P. G. Anderson, *Tetrahedron. Lett.,* 1996, **37**, 7577. *(b)* P. Brandt and P. G. Andersson, *Synlett* 2000, **8**, 1092. (c) H. Nakano, N. Kumagai, C. Kabuto, H. Matsuzaki and H. Hongo, *Tetrahedron: Asymmetry* 1995, **6**, 1233.
10	Synthesis, Application studying collagen stability	(a) C. L. Jenkins, G. Lin, J. Duo, D. Rapolu, I. A. Guzei, R. T. Raines and G. R. Krow, *J. Org. Chem.* 2004*,* **69***,* 8565.
1&2	Synthesis, Application in synthesizing a thrombin inhibitor[d]	(a) A. M. Gil, E. Bunel, M. D. Diaz-de-Villegas and C. Cativiela, *Tetrahedron: Asymmetry* 2003**, 14***,* 1479. *(b)* A. M. Gil, P. Lopez, E. Bunuel and C. Cativiela, *Arkivoc,* 2005, **9**, 90. (c) A. M. Gil, E. Bunel, P. Lopez and C. Cativiela, *Tetrahedron: Asymmetry* 2004**, 15***,* 811. *(d)* W. Han, J. C. Pelletier, L. J. Mersinger, C. A. Kettner and C. N. Hodge, *Org. Lett.* 1999, **1**, 1875.
11	Synthesis	G. R. Krow, Q. Huang, G. Lin, R. A. Centafont, A. M. Thomas, D. Gandla, C. DeBrosse and P. J. Carroll, *J. Org. Chem.,* 2006, **71**, 2090.

Table S5 Relative Energies (in kcal/mol) of *syn* and *anti*-Enamine of Catalysts **1-11** Computed at $CPCM_{(DMSO)}$/B3LYP/6-311+G**//B3LYP/6-31G*

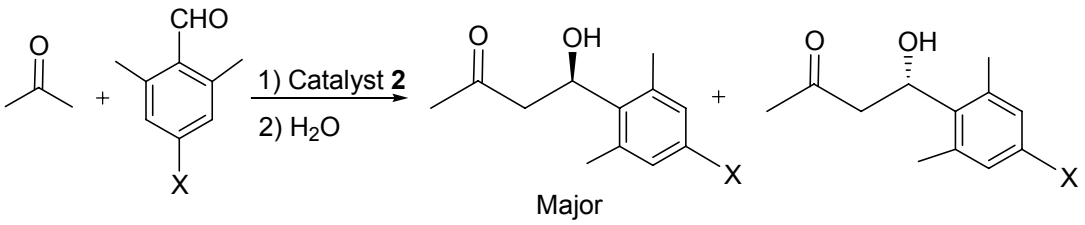
Catalysts	Relative Energy in kcal/mol	
	Syn-enamine	*Anti*-enamine
1	0.00	1.70
2	0.00	6.72
3	0.00	1.41
4	0.00	2.65
5	0.00	4.41
6	0.00	8.70
7	6.53	0.00
8	0.00	0.63
9	0.00	1.50
10	3.42	0.48
11	0.41	0.00

Table S6. Computed Enantiomeric Excess at the B3LYP/6-31G** level (in the gas phase) for the Addition of Enamines to Benzaldehyde with Different *p*-substituents (X)



X	% Enantiomeric excess
$-NO_2$	88
$-CF_3$	89
-F	89
$-NH_2$	87
-OMe	85

Table S7. Computed Enantiomeric Excess at the B3LYP/6-31G** Level (in the gas phase) for the Addition of Enamines to 2,6-dimethyl-4-nitrobenzaldehyde with Different *p*-substituents (X).



X	%Enantiomeric Excess
$-NO_2$	98
$-CF_3$	99
-F	99
$-NH_2$	99
-CN	98

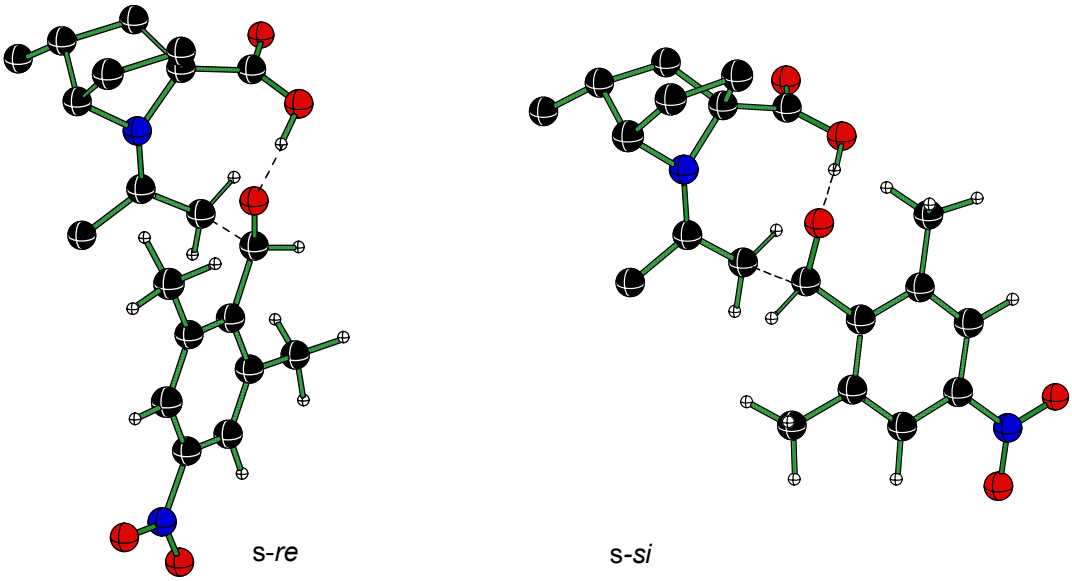


Fig. S2 The lowest energy TSs for the aldol reaction between acetone and 2,6-dimethyl-4-nitrobenzaldehyde catalyzed by **2.** Only selected hydrogens on the catalyst are shown for clarity. [Atom colors: Black = C, Red = O, Blue = N].

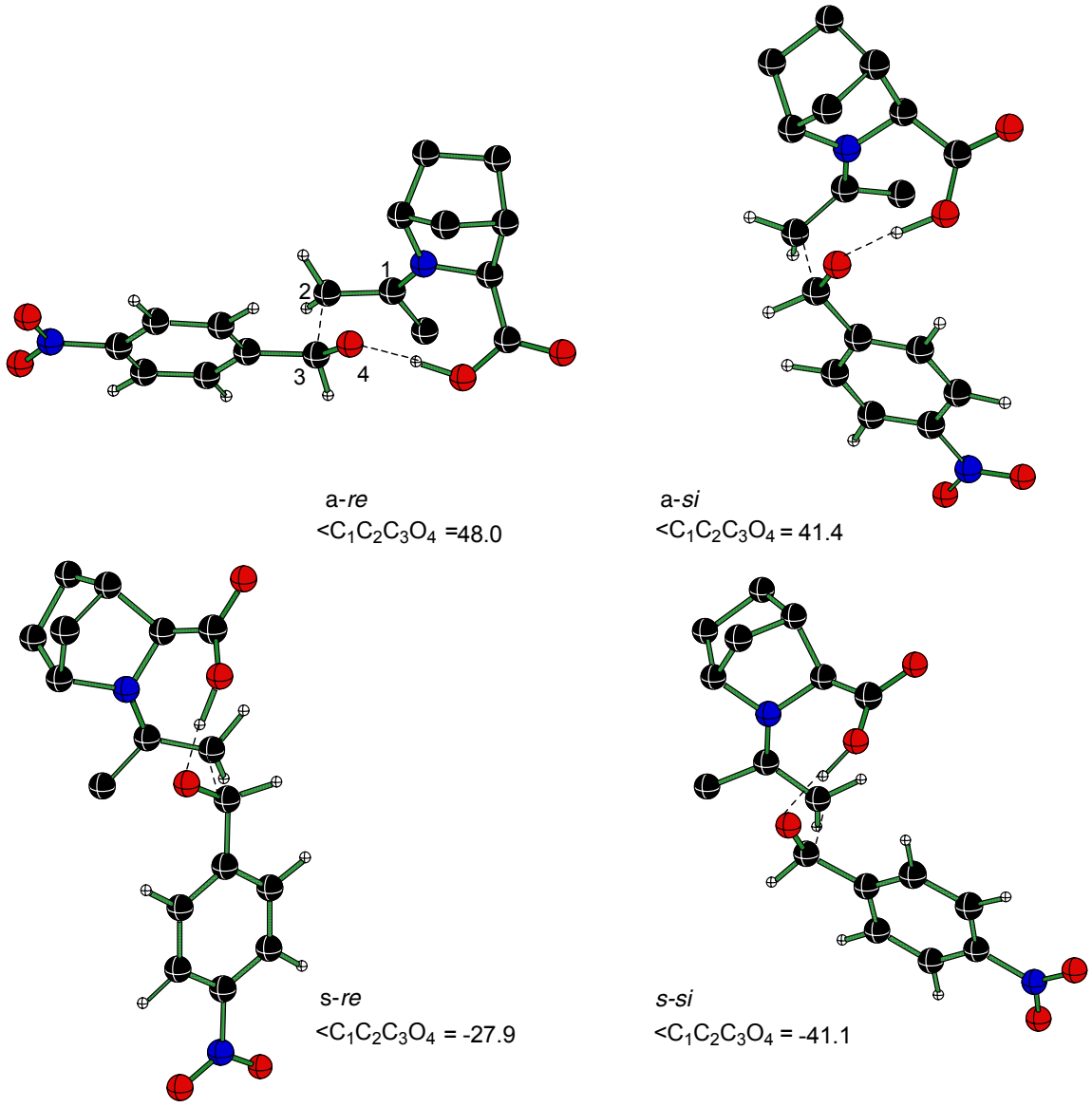


Fig. **S3** The lowest energy transition states for catalyst **9**. Angles describing the orientation of substituents around the forming C-C bond (in º) are provided. Only selected hydrogens on the catalyst are shown for clarity. [Atom colors: Black = C, Red = O, Blue = N].

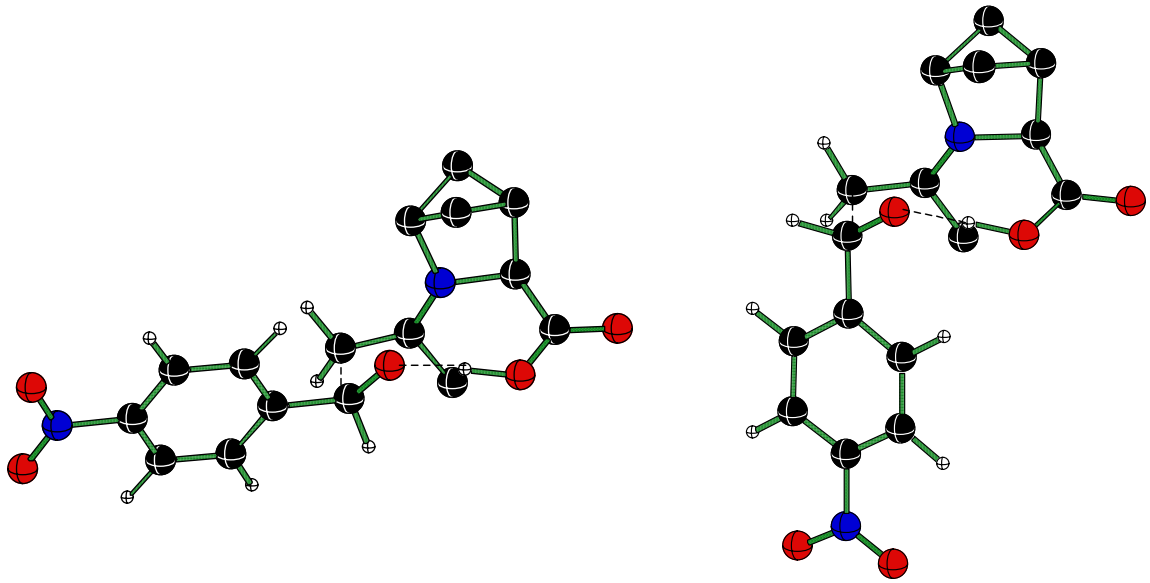


Fig. **S4** The B3LYP/6-31G* optimized structures for the lowest energy TSs for catalyst **10**. Only selected hydrogens on the catalyst are shown for clarity. [Atom colors: Black = C, Red = O, Blue = N]. The aryl group in a-*si* TS occupies a pseudo-axial position.

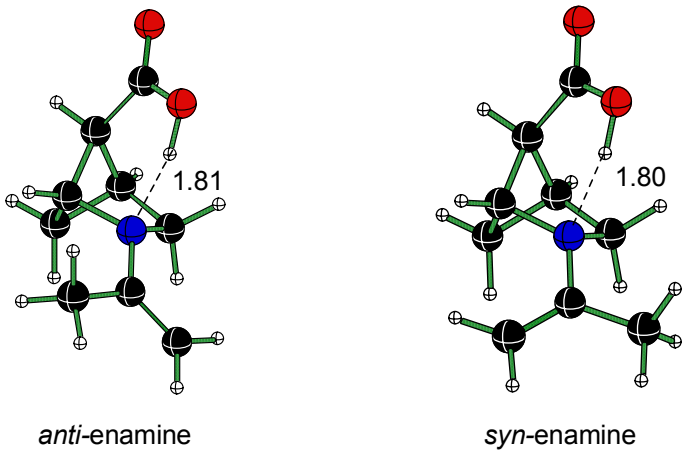
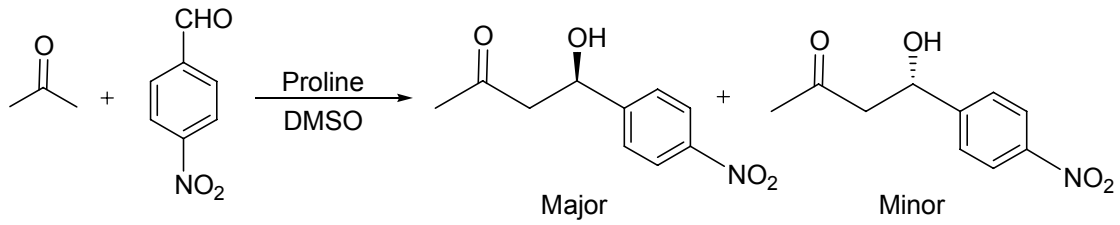


Fig. **S5** Enamines formed from catalyst **11** and acetone. Distances are in Å. [Atom colors: Black = C, Red = O, Blue = N].

Table S8. Enantiomeric Excess Calculated Based on the Energies Obtained at the $CPCM_{(DMSO)}$/B3LYP/6-311+G**//B3LYP/6-31G* Level for Proline Catalyzed Aldol Reaction between Acetone and *p*-Nitrobenzaldehyde



Experimental enantiomeric excess = 76%

	a-*re*	a-*si*	s-*re*	s-*si*	$ee_{calculated}$
E_1	-1068.265271	-1068.263430	-1068.261742	-1068.260989	75
Relative E_1 in kcal	0.0	1.15	2.21	2.67	
E_2	-1068.258867	-1068.256478	-1068.254920	-1068.253780	85
Relative E_2 in kcal	0.0	1.49	2.48	3.19	

E_1 refers to the free energy of solvation with all electrostatic terms (G_{sol}^{el})
E_2 refers to the free energy of solvation with all electrostatic and non-electrostatic energy terms ($G_{sol}^{el+non\text{-}el}$)

Full Citation for Gaussian

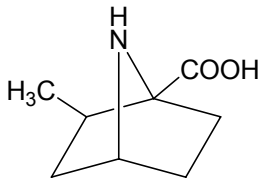
28 (a) **Gaussian 98**, Revision A.11.4, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, Jr., R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam, A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi, V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo, S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui, K. Morokuma, P. Salvador, J. J. Dannenberg, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-

Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres, C. Gonzalez, M. Head-Gordon, E. S. Replogle, J. A. Pople, *Gaussian98*, Revision A.11.4 ; Gaussian, Inc. Pittsburgh, PA, 2002.

(b) **Gaussian 03**, Revision C.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

Optimized Cartesian coordinates of reactants and transition states for the aldol reaction between acetone and *p*-nitrobenzaldehyde catalyzed by catalysts **1- 11** considered in this work. Electronic energies in the gas phase (in a.u) at the B3LYP/6-31G*. The total energies calculated in the gas phase using the B3LYP/6-311+G**//B3LYP/6-31G* are given in parenthesis.

The no. of imaginary frequencies (NImag) and corresponding values (in cm^{-1}) are given after the respective geometries.



1

1. **1-anti-enamine** **Et** = -634.579513 (-634.769726)				2. **1-syn-enamine** **Et** = -634.580854 (-634.772051)			
7	-0.56422	0.22919	-0.75004	7	0.75018	-0.09507	-0.5174
6	0.45773	-0.58423	-0.00137	6	-0.64624	0.33554	-0.20837
6	-0.18435	-0.83846	1.39871	6	-0.57903	1.02804	1.19844
6	-1.69448	-0.95548	0.99459	6	0.88995	1.56516	1.17784
6	-1.67883	-0.74148	-0.54388	6	0.62884	2.12242	-1.2658
6	-1.1169	-1.99555	-1.22159	6	1.37379	1.23588	-0.25476
6	0.37295	-1.93584	-0.7979	6	-0.787600	1.48477	-1.26637
6	0.06899	0.2285	2.46997	1	-1.286440	1.86453	1.19178
1	-0.45134	-0.0528	3.39361	6	-0.894000	0.17646	2.4332
1	-0.31424	1.2079	2.16751	1	-0.82912	0.80315	3.33127
1	1.13554	0.31716	2.69019	1	-0.18496	-0.6475	2.54945
1	0.18786	-1.79338	1.78564	1	-1.90448	-0.23554	2.376
1	-2.13313	-1.9219	1.26382	1	1.49797	1.02537	1.91339
1	-2.28103	-0.17588	1.48922	1	0.96151	2.63356	1.40814
1	-2.61782	-0.39504	-0.97333	1	0.62348	3.17238	-0.95789
1	-1.62244	-2.90512	-0.88367	1	2.45619	1.22682	-0.37937
1	-1.22359	-1.93056	-2.3084	1	1.09119	2.0624	-2.25528
1	1.03716	-1.92061	-1.66589	1	-1.03354	1.06598	-2.24619
1	0.68308	-2.76896	-0.16227	1	-1.58669	2.17556	-0.98683
6	1.89419	-0.09472	-0.08913	6	-1.73617	-0.68696	-0.4832
8	2.70603	-0.17064	0.80047	8	-2.79736	-0.71591	0.09242
8	2.24953	0.33989	-1.32656	8	-1.48483	-1.51008	-1.5298
1	1.43854	0.37366	-1.87141	1	-0.55635	-1.38086	-1.80296
6	-0.82288	1.60005	-0.4481	6	2.85243	-1.33385	-0.23749
6	0.36659	2.53346	-0.39858	1	3.21945	-2.34393	-0.04135
1	0.02131	3.55042	-0.19951	1	3.41515	-0.64803	0.40838
1	1.0782	2.26867	0.39081	1	3.08846	-1.07294	-1.27609
1	0.92306	2.54546	-1.34174	6	1.36236	-1.25991	0.01801

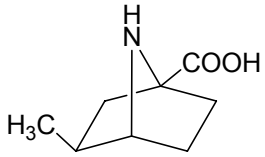
6	-2.06206	2.1085	-0.32227
1	-2.19396	3.17864	-0.2103
1	-2.96778	1.51557	-0.34802
NImag = 0			

6	0.71966	-2.29053	0.59281
1	-0.33957	-2.29987	0.81623
1	1.2701	-3.18977	0.84637
NImag = 0			

3. **1t (a-*re*)**			
Et = -1184.642142 (-1184.991894)			
6	3.431929	1.854384	-1.482450
6	1.955160	1.617437	-1.047831
7	2.075645	0.199267	-0.605877
6	3.173747	0.377429	0.398878
6	4.290654	0.965905	-0.500760
6	2.585047	1.563905	1.249872
6	1.679426	2.349644	0.264382
6	1.462620	-0.871650	-1.044794
6	2.074375	-2.240857	-0.953018
6	3.380369	-0.841396	1.321353
8	4.506118	-1.247688	1.560277
6	0.042707	-0.777052	-1.328165
6	-0.574780	-1.033646	0.278634
8	0.109924	-0.348089	1.192153
6	-2.045610	-0.655868	0.182970
6	-2.510705	0.487503	0.843638
6	-3.850616	0.856238	0.767049
6	-4.723410	0.064372	0.022291
6	-4.292939	-1.088415	-0.634556
6	-2.950498	-1.440902	-0.546638
7	-6.138663	0.449020	-0.068264
8	-6.886918	-0.269776	-0.732163
8	2.277581	-1.329287	1.835162
8	-6.494618	1.469698	0.521429
1	1.273246	-0.866559	1.540398
1	3.412584	2.158841	1.645160
1	2.004421	1.180894	2.087580
1	1.930836	3.411589	0.192957
1	0.630195	2.246051	0.547254
1	1.221971	1.747297	-1.843149
1	3.683408	2.917912	-1.430340
1	4.944588	1.590910	0.114486
1	1.557544	-2.856315	-0.209288
1	3.134419	-2.226119	-0.705200
1	1.945606	-2.724298	-1.929238
1	-0.311404	0.210435	-1.619853
1	-0.348184	-1.551329	-1.988783
1	-0.492791	-2.135320	0.362682
1	-2.605881	-2.345115	-1.043284
1	-5.006004	-1.684089	-1.190951
1	-4.230090	1.734668	1.274765
1	-1.805879	1.060306	1.435579
1	3.580622	1.526690	-2.516766
6	5.155679	-0.055469	-1.242595
1	4.552334	-0.696310	-1.897636
1	5.882665	0.463519	-1.878275
1	5.691306	-0.689918	-0.533546
NImag=1 (-617.5)			

4. **1t (a-*si*)**			
Et = -1184.638223 (-1184.987340)			
6	-2.793260	-1.674967	0.331641
6	-1.842527	-0.941377	-0.398132
6	-2.215835	0.297306	-0.937222
6	-3.495453	0.809680	-0.729583
6	-4.407689	0.062906	0.011400
6	-4.075276	-1.183323	0.544034
6	-0.456655	-1.525485	-0.681456
8	0.323770	-0.847683	-1.521916
7	-5.760048	0.593440	0.231843
8	-6.034331	1.688292	-0.259271
8	-6.541118	-0.088174	0.897824
6	0.318957	-1.842729	0.851257
6	1.108247	-0.635095	1.016523
6	0.457229	0.557219	1.655014
7	2.245235	-0.553519	0.372256
6	3.289574	-1.592504	0.143246
6	3.460451	-1.558375	-1.374524
6	3.330015	-0.039184	-1.661983
6	2.947828	0.602179	-0.274563
6	4.240359	0.663419	0.576825
6	4.490533	-0.874407	0.827252
6	2.038629	1.818148	-0.530750
8	2.420828	2.946785	-0.272610
8	0.888122	1.519302	-1.089301
1	0.635842	0.425866	-1.266519
1	4.258370	0.416392	-2.016540
1	2.549475	0.148269	-2.397350
1	4.422400	-1.979526	-1.680508
1	2.651734	-2.103601	-1.865073
1	3.028548	-2.554209	0.583394
1	5.438218	-1.228612	0.410918
1	5.042284	1.092132	-0.031329
1	-0.461169	0.833433	1.127250
1	1.105137	1.430443	1.711381
1	0.170222	0.264004	2.672487
1	0.902359	-2.746030	0.679079
1	-0.427426	-2.001045	1.628474
1	-0.606199	-2.570865	-1.010220
1	-1.500210	0.856000	-1.528594
1	-3.794116	1.767876	-1.136963
1	-4.817234	-1.740917	1.102201
1	-2.533137	-2.654379	0.727178
1	4.498364	-1.085716	1.901789
6	4.140924	1.461306	1.879066
1	5.091718	1.409166	2.422262
1	3.908219	2.507404	1.669412
1	3.365818	1.057998	2.542500
NImag=1(-637.6)			

5. **1t(s-*re*)** Et= -1184.648346 (-1184.997590)				6. **1t(s-*si*)** **Et** = -1184.645612 (-1184.995101)			
6	-4.061639	0.868403	0.545322	6	2.837299	1.590863	0.041359
6	-3.055576	0.017407	-0.298983	6	1.963932	0.655497	-0.534415
7	-1.754523	0.620620	0.191637	6	2.438602	-0.628835	-0.833846
6	-2.046881	2.032392	-0.194291	6	3.754025	-0.980962	-0.547157
6	-3.390955	2.282809	0.521594	6	4.594491	-0.032495	0.033913
6	-2.284186	1.880034	-1.701840	6	4.154828	1.257566	0.331523
6	-3.073178	0.545426	-1.770233	6	0.543012	1.056900	-0.873892
6	-0.808441	0.222422	1.031100	8	-0.158979	0.344525	-1.683079
6	0.140487	1.266124	1.573837	7	5.985640	-0.396432	0.334703
6	-3.343499	-1.503515	-0.316932	8	6.703689	0.461611	0.850874
8	-4.421925	-1.898908	0.083506	8	6.353966	-1.537389	0.055030
6	-4.277374	0.380687	1.982306	6	-0.258079	0.906744	0.901895
6	-0.505955	-1.145816	1.245252	6	-1.552770	1.398905	0.615655
8	-2.468689	-2.298599	-0.899350	6	-1.792319	2.885578	0.768437
6	0.434807	-1.610154	-0.373794	7	-2.496810	0.684744	0.015066
8	-0.270708	-1.219829	-1.383425	6	-2.811986	-0.790116	-0.088941
6	1.826893	-1.041776	-0.238324	6	-3.300252	-0.872772	-1.573479
6	2.237790	-0.013519	-1.097711	6	-3.884238	0.536429	-1.854890
6	3.521465	0.517640	-1.009145	6	-3.814794	1.190574	-0.468964
6	4.395000	0.003433	-0.052079	6	-4.795190	0.487005	0.493380
6	4.021715	-1.032984	0.805190	6	-4.062958	-0.850786	0.847737
6	2.735724	-1.550846	0.702001	6	-1.765734	-1.901427	0.144828
7	5.749716	0.562106	0.052859	8	-0.634176	-1.840606	-0.534456
8	6.502711	0.083975	0.902126	8	-2.061204	-2.861009	0.829123
8	6.052440	1.479293	-0.711252	1	0.472389	2.154499	-0.994955
1	0.413263	-2.683692	-0.110786	1	-0.479500	-0.960098	-1.073723
1	-1.573397	-1.831791	-1.197602	1	-2.462357	-1.088173	-2.237038
1	-2.582701	-0.166488	-2.434928	1	-4.034436	-1.676444	-1.674570
1	-4.107074	0.668289	-2.103780	1	-3.253211	1.078685	-2.564260
1	-3.985274	3.035007	-0.006165	1	-4.907952	0.515818	-2.239751
1	-2.834477	2.733274	-2.108811	1	-3.872209	2.276683	-0.476522
1	-1.243429	2.715356	0.072547	1	-5.770792	0.334173	0.021770
1	-1.332297	1.793666	-2.232691	1	-4.954628	1.087266	1.395486
1	-3.228499	2.647337	1.541615	1	-4.661539	-1.721627	0.565702
1	-5.024569	0.872364	0.026939	6	-3.746877	-0.933045	2.345412
1	-1.311105	-1.865665	1.155665	1	-1.893914	3.374584	-0.208002
1	0.154681	-1.343886	2.084742	1	-2.702374	3.090002	1.342335
1	0.710540	1.740983	0.766592	1	-0.951764	3.346561	1.289179
1	-0.396266	2.049884	2.119088	1	0.331609	1.525808	1.571375
1	0.855501	0.802670	2.254160	1	-0.116927	-0.155393	1.061825
1	2.434690	-2.366211	1.355923	1	1.773553	-1.348768	-1.295877
1	4.736288	-1.414250	1.524256	1	4.138054	-1.969010	-0.769447
1	3.859027	1.309266	-1.667092	1	4.842486	1.968352	0.772804
1	1.537463	0.336894	-1.848336	1	2.480848	2.595844	0.257558
1	-4.904545	1.100103	2.522373	1	-4.676313	-0.847853	2.921068
1	-4.765085	-0.593983	1.996225	1	-3.263974	-1.878316	2.593692
1	-3.326900	0.305327	2.526137	1	-3.091177	-0.111585	2.661690
NImag=1(-282.1)				NImag=1(-295.8)			



2

7. **2-anti-enamine** **Et** = -634.575509 (-634.766267)				8. **2-syn-enamine** **Et** = -634.584035 (-634.775580)			
6	1.19506	-1.45021	-0.25805	6	-0.05038	-1.04533	1.28868
6	-0.07945	-0.76602	0.27854	6	0.73951	-0.53641	0.06311
7	0.11461	0.60987	-0.2822	7	-0.23236	0.33157	-0.66134
6	1.41047	0.8625	0.38496	6	-1.29848	-0.71047	-0.76888
6	2.25059	-0.29467	-0.2232	6	-1.48723	-1.2286	0.6976
6	1.17771	0.55226	1.88869	6	-0.55713	-1.78371	-1.57985
6	0.0909	-0.55368	1.82314	6	0.86744	-1.71508	-0.95972
6	-0.91469	1.58274	-0.36611	6	-0.57836	1.63266	-0.20243
6	-1.78778	1.44808	-1.59777	6	0.05424	2.30324	0.77466
6	-1.37704	-1.48941	-0.06462	6	2.10517	0.08171	0.31017
8	-2.52477	-0.8989	0.36719	8	2.56054	0.85514	-0.70455
8	-1.42131	-2.55689	-0.6234	8	2.78322	-0.15115	1.28115
6	-1.02601	2.64313	0.45466	6	-1.67723	2.28613	-1.01104
1	-0.84425	-0.21924	2.28406	1	1.62468	-1.49002	-1.71599
1	0.38022	-1.48433	2.32017	1	1.16883	-2.63348	-0.44907
1	0.82446	1.42725	2.44099	1	-0.53784	-1.52012	-2.64132
1	2.09615	0.21068	2.37649	1	-1.01946	-2.77044	-1.48181
1	1.7885	1.86383	0.16801	1	-2.20956	-0.33633	-1.23772
1	3.07873	-0.54419	0.45093	1	-1.75129	-2.29312	0.66383
6	2.81594	0.03633	-1.60547	6	-2.57434	-0.4968	1.49191
1	1.47847	-2.31398	0.35011	1	0.37361	-1.96809	1.69288
1	1.02007	-1.80561	-1.27648	1	-0.04207	-0.30157	2.09033
1	-2.3362	-0.01039	0.72286	1	-1.49855	2.16452	-2.08602
1	-1.74911	3.42566	0.24683	1	-2.66102	1.85245	-0.79249
1	-0.37626	2.79933	1.30838	1	-1.73193	3.35375	-0.78452
1	-2.61147	2.16757	-1.57776	1	0.83259	1.8769	1.39597
1	-1.17996	1.63276	-2.49176	1	-0.19513	3.3418	0.96325
1	-2.21457	0.44732	-1.70607	1	1.82479	0.98998	-1.33282
1	3.30886	-0.8387	-2.04543	1	-2.63295	-0.89062	2.51374
1	2.01335	0.34783	-2.28264	1	-2.36689	0.57556	1.56363
1	3.55518	0.84519	-1.55217	1	-3.56053	-0.62808	1.02946
NImag = 0				NImag = 0			

9**. 2t (a-*re*)** **Et** = -1184.6431337 (-1184.993560)				10**. 2t (a-*si*)** **Et** = -1184.6392783 (-1184.989120)			
6	-3.631582	2.085793	0.438199	6	-2.732765	-1.707915	-0.327647
6	-2.122082	1.768279	0.138767	6	-1.823438	-0.708989	-0.715433
7	-2.144818	0.300199	0.371229	6	-2.255559	0.624469	-0.738568
6	-3.221125	-0.057733	-0.609103	6	-3.552908	0.959472	-0.353629
6	-4.374972	0.785894	-0.052387	6	-4.422812	-0.054081	0.039844
6	-2.676542	0.650827	-1.898168	6	-4.031206	-1.393398	0.052725
6	-1.855651	1.856838	-1.363694	6	-0.420047	-1.089743	-1.183119
6	-1.516121	-0.422634	1.265304	8	0.324470	-0.136717	-1.737135
6	-2.095054	-1.697007	1.811944	7	-5.792659	0.290995	0.444394
6	-3.363564	-1.573575	-0.838883	8	-6.116551	1.478229	0.419961
8	-4.468692	-2.089032	-0.788710	8	-6.537175	-0.629014	0.786995
6	-0.105937	-0.159020	1.476268	6	0.390938	-1.884675	0.172983
6	0.545248	-1.108268	0.168686	6	1.119362	-0.768121	0.739042
8	-0.133044	-0.929794	-0.964645	6	0.431747	0.107237	1.746650
6	2.005593	-0.690834	0.097441	7	2.241156	-0.414778	0.159176
6	2.458251	0.064764	-0.990931	6	3.360303	-1.252110	-0.348246
6	3.788972	0.463908	-1.073202	6	3.559403	-0.708090	-1.762927
6	4.664971	0.094288	-0.053544	6	3.311246	0.810245	-1.549516
6	4.247095	-0.670688	1.035329	6	2.869944	0.929839	-0.048031
6	2.913334	-1.059233	1.101187	6	4.118186	0.776037	0.829627
7	6.070918	0.514774	-0.130360	6	4.503027	-0.733500	0.596577
8	6.823944	0.167286	0.780354	6	1.890132	2.101177	0.130200
8	-2.239596	-2.191240	-1.103369	8	2.201819	3.058077	0.818505
8	6.414448	1.193435	-1.098629	8	0.768132	1.967099	-0.536263
1	-1.247927	-1.592772	-1.051706	1	0.567415	0.972453	-1.083561
1	-3.523197	0.947480	-2.523143	1	4.204464	1.421590	-1.704320
1	-2.045056	-0.028445	-2.469208	1	2.524248	1.171784	-2.209712
1	-2.174189	2.818741	-1.775261	1	4.556894	-0.937944	-2.148221
1	-0.792838	1.714329	-1.569677	1	2.807738	-1.120170	-2.439511
1	-1.418458	2.286635	0.790627	1	3.160879	-2.320142	-0.259919
1	-3.923802	2.950168	-0.168808	1	5.452890	-0.811511	0.055737
6	-3.893962	2.404065	1.910959	6	4.607130	-1.528180	1.899412
1	-5.136531	0.987489	-0.808978	1	4.910078	1.470474	0.540536
1	-4.864442	0.267851	0.778614	1	3.877109	0.968339	1.880061
1	-1.579935	-2.575428	1.408768	1	-0.500198	0.519772	1.347224
1	-3.159807	-1.806860	1.606712	1	1.052940	0.929684	2.100454
1	-1.940445	-1.690796	2.897573	1	0.164997	-0.527745	2.600405
1	0.213941	0.862206	1.273857	1	1.012396	-2.641359	-0.303520
1	0.299646	-0.525467	2.419607	1	-0.345128	-2.333937	0.837847
1	0.481850	-2.128421	0.593889	1	-0.518019	-1.971117	-1.842166
1	2.577860	-1.666595	1.938848	1	-1.574139	1.402307	-1.062717
1	4.962887	-0.949086	1.798861	1	-3.896894	1.986562	-0.360737
1	4.159260	1.045431	-1.908726	1	-4.741115	-2.155216	0.350421
1	1.751996	0.307119	-1.776938	1	-2.424359	-2.751155	-0.336703
1	-4.965801	2.543789	2.090264	1	5.362152	-1.088165	2.560377
1	-3.556155	1.587885	2.561630	1	3.654317	-1.526510	2.443213
1	-3.379259	3.320722	2.222066	1	4.890201	-2.570969	1.713656
NImag=1(-731.9)				NImag=1(-732.0)			

11**. 2t (s-*re*)** **Et** =-1184.651120 (-1185.000854)				12**. 2t (s-*si*)** **Et** = -1184.6483608 (-1184.998340)			
6	-2.166877	-0.232309	1.079032	6	-2.842549	1.571792	0.311437
6	-1.810925	-1.116586	0.051298	6	-2.004689	0.492471	0.630697
6	-2.750834	-1.420741	-0.945316	6	-2.526522	-0.808429	0.606742
6	-4.012905	-0.837823	-0.938004	6	-3.854339	-1.030367	0.254909
6	-4.330398	0.054556	0.087359	6	-4.659542	0.062304	-0.064291
6	-3.425646	0.361387	1.102830	6	-4.172049	1.368981	-0.038448
6	-0.443454	-1.755846	0.062304	6	-0.569863	0.753644	1.037804
8	0.281596	-1.593200	1.115758	8	0.096398	-0.127527	1.692535
7	-5.658409	0.682549	0.099696	7	-6.063657	-0.165489	-0.431595
8	-5.911737	1.470277	1.011943	8	-6.749152	0.818829	-0.713475
8	-6.439984	0.388926	-0.805772	8	-6.474519	-1.326024	-0.437841
6	0.499190	-1.009117	-1.468398	6	0.226531	0.911361	-0.755568
6	0.853209	0.284983	-1.013285	6	1.534998	1.326470	-0.418278
6	-0.070443	1.438465	-1.333912	6	1.798822	2.813903	-0.316931
7	1.835779	0.502208	-0.150721	7	2.490754	0.508141	0.003805
6	3.056459	-0.277869	0.295717	6	2.715384	-0.987828	-0.030603
6	2.980373	-0.060658	1.833548	6	3.112454	-1.244395	1.451994
6	2.338542	1.350754	1.965491	6	3.835755	0.071558	1.860794
6	2.195897	1.793821	0.498259	6	3.824301	0.881672	0.551433
6	3.597077	2.080649	-0.104803	6	4.789357	0.240328	-0.479650
6	4.164985	0.637694	-0.275846	6	3.994851	-1.034430	-0.899415
6	3.255710	-1.759374	-0.110327	6	1.622989	-1.950547	-0.551836
8	2.445729	-2.658709	0.417646	8	0.533004	-2.100423	0.183126
8	4.197776	-2.055508	-0.819012	8	1.834474	-2.607082	-1.551130
1	-0.460890	-2.754961	-0.410032	1	-0.446046	1.805295	1.358080
1	1.581353	-2.246593	0.832992	1	0.383307	-1.349038	0.883745
1	2.353829	-0.818422	2.302272	1	2.227990	-1.405687	2.066981
1	3.982309	-0.120494	2.267686	1	3.752261	-2.128676	1.520185
1	4.183283	2.649349	0.626079	1	3.268411	0.594071	2.635950
1	2.949605	2.054938	2.537619	1	4.854761	-0.087001	2.225525
1	1.455366	2.573166	0.327785	1	3.943382	1.955995	0.679870
1	1.355771	1.283224	2.440029	1	5.722643	-0.026858	0.029138
6	3.557042	2.865530	-1.418350	6	5.118398	1.154103	-1.662879
1	5.110440	0.476823	0.247628	1	4.544066	-1.964307	-0.733141
1	4.331923	0.390651	-1.327281	1	3.715896	-1.007789	-1.955702
1	1.279081	-1.757807	-1.543047	1	1.958364	3.117777	0.724756
1	-0.185937	-1.024055	-2.311333	1	2.683914	3.107555	-0.890242
1	-0.590566	1.788222	-0.434296	1	0.943659	3.370698	-0.702641
1	0.476163	2.284600	-1.762197	1	-0.362165	1.649279	-1.292185
1	-0.827861	1.120064	-2.050629	1	0.062638	-0.101350	-1.103026
1	-2.492637	-2.126732	-1.731390	1	-1.888353	-1.645658	0.863777
1	-4.750982	-1.061362	-1.698472	1	-4.274517	-2.028250	0.227602
1	-3.720733	1.045029	1.889642	1	-4.832858	2.191326	-0.283237
1	-1.443618	-0.043571	1.865193	1	-2.447816	2.585031	0.346047
1	4.568057	2.987388	-1.822897	1	5.749055	0.630252	-2.389816
1	2.965509	2.341852	-2.179282	1	4.208254	1.466818	-2.189324
1	3.129893	3.865991	-1.278977	1	5.656113	2.054205	-1.341012
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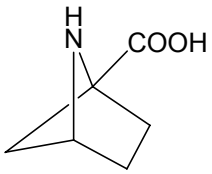
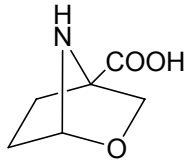


3

13. **3-anti-enamine** **Et** = -555.912376 (-556.082876)				14. **3-syn-enamine** **Et** = -555.914571 (-555.091551)			
6	-1.3674	1.40385	-0.72026	6	-1.18503	1.55387	-0.70471
6	-0.68627	0.30307	0.1411	6	-0.7162	0.30314	0.10235
6	-0.11416	1.09272	1.33194	6	-0.2268	0.92436	1.42841
6	0.76804	1.67522	0.19642	6	0.83391	1.51253	0.46025
6	-0.22967	2.46907	-0.66245	6	0.03296	2.48469	-0.41567
7	0.72149	0.32704	-0.49616	7	0.72373	0.22931	-0.37434
6	-1.46877	-0.97767	0.29984	6	-1.64848	-0.8739	-0.03129
8	-1.89407	-1.38195	1.35246	8	-2.51635	-1.13817	0.76324
8	-1.7327	-1.63825	-0.86015	8	-1.50508	-1.57542	-1.18468
1	1.74761	2.11524	0.37357	1	1.83147	1.80017	0.79219
1	0.17823	2.70277	-1.64885	1	0.57744	2.75904	-1.32266
1	-0.54072	3.39987	-0.17856	1	-0.24278	3.39737	0.12145
1	-1.5722	1.06192	-1.73906	1	-1.30283	1.3211	-1.76611
1	-2.30775	1.73627	-0.27075	1	-2.13512	1.93451	-0.31976
1	-1.25893	-1.20711	-1.59301	1	-0.69631	-1.27874	-1.64094
1	-0.78451	1.76214	1.88124	1	-0.89443	1.60958	1.95992
1	0.4464	0.45329	2.01539	1	0.18821	0.17788	2.10714
6	1.6993	-0.64109	-0.14678	6	1.58473	-0.83995	-0.00134
6	2.87636	-0.34681	0.43219	6	1.20532	-2.02178	0.51148
1	3.14113	0.64247	0.786	1	0.18837	-2.25991	0.79852
1	3.63524	-1.1142	0.53746	1	1.93727	-2.81099	0.64708
6	1.40312	-2.04907	-0.60995	6	3.02755	-0.55986	-0.35594
1	1.08295	-2.05857	-1.65905	1	3.44061	0.26318	0.24137
1	2.29844	-2.66927	-0.52242	1	3.64905	-1.44114	-0.17891
1	0.61459	-2.5282	-0.01957	1	3.11652	-0.26709	-1.4086
NImag = 0				NImag = 0			

15. **3t (a-*re*)** **Et** = -1105.961853 (-1106.291272)				16. **3t (a-*si*)** **Et** = -1105.957877 (-1106.286659)			
6	-2.796558	1.869282	-0.693807	6	3.802523	0.151120	-1.317432
6	-3.476177	0.604115	-0.055938	6	3.336197	0.651064	0.098641
6	-4.105057	1.235415	1.223359	6	4.488471	0.094621	0.988837
6	-2.585442	1.446921	1.582846	6	3.875122	-1.277754	0.514995
6	-2.115930	2.486538	0.562795	6	4.193775	-1.317005	-0.981117
7	-2.387844	0.140797	0.844625	7	2.560529	-0.529791	0.560543
6	-3.920694	-0.421703	-1.101201	6	2.533671	1.950956	0.027782
8	-5.096044	-0.700016	-1.267298	8	2.933404	2.988557	0.524882
8	-2.894035	-0.908359	-1.753364	8	1.414359	1.773541	-0.635234
1	-2.220732	1.467297	2.610157	1	3.923682	-2.182820	1.121144
1	-1.026939	2.513147	0.477444	1	3.575564	-2.042904	-1.514505
1	-2.476841	3.487901	0.814051	1	5.248001	-1.546136	-1.161009
1	-2.080260	1.592812	-1.463600	1	2.999837	0.208786	-2.048539
1	-3.574852	2.504329	-1.126275	1	4.646003	0.765848	-1.644398
1	-1.771109	-0.611860	-1.431870	1	1.107034	0.679500	-1.001129
1	-4.710970	2.135924	1.096720	1	5.514269	0.308440	0.678810
1	-4.598873	0.506623	1.868866	1	4.343391	0.281635	2.054511
6	-1.822265	-1.008726	1.106211	6	1.391286	-0.720880	1.114707
6	-0.401658	-0.982601	1.374502	6	0.680125	-1.915691	0.717577
1	-0.023605	-0.037585	1.765863	1	1.324322	-2.741558	0.412637
1	0.009348	-1.842671	1.903327	1	-0.117144	-2.241187	1.384214
6	-2.480577	-2.317483	0.765933	6	0.660012	0.378627	1.830503
1	-2.078375	-2.756398	-0.152654	1	-0.186091	0.758286	1.250685
1	-2.274000	-3.013407	1.587691	1	0.252098	-0.053506	2.752770
1	-3.559598	-2.221199	0.643012	1	1.308562	1.215931	2.087498
6	0.127097	-1.044040	-0.308971	6	-0.005841	-1.313447	-0.810241
6	1.593179	-0.660840	-0.244654	1	-0.083250	-2.280694	-1.336168
1	0.034837	-2.127889	-0.504962	6	-1.419985	-0.823965	-0.518756
8	-0.603217	-0.261188	-1.105908	8	0.808195	-0.474105	-1.452141
6	2.545348	-1.544344	0.284594	6	-1.791294	0.497433	-0.805867
6	3.887876	-1.187790	0.354917	6	-3.096025	0.934679	-0.584496
6	4.268557	0.069534	-0.113259	6	-4.033629	0.032377	-0.088769
6	3.346571	0.964036	-0.655161	6	-3.702382	-1.295049	0.185549
6	2.007741	0.590108	-0.718712	6	-2.395228	-1.711609	-0.034019
1	2.236768	-2.526189	0.636240	1	-1.053912	1.182198	-1.209894
1	4.637766	-1.858266	0.756197	1	-3.394424	1.954303	-0.795593
7	5.683891	0.459016	-0.038251	7	-5.412513	0.484930	0.144506
1	3.688129	1.924797	-1.020598	1	-4.463814	-1.970311	0.555910
1	1.265105	1.246592	-1.157662	1	-2.132510	-2.748840	0.161952
8	5.993382	1.576291	-0.452659	8	-6.217231	-0.336538	0.586295
8	6.477391	-0.353374	0.438318	8	-5.682292	1.657820	-0.112753
NImag=1(-1029.4)				NImag=1(-1025.2)			

17. **3t (s-*re*)** **Et**= -1105.989682 (-1106.317720)				18. **3t (s-*si*)** **Et** = -1105.986949 (-1106.315023)			
7	-1.964558	0.682789	0.597966	6	3.656807	-0.741744	1.367707
6	-3.259299	0.349242	-0.126965	6	3.209005	-0.781036	-0.124611
6	-3.901147	1.448126	0.755126	6	4.522304	-0.441394	-0.870768
6	-2.493476	2.084823	0.606409	6	4.316977	0.922643	-0.159854
6	-2.431619	2.437700	-0.893794	6	4.514212	0.567198	1.329604
6	-3.013353	1.102633	-1.466942	7	2.850007	0.679430	-0.326245
6	-3.862374	-1.051461	-0.197497	6	2.332714	-1.943060	-0.582268
8	-4.959658	-1.246673	0.282096	8	2.752902	-2.712484	-1.419588
8	-3.174315	-1.977771	-0.849841	8	1.159053	-2.093790	0.020638
1	-2.247767	-1.653396	-1.156806	1	4.717529	1.858234	-0.549006
1	-2.300970	0.567654	-2.093566	1	4.123621	1.342697	1.993925
1	-3.954156	1.237078	-2.007889	1	5.569374	0.401859	1.566494
1	-1.409438	2.629407	-1.230568	1	2.797611	-0.659726	2.032261
1	-3.046252	3.312483	-1.124967	1	4.238600	-1.633522	1.617219
1	-2.074183	2.773090	1.339366	1	0.937119	-1.344166	0.680575
1	-4.116672	1.092603	1.763936	1	5.408625	-1.023269	-0.606332
1	-4.751096	1.991256	0.334463	1	4.382199	-0.397573	-1.951820
6	-1.056741	0.076724	1.346813	6	1.854574	1.432806	-0.768418
6	-0.115315	0.974116	2.115480	6	0.544060	0.963149	-0.967562
1	-0.616956	1.397132	2.994832	1	0.393550	-0.082198	-1.210734
1	0.246943	1.804352	1.500180	1	-0.121912	1.643520	-1.489038
1	0.747295	0.403048	2.462473	6	2.164697	2.904366	-0.929766
6	-0.853726	-1.316729	1.322620	1	2.787564	3.072941	-1.816861
1	-1.707084	-1.955855	1.126155	1	1.240659	3.471197	-1.057640
1	-0.170757	-1.703212	2.073463	1	2.701451	3.305254	-0.063103
6	-0.016699	-1.635847	-0.495596	6	-0.154509	0.781709	0.959280
8	-0.804662	-1.134994	-1.367180	1	-0.011390	1.838005	1.249813
6	1.371945	-1.071962	-0.369309	8	0.578369	-0.090918	1.526509
1	-0.049993	-2.722419	-0.303549	6	-1.591675	0.487176	0.614557
6	2.354315	-1.727010	0.389040	6	-2.476404	1.541233	0.340198
6	3.639441	-1.207307	0.491819	6	-3.813340	1.295940	0.051861
6	3.934892	-0.019970	-0.180274	6	-4.259762	-0.025876	0.042710
6	2.984557	0.644934	-0.954647	6	-3.406957	-1.094019	0.319339
6	1.703550	0.109827	-1.046865	6	-2.072424	-0.830119	0.609920
1	2.108772	-2.655387	0.899657	1	-2.111501	2.565868	0.358363
1	4.411547	-1.699064	1.070607	1	-4.511048	2.096933	-0.158915
7	5.288405	0.540673	-0.073517	1	-3.797095	-2.104336	0.308648
1	3.263218	1.554372	-1.473097	1	-1.395495	-1.645270	0.840014
1	0.943218	0.581216	-1.660085	7	-5.671722	-0.297237	-0.259692
8	5.522540	1.591820	-0.671203	8	-6.400568	0.665744	-0.503413
8	6.109557	-0.070584	0.611348	8	-6.044648	-1.470507	-0.253380
NImag=1(-273.5)				NImag=1(-268.1)			

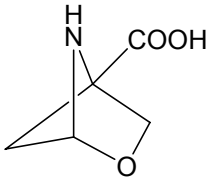


4

19. **4-anti-enamine** **Et** = -631.161090 (-631.354912)				20. **4-syn-enamine** **Et** = -631.163928 (-631.358745)			
6	-1.56449	-0.84449	-0.42217	7	0.60431	-0.08325	-0.4747
8	-0.93817	-1.96837	-1.01918	6	-0.70383	0.35711	0.08632
6	0.44353	-1.8565	-0.65939	6	-0.91483	1.59679	-0.83016
6	0.50051	-0.53116	0.15901	8	0.41267	2.12599	-0.97689
7	-0.55386	0.23088	-0.58816	6	1.24944	1.2364	-0.25298
6	-1.63058	-1.07117	1.11088	6	1.05503	1.49119	1.26084
6	-0.14916	-0.80946	1.53256	6	-0.36568	0.89066	1.50097
1	-0.05528	0.06583	2.18118	1	-0.35179	0.08236	2.23405
1	0.31719	-1.65422	2.04542	1	-1.09777	1.62998	1.83407
1	1.05358	-1.81516	-1.56895	1	1.81665	0.96475	1.84592
1	0.76363	-2.71181	-0.05372	1	1.12344	2.55853	1.48628
1	-2.31626	-0.369	1.5915	1	2.26473	1.30817	-0.64024
1	-1.96823	-2.08854	1.3241	1	-1.30995	1.32043	-1.81482
1	-2.50247	-0.65527	-0.94027	1	-1.57759	2.33617	-0.36847
6	1.90344	0.04735	0.11707	6	-1.84319	-0.63523	-0.066
8	2.67303	0.02145	1.04449	8	-2.75101	-0.73691	0.72183
8	2.26538	0.52624	-1.09943	8	-1.80575	-1.35146	-1.21254
1	1.47383	0.52099	-1.67366	1	-0.95018	-1.1775	-1.65228
6	-0.93397	1.5478	-0.18581	6	1.27486	-1.24228	0.01309
6	0.18091	2.5341	0.06972	6	0.71305	-2.18172	0.78824
1	0.83321	2.65407	-0.80165	1	-0.28787	-2.10993	1.19717
1	0.81924	2.23533	0.90969	1	1.26179	-3.08826	1.01858
1	-0.24346	3.51094	0.31156	6	2.68223	-1.38944	-0.51822
6	-2.21551	1.94646	-0.12221	1	3.37021	-0.66162	-0.06903
1	-3.06184	1.29374	-0.29993	1	2.70846	-1.23563	-1.60343
1	-2.44618	2.98472	0.08686	1	3.06974	-2.38654	-0.29674
NImag = 0				NImag = 0			

21**. 4t (a-*re*)** **Et** = -1181.217009 (-1181.570785)				22**. 4t (a-*si*)** **Et** = -1181.212615 (-1181.565796)			
6	-2.154341	1.699346	0.994218	7	2.407631	-0.511797	0.445430
8	-1.993291	2.304312	-0.258920	6	3.095241	0.741409	0.023910
6	-2.768410	1.493395	-1.174211	6	4.292991	0.751761	0.989567
6	-3.367585	0.356063	-0.284910	6	4.610028	-0.781749	1.106697
7	-2.247827	0.245872	0.693553	6	3.551363	-1.420402	0.168078
6	-3.634079	-0.926312	-1.100436	8	3.889358	-1.162716	-1.166863
8	-4.780508	-1.330148	-1.207415	6	2.169419	1.964881	-0.120753
8	-2.570237	-1.464726	-1.631870	8	2.505173	3.027009	0.375455
1	-1.517637	-1.004014	-1.395093	8	1.081207	1.741721	-0.809467
6	-1.636015	-0.790944	1.223932	1	0.838881	0.651203	-1.171126
6	-2.292982	-2.142200	1.273115	1	4.008772	1.191584	1.948668
1	-1.868254	-2.818434	0.523081	1	5.126647	1.333599	0.590770
1	-3.369744	-2.095683	1.109295	1	4.495289	-1.143545	2.133690
1	-2.100657	-2.577181	2.260481	1	5.610731	-1.047344	0.756756
6	-0.222979	-0.693473	1.461513	1	3.335857	-2.477525	0.313092
1	0.171022	0.306946	1.626795	1	2.865322	0.341973	-2.147780
1	0.198143	-1.424867	2.149998	1	4.532862	0.774126	-1.640262
6	0.338436	-1.104685	-0.205510	6	3.615723	0.244769	-1.363508
1	0.240740	-2.204576	-0.164511	6	1.240526	-0.734718	1.015278
8	-0.380393	-0.496474	-1.132757	6	0.548039	0.336284	1.809337
1	-2.099903	1.110910	-1.945114	1	0.211692	-0.112621	2.751473
1	-3.569976	2.089252	-1.621930	1	1.194237	1.184891	2.033628
1	-1.338172	1.972086	1.660849	1	-0.342752	0.704586	1.290770
1	-3.684994	1.669618	2.570292	6	0.518139	-1.914053	0.640770
1	-3.851647	2.995549	1.403158	1	1.119622	-2.753537	0.298767
1	-4.979855	0.223333	1.172287	1	-0.278905	-2.216445	1.316287
1	-5.197235	1.525079	0.000967	6	-0.227942	-1.316507	-0.943377
6	1.795975	-0.698774	-0.166768	8	0.583113	-0.515253	-1.601412
6	2.756342	-1.521758	0.437180	1	-0.306712	-2.312627	-1.408275
6	4.094116	-1.141534	0.478523	6	-1.620857	-0.822272	-0.589800
6	4.457105	0.077364	-0.092673	6	-1.991578	0.515279	-0.792707
6	3.523743	0.913051	-0.706141	6	-3.287277	0.943580	-0.507792
6	2.190840	0.516882	-0.740731	6	-4.214048	0.019948	-0.032077
1	2.458509	-2.474609	0.868993	6	-3.882644	-1.321682	0.160734
1	4.852864	-1.765396	0.934491	6	-2.585886	-1.730762	-0.122721
7	5.867442	0.490913	-0.049343	1	-1.267195	1.223701	-1.178410
8	6.670180	-0.267149	0.496186	1	-3.586530	1.974161	-0.654767
8	6.162877	1.572348	-0.557820	7	-5.582476	0.465751	0.269167
1	3.852514	1.846772	-1.145762	8	-5.852484	1.651777	0.083102
1	1.437297	1.130265	-1.222461	8	-6.376893	-0.374777	0.692751
6	-3.598225	1.938078	1.512422	1	-4.635987	-2.012863	0.517985
6	-4.455167	0.990859	0.598056	1	-2.321105	-2.777679	0.008213
NImag=1(-820.0)				NImag=1(-865.5)			

23. **4t (s-*re*)** **Et** = -1181.226644 (-1181.579524)				24. **4t (s-*si*)** **Et** = -1181.223526 (-1181.576534)			
6	1.920556	0.014361	-1.054313	6	-2.649771	1.583643	0.159911
6	1.576295	-1.072609	-0.238733	6	-1.769458	0.565195	0.555124
6	2.543929	-1.623929	0.614288	6	-2.250995	-0.744994	0.680672
6	3.827251	-1.092060	0.675022	6	-3.582827	-1.037729	0.402558
6	4.135551	0.000818	-0.136165	6	-4.431042	-0.005421	0.004712
6	3.200746	0.559616	-1.006656	6	-3.983619	1.309751	-0.118901
6	0.183489	-1.650707	-0.323617	6	-0.327882	0.901618	0.883399
8	-0.559434	-1.241773	-1.302033	8	0.381671	0.093088	1.594019
7	5.487228	0.574906	-0.073480	7	-5.839776	-0.307488	-0.286177
8	5.733363	1.541158	-0.795769	8	-6.564314	0.624728	-0.637824
8	6.292995	0.059077	0.701942	8	-6.213554	-1.473755	-0.163022
6	-0.680395	-1.232138	1.325564	6	0.403856	0.939674	-0.905187
6	-0.945700	0.157085	1.210086	6	1.718669	1.399849	-0.654600
6	0.035817	1.147729	1.789420	6	1.982294	2.888475	-0.681492
7	-1.913520	0.635623	0.445245	7	2.697378	0.623968	-0.211991
6	-3.195657	0.099948	-0.145738	6	2.963194	-0.857800	-0.143026
6	-3.052451	0.720857	-1.556492	6	3.463307	-0.911298	1.321983
8	-2.393257	1.987889	-1.308479	8	4.177173	0.338790	1.484617
6	-2.178521	2.053520	0.085411	6	4.048401	1.027092	0.257727
6	-3.507697	2.323231	0.804844	6	4.958116	0.378917	-0.795888
6	-4.224341	0.949979	0.645816	6	4.198599	-0.950958	-1.076129
6	-3.541123	-1.412902	-0.144067	6	1.879633	-1.911377	-0.477913
8	-2.789277	-2.218403	-0.859689	8	0.833079	-1.990226	0.317454
8	-4.541080	-1.771551	0.447345	8	2.083134	-2.681330	-1.394990
1	0.182821	-2.731856	-0.092939	1	-0.232023	1.974917	1.130717
1	-1.854924	-1.803301	-1.154038	1	0.669069	-1.145853	0.930828
1	-2.417385	0.121974	-2.210258	1	2.639875	-0.936801	2.037451
1	-4.029317	0.890715	-2.020026	1	4.141450	-1.754808	1.485176
1	-4.031628	3.151201	0.321120	1	4.160001	2.094957	0.430659
1	-1.348911	2.726317	0.290215	1	5.960349	0.234661	-0.385096
1	-3.346811	2.584102	1.856558	1	5.038923	1.003213	-1.692503
1	-5.168024	1.013184	0.099789	1	4.785220	-1.843089	-0.846344
1	-4.432051	0.469414	1.603052	1	3.865296	-1.035811	-2.111572
1	-1.518077	-1.915196	1.236040	1	2.159210	3.273216	0.330429
1	-0.002693	-1.498335	2.132455	1	2.859150	3.130480	-1.291443
1	0.597135	1.652677	0.994063	1	1.122697	3.414765	-1.098596
1	-0.473087	1.911294	2.387552	1	-0.212776	1.623138	-1.481643
1	0.755085	0.634272	2.427860	1	0.256761	-0.098880	-1.179804
1	2.292507	-2.483551	1.231522	1	-1.579900	-1.534157	0.998448
1	4.588001	-1.504922	1.326006	1	-3.972875	-2.044161	0.492158
1	3.487941	1.397035	-1.630983	1	-4.677343	2.084666	-0.420656
1	1.170486	0.403305	-1.734904	1	-2.286673	2.606011	0.079221
NImag=1(-304.2)				NImag=1(-318.8)			



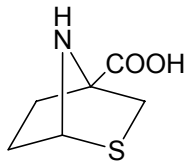
5

25. **5-anti-enamine** **Et** = -591.801011 (-591.985699)				26. **5-syn-enamine** **Et** = -591.811220 (-591.994204)			
7	0.728515	0.275296	-0.517647	6	-0.67545	-1.69114	-0.87795
6	-0.669763	0.333810	0.140479	6	0.82007	-1.48126	-0.58469
6	-1.241207	1.482657	-0.729715	8	0.91635	-1.73569	0.84223
8	-0.125551	2.395268	-0.670911	6	-0.18406	-0.938	1.32974
6	0.796468	1.641826	0.109330	6	-0.72066	-0.39832	-0.0292
6	-0.039139	1.128295	1.304638	7	0.5816	-0.03477	-0.7315
6	-1.541172	-0.886805	0.294443	6	1.49374	0.96005	-0.29794
8	-2.046083	-1.227354	1.333164	6	2.87992	0.5002	0.0838
8	-1.781825	-1.559540	-0.862044	6	-1.93344	0.50674	0.00495
1	-1.231056	-1.191317	-1.576081	8	-3.01359	0.15385	-0.39813
1	0.522630	0.483394	1.981113	6	1.15275	2.2633	-0.31536
1	-0.657838	1.847369	1.848337	8	-1.76151	1.71151	0.59482
1	1.753856	2.153003	0.166618	1	0.18326	-0.14801	1.99525
1	-1.429492	1.183599	-1.766456	1	-0.91243	-1.55953	1.8601
1	-2.141052	1.937174	-0.301493	1	-1.13999	-2.58651	-0.46247
6	1.681939	-0.702488	-0.129006	1	-0.96195	-1.51255	-1.9132
6	1.343268	-2.121426	-0.518197	1	1.65196	-1.95245	-1.10427
1	0.521686	-2.534050	0.077957	1	-0.81388	1.86979	0.78308
1	1.048565	-2.180249	-1.573219	1	3.36265	0.00628	-0.77
1	2.210673	-2.769273	-0.371148	1	2.85331	-0.22546	0.90222
6	2.864750	-0.401070	0.432887	1	3.5021	1.35262	0.36683
1	3.147840	0.601786	0.731545	1	0.21972	2.61391	-0.74398
1	3.611389	-1.174290	0.575529	1	1.85693	3.01853	0.01542
NImag = 0				NImag = 0			

27. **5t (a-*re*)** **Et** = -1141.850182 (-1142.193258)				28. **5t (a-*si*)** **Et**=-1141.8460035 (-1142.214657)			
7	-2.375090	0.174422	0.850378	7	2.555588	-0.558222	0.558107
6	-3.461870	0.586065	-0.076438	6	3.324611	0.629286	0.105444
6	-2.760913	1.835301	-0.707121	6	3.816007	0.066710	-1.271633
8	-2.187988	2.453221	0.486879	8	4.224237	-1.280623	-0.879191
6	-2.602980	1.553649	1.463939	6	3.911959	-1.257942	0.475066
6	-4.114172	1.273388	1.162507	6	4.476953	0.100402	1.012687
6	-3.906642	-0.464643	-1.100283	1	4.298021	0.272034	2.074946
8	-5.085222	-0.729814	-1.258926	1	5.505731	0.328545	0.725168
8	-2.884320	-0.978728	-1.732422	1	3.024691	-0.008362	-2.014409
1	-1.755736	-0.675887	-1.420764	1	4.675344	0.631731	-1.643449
1	-4.583512	0.565319	1.846824	1	4.015057	-2.229438	0.955317
1	-4.733636	2.157262	0.994862	6	2.538648	1.939770	0.001029
1	-2.170965	1.755749	2.442518	8	2.957362	2.971377	0.493761
1	-1.957275	1.579330	-1.393721	8	1.426198	1.776495	-0.670522
1	-3.491746	2.505160	-1.168856	1	1.099807	0.684241	-1.039610
6	-1.791439	-0.956320	1.170123	6	1.375848	-0.765234	1.094639
6	-2.455136	-2.280638	0.903820	6	0.650563	0.327837	1.827921
1	-3.540981	-2.190105	0.848234	6	0.675902	-1.948288	0.681460
1	-2.113934	-2.724772	-0.037072	1	-0.170109	0.743689	1.235862
1	-2.191814	-2.966420	1.716416	1	0.208138	-0.112405	2.729387
6	-0.381388	-0.906807	1.432140	1	1.313668	1.143369	2.118221
1	0.006872	0.061896	1.744293	1	-0.135603	-2.284948	1.323580
1	0.051289	-1.740583	1.983714	1	1.312539	-2.761367	0.333161
6	0.137413	-1.055563	-0.305290	6	-0.020982	-1.287789	-0.882412
8	-0.599964	-0.313144	-1.119171	8	0.799126	-0.448005	-1.495598
1	0.032583	-2.147520	-0.426176	1	-0.083097	-2.256806	-1.403048
6	1.595492	-0.662955	-0.244238	6	-1.426038	-0.805173	-0.563966
6	2.560925	-1.570424	0.214270	6	-1.792675	0.529964	-0.788620
6	3.902514	-1.208924	0.282481	6	-3.094533	0.961121	-0.539701
6	4.265892	0.077309	-0.114000	6	-4.032015	0.040641	-0.078841
6	3.328499	0.998454	-0.580770	6	-3.705199	-1.299291	0.132663
6	1.991412	0.620255	-0.644322	6	-2.401610	-1.710929	-0.114491
1	2.263253	-2.573635	0.510374	1	-1.056524	1.230766	-1.167104
1	4.663891	-1.897283	0.627867	1	-3.390730	1.990086	-0.703145
7	5.680829	0.471389	-0.041240	7	-5.407809	0.488091	0.185121
8	6.486594	-0.362352	0.373432	8	-5.673971	1.671912	-0.019244
8	5.976064	1.612518	-0.395799	8	-6.211403	-0.348962	0.597862
1	3.656763	1.983940	-0.887599	1	-4.467252	-1.987537	0.476862
1	1.237823	1.304383	-1.017747	1	-2.141167	-2.756755	0.031646
NImag=1(-1016.5)				NImag=1(-1020.5)			

29. **5t (s-*re*)** **Et** = -1141.876864 (-1142.219296)			
6	1.650894	0.097804	-1.002182
6	1.347574	-1.094380	-0.329466
6	2.352915	-1.747341	0.399414
6	3.635992	-1.217233	0.476404
6	3.904174	-0.021388	-0.191096
6	2.929351	0.643248	-0.934571
6	-0.039235	-1.673240	-0.422127
8	-0.836352	-1.204352	-1.309864
6	-0.859604	-1.325102	1.357697
6	-1.043204	0.072944	1.375593
6	-0.085530	0.970485	2.121810
7	-1.966372	0.679604	0.649755
6	-2.435750	2.092691	0.512174
8	-2.291656	2.350589	-0.871394
6	-2.848558	1.126442	-1.447505
6	-3.229415	0.378071	-0.141993
6	-3.868725	1.541815	0.664402
6	-3.894916	-0.996044	-0.231684
8	-3.213572	-1.961606	-0.823212
8	-5.023613	-1.124190	0.193656
1	-2.080286	0.607891	-2.019137
1	-3.722986	1.361837	-2.060930
1	-4.665417	2.111852	0.182466
1	-4.135379	1.239599	1.677683
1	-1.976714	2.870101	1.118475
1	-2.255745	-1.680868	-1.106368
1	-0.573798	1.408390	3.001211
1	0.275673	1.787908	1.489046
1	0.775668	0.395701	2.465789
1	-1.730368	-1.946964	1.179106
1	-0.184161	-1.714741	2.114146
1	-0.052086	-2.758488	-0.218091
1	2.128517	-2.683308	0.906109
1	4.426175	-1.707727	1.031362
7	5.255848	0.550313	-0.111297
1	3.185820	1.561705	-1.448485
1	0.872292	0.576383	-1.586142
8	5.466441	1.608227	-0.704957
8	6.097587	-0.060083	0.548689
NImag=1(-291.1)			

30. **5t (s-*si*)** **Et** = -1141.874315 (-1142.216602)			
6	4.314315	0.915723	-0.123781
8	4.404231	0.665214	1.267127
6	3.619362	-0.564654	1.384354
6	3.231818	-0.763440	-0.108343
7	2.872807	0.676675	-0.431509
6	4.591826	-0.447473	-0.788538
1	2.753551	-0.387967	2.021613
1	4.247126	-1.377134	1.761713
1	5.468992	-0.992360	-0.435306
1	4.515296	-0.449169	-1.876038
1	4.767950	1.867010	-0.392605
6	2.401212	-1.976172	-0.528970
8	2.877389	-2.769453	-1.311910
8	1.209179	-2.120588	0.028892
1	0.946183	-1.356148	0.669276
6	1.847491	1.442340	-0.771025
6	2.143035	2.920468	-0.877221
1	2.781304	3.127837	-1.744492
1	2.659214	3.287884	0.016681
1	1.215593	3.482272	-1.000804
6	0.534700	0.960947	-0.944139
1	0.404445	-0.078861	-1.224244
1	-0.142131	1.643241	-1.449551
6	-0.151917	0.752153	0.925809
8	0.569644	-0.139034	1.492734
1	-0.012055	1.797398	1.253804
6	-1.597180	0.467767	0.592424
6	-2.078258	-0.848642	0.566092
6	-3.415600	-1.106233	0.281676
6	-4.269244	-0.032285	0.032359
6	-3.822293	1.288713	0.063774
6	-2.482528	1.527594	0.345964
1	-1.400027	-1.668159	0.776599
1	-3.806800	-2.115843	0.254897
7	-5.684196	-0.297095	-0.265730
8	-6.057228	-1.469997	-0.279347
8	-6.413298	0.670895	-0.486277
1	-4.521180	2.094049	-0.125444
1	-2.117498	2.551756	0.382206
NImag=1(-293.6)			

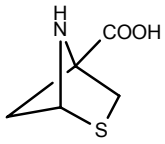


6

31. **6-anti-enamine** **Et** = -954.135755 (-954.332675)				32. **6-syn-enamine** **Et** = -954.141231 (-954.338373)			
6	-1.40006	0.96334	0.10865	7	-0.08815	0.62116	-0.37849
16	-2.4952	-0.31765	-0.65537	6	0.15635	-0.74537	0.16086
6	-1.08015	-1.50866	-0.55778	6	-0.88005	-1.61242	-0.6132
6	0.05193	-0.724	0.17393	16	-2.40849	-0.56831	-0.68986
7	-0.05717	0.63717	-0.42315	6	-1.46498	0.78462	0.14677
6	-1.26178	0.69811	1.62601	6	-1.31636	0.46967	1.65394
6	-0.34134	-0.55687	1.66777	6	-0.2537	-0.66844	1.65683
1	0.54272	-0.40722	2.29104	6	1.54204	-1.3088	-0.14693
1	-0.7798	-1.79543	-1.56846	8	2.1489	-2.0312	0.60421
1	-0.85282	-1.44502	2.04665	8	2.00661	-1.01401	-1.38259
1	-1.35381	-2.40583	0.00164	1	1.41545	-0.34826	-1.78415
1	-2.22753	0.54506	2.112	1	0.60609	-0.424	2.28294
1	-1.73607	1.9593	-0.16883	1	-0.65287	-1.62288	2.00772
1	-0.77322	1.56049	2.09591	1	-2.26485	0.18252	2.1123
6	1.36241	-1.44393	-0.1228	1	-0.93636	1.35576	2.17633
8	1.91459	-2.18544	0.64926	1	-1.90595	1.74886	-0.09941
8	1.82891	-1.24871	-1.38251	1	-0.54036	-1.8301	-1.62852
1	1.26858	-0.57579	-1.81719	1	-1.06824	-2.5517	-0.08897
6	0.93733	1.66499	-0.24076	6	0.80638	1.70302	-0.09145
6	2.23568	1.35205	0.46815	6	0.36387	3.01839	-0.69208
1	2.07872	0.92355	1.4635	1	-0.47182	3.46542	-0.1386
1	2.85568	0.64823	-0.09649	1	0.03373	2.8836	-1.72839
1	2.81337	2.27235	0.58411	1	1.18534	3.73872	-0.67531
6	0.71069	2.88855	-0.74309	6	1.9714	1.59039	0.56281
1	-0.1842	3.13199	-1.30669	1	2.63693	2.44473	0.62473
1	1.43546	3.68215	-0.60386	1	2.3221	0.6774	1.02824
NImag=0				NImag=0			

33**. 6t (a-*re*)** **Et =** -1504.193860 (-1504.525388)				34**. 6t (a-*si*)** **Et =** - 1504.1894313 (-1504.545209)			
6	-2.104588	1.454949	1.169698	6	-2.727242	-1.744415	0.028199
16	-1.863989	2.453618	-0.197370	6	-1.779843	-0.849373	-0.497139
6	-2.902174	1.436330	-1.082186	6	-2.182295	0.455679	-0.819249
6	-3.348212	0.194619	-0.233309	6	-3.495136	0.867053	-0.595218
7	-2.166951	0.052172	0.676809	6	-4.404799	-0.041097	-0.060320
6	-3.557486	1.568028	1.732304	6	-4.040467	-1.351338	0.251974
6	-4.409811	0.662885	0.771699	6	-0.372421	-1.331331	-0.782966
1	-4.848959	-0.189372	1.295365	8	0.427795	-0.583581	-1.508024
1	-2.356090	1.115899	-1.967489	7	-5.792138	0.387255	0.175544
1	-5.221239	1.202092	0.280322	8	-6.090244	1.545515	-0.113032
1	-3.791340	1.985563	-1.400723	8	-6.571824	-0.439233	0.650419
1	-3.885488	2.610743	1.740193	6	0.375496	-1.739857	0.904852
1	-1.361849	1.593614	1.954176	6	1.052004	-0.505659	1.137808
1	-3.597504	1.198479	2.760533	6	0.304760	0.632143	1.775860
6	-3.632174	-1.061299	-1.076249	7	2.252583	-0.331868	0.601265
8	-4.765055	-1.510063	-1.130805	6	3.403788	-1.252604	0.651625
8	-2.588442	-1.538988	-1.709044	16	3.988011	-1.394535	-1.086218
1	-1.568147	-1.069867	-1.513731	6	3.433654	0.360127	-1.352689
6	-1.535328	-1.017597	1.098491	6	2.907496	0.879885	0.021209
6	-2.140147	-2.388480	0.993535	6	4.087386	1.075028	0.992773
1	-3.215108	-2.367406	0.821180	6	4.386236	-0.382313	1.480987
1	-1.679758	-2.965364	0.185500	6	1.926665	2.056242	-0.232342
1	-1.939837	-2.913051	1.933749	8	2.211731	3.165021	0.190041
6	-0.118116	-0.905778	1.357979	8	0.863574	1.735804	-0.916073
1	0.232841	0.082665	1.646828	1	0.651893	0.582954	-1.188990
1	0.305717	-1.686666	1.987689	1	4.268557	0.981659	-1.683206
6	0.467568	-1.123330	-0.294881	1	2.646610	0.356520	-2.104145
8	-0.249098	-0.429490	-1.170390	1	3.158126	-2.222673	1.079944
1	0.393923	-2.223914	-0.387006	1	5.418933	-0.694302	1.314752
6	1.931137	-0.724022	-0.214416	1	4.160934	-0.492013	2.548687
6	2.361520	0.455267	-0.834182	1	4.941703	1.537650	0.494024
6	3.695894	0.844284	-0.768658	1	3.790428	1.732842	1.812563
6	4.596811	0.036270	-0.076859	1	-0.574306	0.922629	1.193253
6	4.201050	-1.151474	0.537595	1	0.924065	1.515033	1.931217
6	2.863600	-1.524014	0.461907	1	-0.054919	0.277123	2.749268
1	1.633243	1.038961	-1.384980	1	0.996615	-2.595476	0.650955
1	4.051774	1.749837	-1.243903	1	-0.438169	-1.980621	1.584336
7	6.007176	0.442108	0.001835	1	-0.396082	-2.377313	-1.122914
8	6.332997	1.493544	-0.549905	1	-1.469415	1.150615	-1.249069
8	6.781052	-0.291264	0.618618	1	-3.820589	1.871994	-0.834671
1	4.937334	-1.755842	1.051980	1	-4.781565	-2.031820	0.652682
1	2.543837	-2.453956	0.925133	1	-2.434034	-2.767187	0.254284
NImag=1(-906.0)				NImag=1(-949.3)			

35. **6t (s-*re*)** **Et** = -1504.2052707 (-1504.560968)				36. **6t (s-*si*)** **Et** = - 1504.2023354 (-1504.558062)			
6	1.983191	0.115881	-1.008884	6	2.823817	-1.575786	0.156922
6	1.690765	-1.104126	-0.383322	6	1.955467	-0.536933	0.523207
6	2.689037	-1.752961	0.358549	6	2.461233	0.763107	0.659773
6	3.953648	-1.191356	0.496195	6	3.806711	1.026002	0.421599
6	4.210812	0.031640	-0.124679	6	4.643697	-0.026606	0.053318
6	3.243870	0.692553	-0.881372	6	4.171632	-1.331958	-0.080750
6	0.322403	-1.717692	-0.553278	6	0.497790	-0.837336	0.807065
8	-0.444972	-1.208814	-1.458860	8	-0.196787	-0.029688	1.529667
7	5.542860	0.636177	0.019282	7	6.067156	0.243473	-0.195184
8	5.744124	1.717569	-0.533880	8	6.781456	-0.705802	-0.520925
8	6.378384	0.027894	0.689056	8	6.462215	1.401901	-0.064933
6	-0.550904	-1.562820	1.153511	6	-0.190869	-0.771453	-1.009714
6	-0.838511	-0.181062	1.283569	6	-1.507551	-1.272011	-0.874412
6	0.138839	0.689068	2.039050	6	-1.715240	-2.760512	-1.045873
7	-1.830600	0.428164	0.639453	7	-2.554791	-0.558548	-0.464612
6	-3.076363	-0.044059	-0.079623	6	-2.802295	0.908188	-0.197093
6	-2.954220	0.632879	-1.466567	6	-3.164858	0.924994	1.309612
16	-2.239699	2.317808	-1.133185	16	-4.193737	-0.601689	1.584188
6	-2.105491	1.879634	0.660877	6	-3.904503	-1.083559	-0.182674
6	-3.484269	1.935054	1.329647	6	-4.779305	-0.238096	-1.114195
6	-4.173693	0.664277	0.763826	6	-4.076417	1.143939	-1.056716
6	-3.372421	-1.575787	-0.210863	6	-1.697045	1.957329	-0.548857
8	-2.657113	-2.269145	-1.069841	8	-0.671834	2.069893	0.272652
8	-4.301528	-2.046928	0.414235	8	-1.858820	2.689401	-1.503185
1	0.360315	-2.819112	-0.464942	1	0.354450	-1.915564	1.002546
1	-1.744811	-1.812768	-1.348515	1	-0.494929	1.234537	0.881846
1	-2.265817	0.097236	-2.115974	1	-2.278857	0.844441	1.935166
1	-3.935987	0.719592	-1.937361	1	-3.736614	1.821771	1.558551
1	-4.008509	2.862050	1.090519	1	-3.985337	-2.160539	-0.294612
1	-1.318075	2.463333	1.128292	1	-5.817128	-0.217082	-0.776953
1	-3.373462	1.874198	2.419606	1	-4.754762	-0.653310	-2.129504
1	-5.039570	0.893097	0.138013	1	-4.698086	1.918701	-0.601500
1	-4.508493	-0.012246	1.549891	1	-3.777961	1.499357	-2.042566
1	-1.372204	-2.242217	0.959297	1	-2.012870	-3.230177	-0.100577
1	0.143374	-1.945315	1.896590	1	-2.490775	-2.975602	-1.789302
1	0.639983	1.396357	1.368069	1	-0.789245	-3.229540	-1.380494
1	-0.363296	1.260596	2.827797	1	0.463752	-1.407015	-1.598621
1	0.907010	0.070345	2.502812	1	-0.042549	0.282915	-1.208743
1	2.476480	-2.712246	0.825404	1	1.796596	1.567026	0.954550
1	4.738050	-1.678263	1.062401	1	4.216146	2.023934	0.519346
1	3.492432	1.632177	-1.359730	1	4.857434	-2.122771	-0.358417
1	1.210632	0.586527	-1.607843	1	2.440547	-2.590024	0.067373
NImag=1(-305.8)				NImag=1(-318.4)			

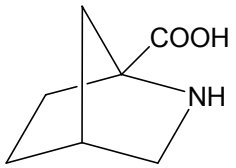


7

37. **7-anti-enamine** **Et** = -914.794098 (-914.980619)				38. **7-syn-enamine** **Et** = -914.785627 (-914.972675)			
7	-0.46041	0.45415	0.68006	7	-0.04454	0.7294	-0.2988
6	0.64589	-0.36707	0.11972	6	-0.06525	-0.71923	0.14118
6	0.0774	-1.07098	-1.15792	6	-1.28956	-1.28985	-0.63475
16	-1.56233	-1.6904	-0.54788	16	-2.58503	0.0069	-0.30042
6	-1.06932	-0.80787	1.07186	6	-1.23143	0.84062	0.63776
6	0.35146	-1.34679	1.30244	6	-0.60713	-0.2706	1.51408
6	2.04303	0.23238	0.04082	6	1.14351	-1.61182	-0.05045
8	2.35808	1.30882	0.47528	8	1.47701	-2.45613	0.74193
8	2.97961	-0.58432	-0.51226	8	1.77718	-1.46119	-1.23903
1	2.57674	-1.4166	-0.81084	1	1.44622	-0.66205	-1.68821
1	-0.05776	-0.36047	-1.97734	1	-1.09094	-1.36407	-1.70593
1	0.68819	-1.90917	-1.5111	1	-1.58728	-2.26436	-0.24155
1	0.52839	-2.41218	1.14963	1	-1.26738	-0.93883	2.07086
1	0.79441	-0.97938	2.23074	1	0.19603	0.11383	2.14718
1	-1.86364	-0.81715	1.81707	1	-1.49401	1.82666	1.01628
6	-1.13989	1.51798	0.0388	6	1.04764	1.60486	-0.02768
6	-0.26074	2.57517	-0.57652	6	0.72998	3.03446	-0.40064
1	0.32985	2.18106	-1.41349	1	-0.07483	3.44801	0.22057
1	0.45441	2.96705	0.15189	1	0.39208	3.09562	-1.44125
1	-0.87626	3.39245	-0.96039	1	1.60784	3.67214	-0.27124
6	-2.47672	1.61486	0.07066	6	2.26123	1.24172	0.416
1	-2.97057	2.49086	-0.33455	1	3.05417	1.97942	0.4777
1	-3.11172	0.84861	0.50067	1	2.5228	0.23497	0.71776
NImag = 0				NImag = 0			

39. **7t (a-*re*)** **Et** = -1464.831377 (-1465.177618)				40. **7t (a-*si*)** **Et** = -1464.827188 (-1465.172659)			
6	2.062357	0.508058	-0.670275	6	4.241740	0.458028	1.108410
6	1.699367	-0.772143	-0.228898	6	3.103120	0.815332	0.112307
6	2.685395	-1.639790	0.262406	6	3.614656	0.260802	-1.259369
6	4.017122	-1.242290	0.320060	16	4.251053	-1.441880	-0.823569
6	4.348237	0.038612	-0.118958	6	3.705167	-0.996193	0.869924
6	3.389390	0.920917	-0.616337	7	2.370622	-0.335322	0.701669
6	0.262058	-1.210145	-0.286486	6	1.172509	-0.516499	1.232162
8	-0.491438	-0.546087	-1.141822	6	0.400745	0.624873	1.836556
7	5.753667	0.469773	-0.058397	6	2.251919	2.082471	-0.085025
8	6.578492	-0.330816	0.382577	8	2.620603	3.159484	0.351340
6	-0.282657	-0.940922	1.502004	6	0.529743	-1.760916	0.979261
6	-1.670534	-1.043449	1.201264	8	1.155720	1.821275	-0.744386
6	-2.296691	-2.401893	1.018387	6	-0.174690	-1.272945	-0.730473
7	-2.284338	0.060661	0.811822	8	0.638843	-0.482234	-1.400659
6	-3.368853	0.382022	-0.153737	1	-0.164933	-2.301246	-1.116843
6	-2.773177	1.556526	-0.997312	1	3.768566	-1.790652	1.612247
16	-1.980058	2.653160	0.292349	1	2.817961	0.171987	-1.993332
6	-2.583792	1.376586	1.464141	1	4.421288	0.897074	-1.630158
6	-4.066638	1.095205	1.038638	1	0.862788	0.648304	-1.054410
6	-3.790553	-0.788829	-1.060548	1	5.272680	0.658048	0.812365
8	-2.763165	-1.323710	-1.657623	1	4.030482	0.820674	2.117446
8	-4.963153	-1.112532	-1.153024	1	1.178571	-2.592503	0.709874
8	6.020502	1.605716	-0.449296	1	-0.302147	-2.034772	1.623651
1	-2.265156	1.496234	2.498742	1	-0.437805	0.943849	1.211569
1	-2.020632	1.217834	-1.705146	1	-0.020113	0.265989	2.783662
1	-3.581613	2.080911	-1.511527	1	1.029491	1.492871	2.034775
1	-1.595433	-0.951408	-1.386507	6	-1.591942	-0.815877	-0.475807
1	-4.693622	1.963530	0.830064	6	-1.995703	0.491255	-0.789086
1	-4.564141	0.385969	1.704808	6	-3.318691	0.887392	-0.602319
1	0.096200	0.053537	1.728969	6	-4.236378	-0.038473	-0.113374
1	0.171568	-1.735987	2.090402	6	-3.870165	-1.350303	0.189502
1	-1.953323	-2.899342	0.106057	6	-2.546695	-1.728671	0.003453
1	-2.010314	-3.023695	1.873621	1	-1.275041	1.198049	-1.186432
1	-3.384669	-2.344740	0.964779	1	-3.645979	1.892971	-0.836373
1	0.166713	-2.306714	-0.301681	7	-5.635780	0.372625	0.081131
1	2.411822	-2.639394	0.591681	1	-4.617844	-2.043834	0.553938
1	4.795002	-1.899289	0.688824	1	-2.252022	-2.752463	0.221950
1	3.693605	1.904181	-0.953415	8	-6.421834	-0.468550	0.517631
1	1.293533	1.163419	-1.063806	8	-5.935668	1.531643	-0.201822
NImag=1(-1005.6)				NImag=1(-1030.7)			

41. **7t (s-*re*)** **Et** = -1464.8624207 (-1465.207105)				42. **7t (s-*si*)** **Et** = -1464.860160 (-1465.204588)			
6	1.719273	0.122928	-0.967119	7	-2.677389	-0.550712	-0.633353
6	1.466342	-1.153669	-0.445793	6	-4.120329	-0.845847	-0.519438
6	2.501008	-1.852242	0.194360	6	-4.368319	0.618431	-0.938304
6	3.763674	-1.286745	0.333690	6	-3.032139	0.854715	-0.192708
6	3.981703	-0.008803	-0.182341	6	-3.364282	0.693153	1.317124
6	2.976851	0.704192	-0.835804	16	-4.416746	-0.858793	1.315430
6	0.103251	-1.774220	-0.604858	6	-2.177409	2.075059	-0.573038
8	-0.715070	-1.251882	-1.440521	8	-2.629976	2.885272	-1.352411
7	5.311095	0.600591	-0.035272	8	-0.996995	2.204669	0.012073
8	6.178601	-0.051517	0.546958	1	-0.739588	1.426605	0.636434
8	5.478583	1.728961	-0.498569	1	-2.466535	0.526631	1.909702
6	-0.724588	-1.647859	1.198914	1	-3.937103	1.548592	1.682185
6	-0.946718	-0.273900	1.422271	1	-4.520561	-1.707823	-1.049717
6	-0.007122	0.530233	2.286709	1	-4.250200	0.782240	-2.011228
7	-1.905035	0.414409	0.816200	1	-5.259513	1.111247	-0.548917
6	-3.123954	0.202386	-0.060476	6	-1.629782	-1.293358	-0.969549
6	-2.780383	0.981929	-1.358620	6	-1.923171	-2.755525	-1.204617
16	-2.063717	2.573470	-0.675280	1	-2.477701	-3.186560	-0.363072
6	-2.389311	1.802311	0.982166	1	-2.526168	-2.891969	-2.110649
6	-3.818969	1.230258	0.866053	1	-0.992913	-3.311028	-1.334365
6	-3.765140	-1.179933	-0.266976	6	-0.308096	-0.807553	-1.039392
8	-3.086027	-2.068482	-0.972206	1	-0.163487	0.245530	-1.254912
8	-4.875230	-1.378822	0.178566	1	0.383751	-1.461123	-1.562149
1	-2.139997	-1.753565	-1.249754	6	0.337281	-0.705771	0.844320
1	-2.029262	0.464803	-1.951574	8	-0.361991	0.188811	1.435178
1	-3.683073	1.181691	-1.940155	1	0.154025	-1.757674	1.125878
1	-2.030281	2.381379	1.830450	6	1.799426	-0.456475	0.557261
1	-4.164275	0.755176	1.786681	6	2.318944	0.844759	0.593674
1	-4.586156	1.870381	0.429108	6	3.669652	1.073097	0.350555
1	-0.507145	0.855081	3.207636	6	4.497158	-0.015914	0.078957
1	0.352016	1.421311	1.760449	6	4.011286	-1.323120	0.048339
1	0.855299	-0.076264	2.566756	6	2.658522	-1.532451	0.289753
1	-1.580469	-2.263326	0.944473	1	1.658179	1.673997	0.821611
1	-0.033608	-2.118128	1.892813	1	4.090819	2.070693	0.372429
1	0.135725	-2.874690	-0.512969	7	5.926063	0.217386	-0.176340
1	2.316427	-2.852141	0.580792	8	6.333465	1.378122	-0.135121
1	4.575464	-1.811299	0.822345	8	6.631499	-0.762848	-0.418577
1	3.193887	1.688750	-1.231966	1	4.690971	-2.141084	-0.156114
1	0.920117	0.643056	-1.483975	1	2.262780	-2.545711	0.277096
NImag=1(-295.3)				NImag=1(-305.5)			

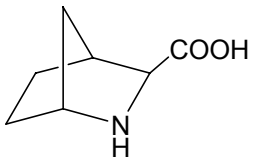


8

43. **8-anti-enamine** **Et** = -595.2726134 (-595.453001)				44. **8-syn-enamine** **Et** = -595.273117 (-595.453921)			
7	-0.220541	-0.691979	-0.481748	6	1.208884	-1.984988	1.009910
6	0.334209	0.592106	0.033780	6	0.891338	-2.029909	-0.505583
6	0.985200	0.385786	1.418959	6	0.702375	0.152204	-0.003558
6	2.232388	-0.492358	1.066041	6	1.088356	-0.465101	1.360155
6	2.147892	-0.634834	-0.476266	1	0.519121	-2.606395	1.591342
6	0.955648	-1.540636	-0.823707	1	2.221439	-2.357227	1.199131
6	1.586306	0.735330	-0.876340	1	0.327008	-0.267690	2.117582
6	-0.596505	1.784082	-0.146165	1	2.030317	-0.037457	1.712331
8	-1.354614	1.719627	-1.267169	6	1.529811	-0.718370	-0.987026
6	-1.343017	-1.328542	0.100689	1	1.329282	-0.475359	-2.035394
6	-1.574275	-2.648699	-0.036093	1	2.603578	-0.646929	-0.791911
8	-0.603181	2.752665	0.573341	6	-0.601438	-1.714372	-0.710054
6	-2.352383	-0.455917	0.814557	1	-0.932922	-1.909708	-1.737764
1	2.214254	-1.465605	1.567344	1	-1.229313	-2.303207	-0.032484
1	3.162743	0.007787	1.355431	7	-0.673379	-0.251037	-0.397385
1	0.303850	-0.111869	2.114111	1	1.211987	-2.944709	-1.011390
1	1.259695	1.349812	1.854879	6	0.966084	1.640855	-0.204535
1	1.330097	0.826083	-1.936569	8	1.774785	2.270492	0.434196
1	2.210670	1.581745	-0.576060	8	0.285489	2.186403	-1.235432
1	0.934790	-1.833264	-1.881633	6	-1.808941	0.249733	0.284054
1	0.955370	-2.454554	-0.218744	6	-3.124869	-0.315835	-0.200530
1	3.081268	-0.938557	-0.957647	1	-3.244076	-1.375335	0.056540
1	-2.898471	0.190132	0.118160	1	-3.958132	0.229035	0.248884
1	-3.080866	-1.089138	1.325563	1	-3.209675	-0.237995	-1.291883
1	-1.894374	0.198105	1.563883	6	-1.772127	1.223317	1.210732
1	-2.478386	-3.080897	0.376355	1	-2.699107	1.627720	1.601231
1	-0.926071	-3.317839	-0.588681	1	-0.857838	1.670355	1.581891
1	-1.221212	0.825662	-1.646263	1	-0.357043	1.511794	-1.537917
NImag = 0				NImag = 0			

45. **8t (a-*re*)** **Et** = -1145.3397843 (-1145.679261)			46. **8t (a-*si*)** **Et** = -1145.336393 (-1145.675554)		
7	-2.198985	0.241311	0.650732	7	2.351610	-0.582175	0.366972
6	-3.428058	0.186017	-0.208586	6	3.036904	0.720416	0.078444
6	-4.614308	0.574228	0.691744	6	4.166657	0.863433	1.113632
6	-4.292238	2.070611	1.032401	6	5.116883	-0.321945	0.724272
6	-3.025491	2.377071	0.185819	6	4.470282	-0.907485	-0.562593
6	-1.801996	1.676060	0.796619	6	3.191696	-1.679072	-0.203008
6	-3.235355	1.480768	-1.041743	6	3.834051	0.336078	-1.196662
6	-3.517285	-1.075081	-1.090011	6	2.068856	1.889539	-0.176814
8	-2.399110	-1.462873	-1.656867	8	1.015489	1.602631	-0.904316
6	-1.568149	-0.771427	1.198867	6	1.223738	-0.764671	1.015153
6	-0.141789	-0.652662	1.402269	6	0.439570	-1.932397	0.687262
8	-4.602779	-1.604461	-1.253914	8	2.352091	2.998264	0.242061
6	-2.200583	-2.128522	1.315923	6	0.604181	0.319707	1.846883
1	-4.118071	2.228579	2.102368	1	5.196787	-1.071388	1.519302
1	-5.115524	2.728997	0.738563	1	6.129768	0.035304	0.514291
1	-4.684071	-0.061558	1.578831	1	3.797319	0.796126	2.140788
1	-5.543060	0.457555	0.128957	1	4.638081	1.841521	0.995216
1	-2.373446	1.424763	-1.710654	1	3.183922	0.124305	-2.048783
1	-4.139520	1.705657	-1.614275	1	4.545802	1.124865	-1.454861
1	-0.892844	1.872686	0.226465	1	2.707164	-2.098005	-1.087557
1	-1.636703	1.896425	1.855963	1	3.332526	-2.456623	0.554348
1	-2.846557	3.437729	-0.005139	1	5.146687	-1.489535	-1.192766
1	-1.781542	-2.810386	0.566022	1	-0.279308	0.726123	1.340665
1	-1.965101	-2.536464	2.304733	1	0.264884	-0.120812	2.790731
1	-3.282845	-2.115947	1.186277	1	1.283000	1.144362	2.063958
1	0.284708	-1.401558	2.069267	1	-0.345847	-2.160245	1.405241
1	0.223435	0.342801	1.645633	1	1.016645	-2.820887	0.439895
1	-1.467965	-0.901833	-1.438321	1	0.827080	0.538908	-1.208143
6	0.424939	-0.956725	-0.240764	6	-0.286204	-1.453165	-0.877608
6	1.899263	-0.586724	-0.179588	1	-0.420294	-2.469227	-1.290668
1	0.330312	-2.060054	-0.288552	6	-1.672396	-0.897081	-0.556656
8	-0.284655	-0.287949	-1.136745	8	0.534818	-0.713152	-1.604422
6	2.820398	-1.389049	0.509058	6	-2.014405	0.429032	-0.855649
6	4.166769	-1.044750	0.563759	6	-3.295790	0.910353	-0.590481
6	4.584039	0.117559	-0.084692	6	-4.239638	0.049697	-0.036288
6	3.693849	0.927061	-0.789516	6	-3.937728	-1.281789	0.253003
6	2.350732	0.565733	-0.833997	6	-2.654736	-1.742548	-0.013063
1	2.484460	-2.300274	0.998820	1	-1.277291	1.087088	-1.300031
1	4.892648	-1.653888	1.088102	1	-3.570892	1.934464	-0.811535
7	6.003056	0.493532	-0.028861	7	-5.591678	0.550788	0.245519
1	4.063348	1.812485	-1.292422	1	-4.702786	-1.925247	0.669669
1	1.631240	1.152187	-1.394649	1	-2.414113	-2.783185	0.194425
8	6.347166	1.523447	-0.609739	8	-6.402866	-0.235578	0.737331
8	6.766903	-0.241014	0.599206	8	-5.835804	1.726982	-0.023224
NImag =1(-291.4)				NImag =1(-490.4)			

47. **8t (s-*re*)** **Et** = -1145.3255531 (-1145.664874)				48. **8t (s-*si*)** **Et** = -1145.328359 (-1145.667378)			
7	1.747533	-0.731578	0.454480	7	2.595943	-0.847098	-0.052270
6	2.908964	-0.181787	-0.340774	6	3.436728	0.395415	0.139540
6	4.162994	-0.388623	0.532330	6	4.563623	0.117545	-0.877468
6	4.321999	-1.945535	0.538468	6	4.894707	-1.271460	-0.309722
6	3.157276	-2.425957	-0.367700	6	3.522154	-1.948202	-0.437917
6	1.830587	-2.218088	0.377320	6	5.158927	-0.956584	1.186210
6	3.066500	-1.293128	-1.401135	6	4.163928	0.212261	1.487687
6	2.643548	1.211054	-0.909974	1	3.463210	-0.009490	2.297075
8	1.511889	1.244005	-1.580613	1	4.673108	1.143690	1.746434
6	0.925558	-0.085071	1.276265	1	4.993460	-1.831259	1.825120
6	0.886052	1.329179	1.488483	1	6.197486	-0.642592	1.331875
8	3.424479	2.126500	-0.720392	1	5.378025	0.840753	-0.775070
6	-0.070492	-0.937431	2.026760	1	4.200211	0.119481	-1.908198
1	4.262762	-2.373954	1.545016	1	5.687294	-1.834161	-0.809083
1	5.284802	-2.248146	0.114615	1	3.403374	-2.808241	0.228634
1	4.036619	0.040418	1.530000	1	3.320958	-2.272753	-1.466724
1	5.010049	0.119769	0.065290	6	1.317076	-1.040758	0.265309
1	2.206623	-1.351079	-2.073138	6	0.772371	-2.433907	0.046459
1	3.980670	-1.156162	-1.985915	1	1.032775	-2.823703	-0.944070
1	0.976969	-2.616515	-0.184652	1	1.178517	-3.132665	0.788840
1	1.826852	-2.659877	1.378360	1	-0.313893	-2.433605	0.147311
1	3.264731	-3.441443	-0.756384	6	0.411303	-0.040747	0.714602
1	0.435413	-1.530703	2.799363	1	0.819305	0.865495	1.147834
1	-0.815876	-0.309916	2.514182	1	-0.416175	-0.450675	1.286036
1	-0.591154	-1.633673	1.361295	6	2.668295	1.702517	-0.089900
1	0.508384	1.558641	2.483047	8	2.646113	2.563594	0.776839
1	1.777011	1.898696	1.242672	8	2.081909	1.724673	-1.258622
1	0.910181	2.137189	-1.276530	1	0.983614	2.089564	-1.136731
6	-0.405754	2.382044	0.445009	6	-0.558113	0.793027	-0.837390
1	-0.622777	3.057632	1.288087	8	-0.244682	2.049106	-0.851953
8	0.184604	2.947886	-0.553261	6	-1.986313	0.462785	-0.520086
6	-1.564237	1.439846	0.200208	1	-0.127006	0.153656	-1.620510
6	-2.621502	1.394126	1.121264	6	-2.768163	1.377990	0.199624
6	-3.716764	0.559200	0.919239	6	-4.095633	1.091603	0.497172
6	-3.744411	-0.233955	-0.226467	6	-4.636955	-0.118112	0.060006
6	-2.716206	-0.198370	-1.170071	6	-3.889354	-1.039337	-0.672207
6	-1.631360	0.645203	-0.955426	6	-2.561614	-0.738444	-0.959007
1	-2.591598	2.031539	2.002355	1	-2.318575	2.316628	0.505133
1	-4.541894	0.517474	1.619687	1	-4.716855	1.783435	1.052706
7	-4.886739	-1.130306	-0.446260	7	-6.038942	-0.429531	0.372567
1	-2.785124	-0.821871	-2.053287	1	-4.354164	-1.958270	-1.007386
1	-0.823652	0.685241	-1.677553	1	-1.970649	-1.436645	-1.547055
8	-4.879274	-1.831271	-1.459081	8	-6.488538	-1.506003	-0.023256
8	-5.783080	-1.135411	0.398743	8	-6.681156	0.401656	1.014279
NImag =1(-676.1)				NImag =1 (-837.5)			

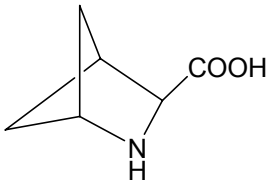


9

49. **9-anti-enamine** **Et** = -595.278257 (-595.458687)				50. **9-syn-enamine** **Et** = -595.278607 (-595.465475)			
6	0.27794	-1.72513	1.13488	6	0.75623	0.03572	-0.47792
6	-0.23316	-1.73845	-0.32073	6	0.8473	1.56342	-0.22585
6	1.07962	-1.96888	-1.10719	6	0.26245	1.66423	1.19806
6	2.13427	-1.16247	-0.28062	6	-1.02889	0.92391	0.81912
6	1.27424	-0.58576	0.87145	7	-0.46235	-0.34543	0.27788
7	0.36302	0.46007	0.33465	6	-1.57467	1.78362	-0.34801
6	-0.64595	-0.25348	-0.50155	6	-0.26202	2.24631	-1.06172
6	-2.08584	-0.0086	-0.01826	6	-1.30826	-1.36285	-0.22356
8	-3.04991	-0.40121	-0.63028	6	-0.95302	-2.20891	-1.2063
6	0.87202	1.72135	-0.05681	6	2.00709	-0.7088	0.01761
6	2.11336	2.14286	0.24274	8	1.82621	-1.42644	1.14155
6	-0.11117	2.62884	-0.76047	8	3.07477	-0.61973	-0.54048
8	-2.179	0.64173	1.15832	6	-2.62393	-1.51816	0.50295
1	-0.60493	0.02926	-1.55796	1	0.65909	-0.16556	-1.55037
1	-1.04476	-2.42608	-0.56472	1	1.85365	1.95314	-0.38749
1	-0.48567	-1.47462	1.87743	1	0.85002	1.14582	1.96189
1	0.77011	-2.65875	1.42422	1	0.08276	2.69584	1.51638
1	1.82775	-0.20805	1.73268	1	-1.73443	0.72792	1.62699
1	2.92594	-1.80992	0.11271	1	-2.15565	2.63234	0.03006
1	2.61261	-0.3694	-0.86018	1	-2.22846	1.20169	-1.00481
1	1.32244	-3.03655	-1.13299	1	-0.15053	3.33512	-1.02132
1	1.00231	-1.62676	-2.14463	1	-0.22585	1.95129	-2.11532
1	2.84817	1.52828	0.74865	1	-2.46856	-1.6437	1.58212
1	2.41253	3.15552	-0.00171	1	-3.27661	-0.64708	0.36837
1	-1.24737	0.84035	1.41498	1	-3.15665	-2.3961	0.1315
1	0.32314	3.62271	-0.88871	1	-0.0067	-2.15944	-1.73179
1	-0.38138	2.25503	-1.7557	1	-1.6168	-3.01967	-1.48338
1	-1.04282	2.73265	-0.19171	1	0.86965	-1.33512	1.35725
NImag = 0				NImag = 0			

51. **9t (a-*re*)** $\mathbf{E_t}$ = -1145.344040 (-1145.683959)				52**. 9t (a-*si*)** **Et** = -1145.341517 (-1145.680922)			
6	-4.274088	2.159975	0.802552	7	2.269421	-0.419213	0.424362
6	-4.086904	1.220322	-0.416116	6	2.825217	0.938290	0.646527
6	-3.641022	-0.169325	0.095126	6	4.219564	0.808001	-0.009118
7	-2.293270	0.136325	0.635888	6	3.858794	-0.020008	-1.260254
6	-1.982175	1.561432	0.293324	6	3.234144	-1.163512	-0.451377
6	-2.805711	2.417354	1.282553	6	4.395573	-1.578066	0.480791
6	-2.761949	1.735540	-1.016345	6	5.063118	-0.200395	0.812662
6	-1.554850	-0.697692	1.348745	1	2.889659	1.166613	1.713418
6	-0.149507	-0.488988	1.481935	6	1.997523	2.081563	-0.011025
6	-3.661028	-1.231370	-1.043226	8	2.297583	3.215935	0.305904
8	-2.530145	-1.620263	-1.592091	8	1.058216	1.774631	-0.876408
8	-4.754951	-1.645174	-1.372822	1	0.884226	0.747707	-1.150884
6	-2.145814	-2.026112	1.742061	1	4.681886	1.782679	-0.166774
6	0.412611	-1.060053	-0.201361	1	3.150649	0.458468	-1.938724
6	1.874216	-0.658860	-0.168203	1	4.735302	-0.356363	-1.822057
8	-0.321948	-0.513703	-1.124506	1	2.741279	-1.945598	-1.017919
1	-4.302018	-0.545505	0.880322	1	5.080149	-2.242912	-0.056368
1	-1.628207	-1.125498	-1.338614	1	4.042053	-2.112235	1.367734
1	-4.946469	1.146200	-1.082672	1	6.108108	-0.177548	0.488051
1	-2.362652	1.131041	-1.832650	1	5.050232	0.027331	1.883554
1	-2.808097	2.784357	-1.324698	6	1.163213	-0.883815	0.971759
1	-0.913792	1.741444	0.252818	6	0.438598	-0.030896	1.977329
1	-2.524249	3.471058	1.183205	1	1.091778	0.237039	2.815493
1	-2.632654	2.124982	2.322475	1	0.088487	0.902112	1.519021
1	-4.759648	3.091270	0.494458	1	-0.429951	-0.561953	2.367849
1	-4.899930	1.708861	1.579587	6	0.515551	-2.034380	0.410130
1	-2.344205	-2.640709	0.855333	1	1.173813	-2.799839	0.007453
1	-1.455745	-2.570227	2.388967	1	-0.255500	-2.465647	1.044154
1	-3.094469	-1.901752	2.275283	6	-0.244946	-1.352919	-1.096711
1	0.206606	0.536416	1.504043	8	0.573881	-0.526961	-1.695645
1	0.338177	-1.107653	2.232044	6	-1.629337	-0.852835	-0.691959
1	0.309675	-2.152773	-0.052972	1	-0.363707	-2.323482	-1.614994
6	2.811710	-1.397394	0.567581	6	-1.981898	0.493905	-0.851478
6	4.151034	-1.023980	0.594839	6	-3.260079	0.939396	-0.518477
6	4.543769	0.102135	-0.128730	6	-4.189649	0.022462	-0.034370
6	3.636448	0.847297	-0.881743	6	-3.877323	-1.329610	0.115254
6	2.301141	0.457619	-0.898631	6	-2.597971	-1.754782	-0.219827
1	2.492069	-2.279436	1.118042	1	-1.256506	1.194196	-1.248464
1	4.890132	-1.583080	1.155221	1	-3.544733	1.978136	-0.634272
7	5.955083	0.508975	-0.101528	7	-5.537793	0.485496	0.320930
1	3.987747	1.705524	-1.441624	1	-4.632116	-2.015515	0.479724
1	1.569563	0.993513	-1.493761	1	-2.350446	-2.809938	-0.124559
8	6.276883	1.507776	-0.746057	8	-6.335304	-0.349306	0.751624
8	6.734934	-0.170203	0.567787	8	-5.792704	1.680497	0.171075
NImag =1(-236.5cm^{-1})				NImag =1 (-272.3)			

53. **9t (s-*re*)** **Et** = -1145.337110 (-1145.678273)				54. **9t (s-*si*)** **Et** = -1145.336435 (-1145.677349)			
6	2.367957	-0.004143	1.124616	6	-2.718710	1.692271	-0.064727
6	1.854542	0.789876	0.090058	6	-1.799863	0.813469	0.529686
6	2.706349	1.188247	-0.952335	6	-2.196083	-0.500495	0.816834
6	4.035312	0.783070	-0.982994	6	-3.481408	-0.933013	0.502274
6	4.510135	-0.027516	0.049460	6	-4.368563	-0.038786	-0.095034
6	3.695636	-0.422786	1.108827	6	-4.006217	1.277130	-0.382859
6	0.418637	1.250384	0.151303	6	-0.413785	1.312395	0.889446
8	-0.238841	0.945741	1.233377	8	0.308118	0.675005	1.754990
7	5.911778	-0.468509	0.021171	7	-5.727376	-0.489967	-0.426353
8	6.610130	-0.097016	-0.922796	8	-6.027842	-1.652888	-0.157135
8	6.305168	-1.187296	0.940250	6	0.427962	1.281695	-0.824341
6	-0.424467	0.481820	-1.391266	6	1.771575	1.498741	-0.418531
6	-1.043191	-0.657642	-0.803781	6	2.186446	2.890729	-0.025185
6	-0.214823	-1.888833	-0.569741	7	2.575508	0.488234	-0.120437
7	-2.225403	-0.564412	-0.218905	6	3.929479	0.632085	0.494136
6	-2.864121	-1.642478	0.593124	6	4.188664	-0.802514	0.974632
6	-3.938104	-0.844474	1.346678	6	3.903801	-1.420019	-0.410049
6	-4.530174	-0.239012	0.057393	6	2.456729	-0.910340	-0.641429
6	-3.272842	0.467783	-0.513556	6	4.942062	0.774421	-0.666907
6	-3.712630	-2.497663	-0.376693	6	4.882983	-0.643227	-1.324163
6	-4.847110	-1.500815	-0.782412	6	1.469430	-1.921271	0.015419
6	-3.178986	1.901624	0.099899	8	0.853082	-1.634260	1.133218
8	-2.314637	2.182750	1.032368	8	1.404088	-2.999883	-0.546036
8	-4.028015	2.671326	-0.318130	8	-6.487575	0.322321	-0.956129
1	0.310157	2.282484	-0.224211	1	-0.429849	2.410965	1.012869
1	-3.334487	0.601435	-1.596718	1	2.198442	-0.870411	-1.702934
1	-1.417863	1.546263	1.163423	1	0.693486	-0.598167	1.396910
1	-5.357487	0.461205	0.166186	1	3.955912	-2.504591	-0.495629
1	-3.523563	-0.102248	2.033427	1	3.498123	-1.128314	1.756656
1	-4.631367	-1.499321	1.882869	1	5.220202	-0.940216	1.311926
1	-2.125141	-2.171529	1.192603	1	3.936223	1.418510	1.247094
1	-4.105298	-3.374653	0.148811	1	5.936397	1.000407	-0.267082
1	-3.132499	-2.857324	-1.231653	1	4.674105	1.578174	-1.358856
1	-5.833809	-1.895848	-0.520737	1	5.867178	-1.122075	-1.323700
1	-4.855806	-1.287931	-1.856079	1	4.536957	-0.610807	-2.362130
1	0.189111	-1.849077	0.451177	1	3.219004	3.117035	-0.302924
1	-0.791698	-2.811146	-0.675679	1	1.529381	3.628040	-0.489919
1	0.629435	-1.917777	-1.259903	1	2.095407	2.992640	1.064820
1	-1.084132	1.281661	-1.718589	1	0.175260	0.303935	-1.226489
1	0.363673	0.263707	-2.105952	1	-0.036616	2.098263	-1.370855
1	2.326207	1.827815	-1.745639	1	-1.495051	-1.181789	1.285172
1	4.706431	1.081381	-1.778890	1	-3.805398	-1.944550	0.714357
1	4.109918	-1.036259	1.899662	1	-4.728307	1.944026	-0.837442
1	1.710430	-0.261077	1.947998	1	-2.423738	2.719086	-0.270797
NImag =1 (-451.3)				NImag =1 (-398.3)			

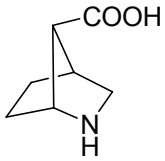


10

55. **10-anti-enamine** **Et** = -555.925346 (-556.095023)				56. **10-syn-enamine** **Et** = -555.925030 (-556.095795)			
7	-0.58304	-0.03624	0.3602	7	-0.57021	-0.03784	0.26034
6	0.58004	-0.00514	-0.59396	6	0.66648	-0.0685	-0.57387
6	0.82931	1.52259	-0.62251	6	0.97939	1.44708	-0.60657
6	-0.62708	2.05546	-0.79315	6	0.69124	1.85698	0.86821
6	-0.77551	1.41918	0.61961	6	-0.74256	1.43405	0.46902
6	0.67576	1.88683	0.88359	6	-0.43171	2.02598	-0.93519
6	1.78196	-0.80723	-0.08322	6	1.78667	-0.90979	0.0468
8	2.78024	-0.97192	-0.74252	8	2.83686	-1.10546	-0.51658
8	1.63737	-1.2849	1.16791	8	1.51618	-1.37984	1.27916
1	0.72989	-1.00751	1.44357	1	0.59631	-1.08656	1.47581
1	0.31917	-0.37716	-1.58927	1	0.47491	-0.44681	-1.58301
1	1.66856	1.85394	-1.23491	1	1.88594	1.7328	-1.14042
1	1.2699	1.34336	1.62386	1	1.18428	1.30784	1.67562
1	0.73798	2.96309	1.06024	1	0.77941	2.93422	1.02756
1	-0.67699	3.14756	-0.78345	1	-0.44427	3.11906	-0.95632
1	-1.24182	1.64738	-1.60105	1	-0.97521	1.61593	-1.79298
1	-1.59462	1.6242	1.30728	1	-1.6188	1.6911	1.06104
6	-1.70889	-0.83162	0.00896	6	-1.67376	-0.84637	-0.11356
6	-1.37731	-2.27351	-0.29300	6	-2.99408	-0.46433	0.51094
1	-0.83084	-2.73745	0.53713	1	-2.90423	-0.36284	1.59982
1	-0.74566	-2.37465	-1.18462	1	-3.37186	0.49055	0.12405
1	-2.29049	-2.84657	-0.46922	1	-3.74491	-1.2291	0.30085
6	-2.97366	-0.38414	0.023300	6	-1.55705	-1.93922	-0.88638
1	-3.23841	0.64685	0.22685	1	-0.62179	-2.26468	-1.32723
1	-3.79398	-1.06934	-0.15871	1	-2.42055	-2.56949	-1.0643
NImag = 0				NImag=0			

57. **10t (a-*re*)** **Et** = -1105.990047 (-1106.319199)				58. **10t (a-*si*)** **Et** = -1105.987399 (-1106.315966)			
7	-2.442879	0.121113	0.834169	7	2.488794	-0.515319	0.576065
6	-3.802932	0.074714	0.235698	6	3.113930	0.828312	0.705229
6	-4.036320	1.602595	0.138872	6	4.454814	0.499451	0.003020
6	-2.677138	2.096331	-0.447572	6	3.968765	-0.278078	-1.259106
6	-2.151954	1.581479	0.914229	6	3.507216	-1.294623	-0.187983
6	-3.496447	2.082750	1.519299	6	4.783928	-0.896735	0.610167
1	-4.517881	-0.401784	0.912175	1	3.257550	1.101073	1.754022
6	-3.922828	-0.647026	-1.130258	6	2.345403	1.989841	0.025933
8	-5.050229	-0.881585	-1.517471	8	2.704425	3.115301	0.310158
8	-2.833910	-0.955459	-1.804465	8	1.385486	1.710097	-0.829174
1	-1.898296	-0.620553	-1.451778	1	1.170185	0.690815	-1.068971
1	-5.004315	1.897629	-0.263808	1	5.168429	1.321218	-0.037445
1	-3.861706	1.595332	2.429108	1	4.802732	-0.670683	-1.845372
1	-3.520424	3.169686	1.626001	1	3.205390	0.151892	-1.905684
1	-1.170749	1.812799	1.317298	1	3.208292	-2.314546	-0.407851
1	-2.273499	1.635737	-1.348294	1	5.688286	-1.338951	0.185941
1	-2.628825	3.185967	-0.509096	1	4.766772	-1.018066	1.698263
6	-1.729151	-0.903731	1.261532	6	1.346860	-0.912156	1.096964
6	-2.367924	-2.267677	1.257460	6	0.611771	0.026172	2.014654
1	-3.363665	-2.251383	1.711556	1	1.276980	0.467221	2.763688
1	-2.480085	-2.633686	0.228792	1	0.165417	0.846957	1.439075
1	-1.746642	-2.977238	1.806877	1	-0.194635	-0.500637	2.526876
6	-0.316627	-0.790963	1.414853	6	0.676924	-2.061526	0.561833
1	0.085229	0.182977	1.677995	1	1.319048	-2.857280	0.192814
1	0.156330	-1.598242	1.969803	1	-0.121200	-2.449325	1.190539
6	0.193689	-0.932220	-0.382082	6	-0.023497	-1.403245	-0.993337
8	-0.543837	-0.154004	-1.113054	8	0.827556	-0.608046	-1.582949
1	0.060031	-2.024998	-0.503857	1	-0.142440	-2.386809	-1.487088
6	1.665366	-0.583769	-0.286511	6	-1.409469	-0.870561	-0.642522
6	2.600658	-1.509064	0.197680	6	-1.730198	0.480113	-0.834178
6	3.949549	-1.180854	0.282629	6	-3.009131	0.955612	-0.548900
6	4.353116	0.090344	-0.126114	6	-3.971496	0.063874	-0.081871
6	3.447010	1.026703	-0.624251	6	-3.691079	-1.291708	0.097059
6	2.102400	0.680090	-0.703805	6	-2.410292	-1.746442	-0.189423
1	2.271322	-2.499416	0.504012	1	-0.978063	1.158392	-1.220421
1	4.687545	-1.882679	0.651099	1	-3.269852	1.997601	-0.689284
1	3.806445	1.997085	-0.944406	7	-5.321101	0.557712	0.222722
1	1.369068	1.369211	-1.108492	8	-5.547638	1.755036	0.047871
7	5.774535	0.449959	-0.034623	8	-6.148129	-0.255359	0.638952
8	6.553893	-0.397585	0.403153	1	-4.470965	-1.957240	0.446095
8	6.104798	1.579612	-0.397134	1	-2.186055	-2.804404	-0.070802
NImag =1(-226.7)				NImag =1(-237.4)			

59**. 10t (s-*re*)** **Et** = -1105.985249 (-1106.315111)				60**. 10t (s-*si*)** **Et** = -1105.984315 (-1106.313931)			
7	2.299166	0.719644	-0.399026	7	2.788303	0.544228	-0.244472
6	3.490035	-0.190960	-0.542681	6	2.734664	-0.855420	-0.784305
6	4.540819	0.780148	0.051869	6	4.212861	-1.226215	-0.499844
6	3.790702	1.286255	1.321994	6	4.366789	-0.710172	0.964432
6	2.872732	1.927916	0.249687	6	4.181816	0.659072	0.262945
6	4.156782	2.139925	-0.599641	6	4.977331	0.059073	-0.930469
1	3.657675	-0.373642	-1.607698	1	2.516910	-0.813479	-1.855154
6	3.596407	-1.573902	0.161314	6	1.809296	-1.943818	-0.179154
8	4.596095	-2.199263	-0.149383	8	1.846875	-3.012012	-0.762163
8	2.723486	-1.963611	1.046767	8	1.128736	-1.725883	0.917197
1	1.785906	-1.412879	1.140860	1	0.961385	-0.711599	1.229711
1	5.556112	0.389006	0.072794	1	4.496190	-2.229084	-0.813208
1	3.345865	0.552705	1.997686	1	3.623196	-1.004881	1.708009
1	4.355237	2.040355	1.874916	1	5.380893	-0.833117	1.350772
1	2.137121	2.697897	0.468731	1	4.397259	1.612590	0.738421
1	4.047446	2.191664	-1.687986	1	6.049204	-0.001335	-0.727346
1	4.764538	2.970001	-0.231687	1	4.793573	0.473772	-1.927119
6	1.141836	0.632444	-1.028286	6	1.963982	1.541395	-0.520701
6	0.226806	1.825517	-1.035518	6	2.387499	2.944281	-0.175984
1	0.739922	2.730580	-1.375989	1	2.441825	3.057668	0.914657
1	-0.156296	2.007141	-0.023080	1	3.368768	3.191311	-0.593470
1	-0.629183	1.642721	-1.686128	1	1.659270	3.663189	-0.555212
6	0.647741	-0.634187	-1.445001	6	0.611469	1.293367	-0.870575
1	1.391156	-1.405201	-1.634258	1	0.371167	0.311718	-1.271975
1	-0.137190	-0.607413	-2.195288	1	0.101432	2.102281	-1.386906
6	-0.137987	-1.266692	0.177306	6	-0.162357	1.243686	0.874329
8	0.554407	-0.861356	1.199302	8	0.589317	0.554435	1.669005
1	-0.035172	-2.327420	-0.114396	1	-0.170043	2.333933	1.059733
6	-1.582216	-0.825073	0.128494	6	-1.563061	0.767400	0.538762
6	-2.468628	-1.324987	-0.838128	6	-1.949384	-0.561633	0.762511
6	-3.801811	-0.932194	-0.856186	6	-3.246397	-0.976549	0.473574
6	-4.245536	-0.031283	0.113151	6	-4.155088	-0.049612	-0.034953
6	-3.395478	0.466716	1.098920	6	-3.802528	1.281311	-0.258519
6	-2.063919	0.060371	1.102372	6	-2.503191	1.678639	0.033662
1	-2.113162	-2.035492	-1.580919	1	-1.232192	-1.268502	1.163747
1	-4.499247	-1.308299	-1.594449	1	-3.563322	-1.999070	0.638427
7	-5.651312	0.396575	0.097622	7	-5.526021	-0.482371	-0.339352
8	-6.381048	-0.065258	-0.780444	8	-5.817434	-1.658972	-0.125051
8	-6.016960	1.195339	0.960472	8	-6.304679	0.357876	-0.793177
1	-3.786002	1.148841	1.844347	1	-4.540843	1.972963	-0.644978
1	-1.377253	0.399023	1.870660	1	-2.215341	2.716249	-0.122114
NImag =1 (-363.1)				NImag =1 (-364.3)			



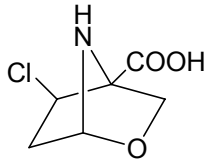
11

61. **11-anti-enamine** **Et** =-555.9252267 (-556.095608)				62. **11-syn-enamine** **Et** = -555.924992(-556.095073)			
6	-1.445559	.549479	-.465164	6	-1.461904	.683968	-.261233
6	-0.812083	1.512007	.605883	6	-0.777181	1.223211	1.047668
6	0.198432	.604631	1.325866	6	0.237211	.116752	1.374244
7	0.731280	-.140408	.140173	7	0.723068	-.173195	-.027342
6	0.023122	.557724	-.980378	6	-0.013455	.866442	-.801833
6	0.067310	2.050049	-.564917	6	0.067066	2.127767	.097459
1	-0.247585	-.079460	2.054359	1	-0.206288	-.773503	1.829954
1	0.983956	1.187845	1.817295	1	1.046011	.482943	2.014726
1	-1.431047	2.158837	1.229062	1	-1.365007	1.618166	1.877704
6	-2.181999	-.725261	-.065499	6	-2.199344	-.651468	-.286272
1	-2.105926	1.111002	-1.127936	1	-2.138481	1.437753	-.667106
1	-0.479356	2.705314	-1.247307	1	-0.496854	2.976759	-.295939
1	1.045094	2.475832	-.316648	1	1.058933	2.442748	.435213
1	0.294873	.187267	-1.966782	1	0.216521	.847454	-1.866139
8	-1.420843	-1.780106	.284989	8	-1.438047	-1.760875	-.352433
8	-3.390382	-.781507	-.057875	8	-3.406901	-.708641	-.238600
6	2.115009	-.432327	.057455	6	2.118396	-.349167	-.230146
6	2.924434	-.448525	1.129003	6	2.831454	.319521	-1.148365
1	2.593214	-.196865	2.129834	1	2.415718	1.109072	-1.763808
1	3.956052	-.763256	1.022950	1	3.871966	.066812	-1.318940
6	2.611153	-.832468	-1.311171	6	2.722472	-1.436262	.624217
1	2.596267	.007828	-2.016719	1	2.206742	-2.391117	.462371
1	3.639778	-1.193923	-1.247011	1	3.781105	-1.567930	.388633
1	1.994510	-1.631883	-1.740919	1	2.643434	-1.207153	1.694342
1	-0.467903	-1.504636	.225234	1	-0.483992	-1.478089	-.365786
NImag = 0				NImag = 0			

63. **11t (a-*re*)** **Et** = -1105.991543 (-1106.321334)				64. **11t(a-*si*)** **Et** = -1105.989990 (-1106.319877)			
6	-2.351436	-1.092481	0.482861	7	2.22442	-0.69465	0.75107
6	-1.752449	-0.180115	-0.395520	6	2.84516	0.2212	1.75545
6	-2.553454	0.749204	-1.074284	6	4.14387	0.52775	0.98673
6	-3.928550	0.785418	-0.873176	6	3.58335	0.7981	-0.442
6	-4.495143	-0.124890	0.019766	6	3.22375	-0.71867	-0.34974
6	-3.725181	-1.068473	0.699744	1	2.23258	1.11087	1.9231
6	-0.260816	-0.236028	-0.622921	1	3.00869	-0.29983	2.70456
8	0.368950	-1.283745	-0.236419	1	4.84322	1.2054	1.47406
7	-5.946652	-0.090635	0.244566	1	4.39157	0.94868	-1.16492
8	-6.602354	0.752144	-0.369672	1	2.91308	-1.30188	-1.20905
6	0.272785	1.256039	0.562469	6	4.54095	-0.88186	0.45533
6	1.599926	1.629681	0.230654	1	4.59729	-1.71264	1.16627
6	1.855867	2.840849	-0.631213	1	5.42671	-0.86046	-0.18337
7	2.660880	0.908464	0.567064	6	2.56674	1.93042	-0.59459
6	4.096925	1.215690	0.297573	8	2.75902	2.96946	0.00817
6	4.704411	-0.050130	0.930396	8	1.53712	1.75976	-1.41034
6	3.891877	-0.160773	2.253567	1	1.33609	0.79154	-1.68479
6	2.717873	-0.398598	1.269641	6	1.12973	-1.42471	0.89818
6	3.751927	-1.149153	0.366782	6	0.28471	-1.15056	2.11437
6	3.635556	-1.255857	-1.156740	1	-0.64833	-1.71312	2.06583
8	2.459332	-1.544023	-1.687261	1	0.81404	-1.44087	3.03078
8	4.636010	-1.091309	-1.831486	1	0.04224	-0.08479	2.1955
8	-6.423883	-0.903747	1.036685	6	0.69584	-2.34401	-0.09658
1	4.300210	1.289687	-0.773421	1	1.4789	-2.83797	-0.66587
1	4.396450	2.142741	0.798605	1	-0.07355	-3.03131	0.24597
1	5.788658	-0.139331	0.881781	6	-0.05402	-1.36936	-1.55864
1	3.980146	-2.134056	0.787049	6	-1.34002	-0.78421	-0.99985
1	4.138069	-1.054844	2.830801	8	0.85388	-0.61915	-2.07041
1	3.833325	0.716063	2.906687	1	-0.2817	-2.29983	-2.11434
1	1.744699	-0.807283	1.517896	6	-1.46784	0.58417	-0.72069
1	2.356543	2.562545	-1.566540	6	-2.66195	1.09547	-0.2161
1	0.918695	3.343688	-0.873965	6	-3.73135	0.22906	0.00158
1	2.505124	3.558544	-0.115382	6	-3.64155	-1.13394	-0.2843
1	1.666536	-1.519280	-1.034187	6	-2.44384	-1.62691	-0.78722
1	0.125743	0.696601	1.481475	1	-0.6391	1.2567	-0.91177
1	-0.456595	2.048612	0.423676	1	-2.77674	2.15013	0.00322
1	0.027569	0.225522	-1.584400	7	-4.98947	0.76239	0.53994
1	-2.094801	1.446889	-1.771553	1	-4.50002	-1.77303	-0.11802
1	-4.565153	1.492737	-1.390166	1	-2.36353	-2.68474	-1.0289
1	-4.208954	-1.764043	1.374606	8	-5.91717	-0.02868	0.71911
1	-1.721014	-1.826459	0.973251	8	-5.04377	1.96752	0.78633
NImag = 1 (-272.6)				NImag = 1 (-263.6)			

65. **11t (s-*re*)** **Et** = -1105.978979 (-1106.319877)			
6	-4.341918	-0.607428	1.509147
6	-4.357901	-0.178177	0.008987
6	-3.283493	-1.110559	-0.566783
7	-2.253666	-0.908506	0.511003
6	-2.923021	0.027596	1.445594
6	-3.556988	1.085767	0.492670
6	-2.791282	2.107670	-0.367988
8	-3.244724	3.236875	-0.392245
6	-1.112950	-1.542287	0.670228
6	-0.274756	-1.239602	1.883868
8	-1.664567	1.804887	-0.989744
6	-0.589701	-2.353881	-0.393326
1	-2.868619	-0.831264	-1.533068
1	-3.602507	-2.159230	-0.579705
1	-5.278732	-0.084375	-0.566397
1	-4.235132	1.708107	1.078672
1	-5.027884	-0.033912	2.134223
1	-4.402725	-1.675992	1.740203
1	-2.325200	0.288492	2.315109
1	-1.344016	-2.843023	-1.007405
1	0.181512	-3.049717	-0.068136
1	-0.815612	-1.468768	2.809215
1	0.643382	-1.827175	1.864453
1	0.005935	-0.179678	1.908123
1	-1.374587	0.836312	-1.199375
6	0.107688	-1.209720	-1.585498
1	0.347356	-1.982311	-2.345294
8	-0.794578	-0.345441	-1.943732
6	1.419923	-0.691820	-0.996865
6	2.505012	-1.559032	-0.788709
6	3.707639	-1.095883	-0.268602
6	3.821186	0.261109	0.038425
6	2.772239	1.152093	-0.178054
6	1.573812	0.669445	-0.701523
1	2.410602	-2.611471	-1.048709
1	4.552313	-1.753495	-0.103574
7	5.084226	0.761130	0.597177
1	2.906937	2.201479	0.054918
1	0.756092	1.352881	-0.902776
8	5.160823	1.961474	0.860301
8	5.993549	-0.051168	0.775776
NImag = 1 (-138)			

66. **11t (s-*si*)** **Et** = -1105.978918 (-1106.309690)			
7	-2.490561	0.926054	0.483085
6	-2.347825	-0.074557	1.591124
6	-3.826452	-0.476036	1.687874
6	-4.296564	-0.593405	0.189769
6	-3.946362	0.922978	0.208223
6	-4.507700	0.928048	1.658916
1	-1.986899	0.422005	2.499773
1	-1.661094	-0.865074	1.298862
1	-4.077789	-1.237488	2.426030
1	-4.129716	1.697414	2.340162
1	-5.597474	0.884136	1.687157
1	-4.252149	1.616623	-0.570704
1	-5.382866	-0.699554	0.194623
6	-3.841246	-1.604917	-0.878631
8	-4.640384	-2.472238	-1.177054
8	-2.696329	-1.460458	-1.530400
1	-1.857218	-1.102828	-1.058888
6	-1.561344	1.719214	-0.018886
6	-1.957094	2.687353	-1.105099
1	-2.709124	3.401746	-0.751380
1	-2.379218	2.156093	-1.966865
1	-1.086256	3.250879	-1.443513
6	-0.189040	1.537656	0.301904
1	0.040057	1.091590	1.266239
1	0.451685	2.380934	0.057400
6	0.302497	0.085215	-0.827197
8	-0.430312	-0.927206	-0.523717
6	1.782935	-0.000570	-0.512589
1	0.141872	0.571573	-1.810346
6	2.250376	-1.018863	0.327697
6	3.605433	-1.125974	0.624088
6	4.489769	-0.204017	0.064291
6	4.055059	0.811260	-0.788270
6	2.697051	0.903405	-1.071802
1	1.532993	-1.731096	0.720860
1	3.988630	-1.907572	1.268788
7	5.922188	-0.307475	0.373965
1	4.777120	1.498193	-1.212069
1	2.342881	1.683478	-1.742338
8	6.680330	0.518988	-0.135828
8	6.282473	-1.211818	1.128047
NImag = 1 (-262)			



4-C(β')Cl

67. **4**-C(β')Cl **t(a-*re*)** **Et** = -1640.8070012 (-1641.1896979)				68. **4**-C(β')Cl **t(a-*si*)** **Et** = -1640.8024105 (-1641.1846493)			
6	3.999224	1.051089	-0.296117	6	-4.310785	-0.868461	-0.872243
6	2.886973	0.380611	0.530952	6	-3.105031	-1.684873	-0.333064
6	2.228872	1.547279	1.359849	7	-2.056924	-0.633753	-0.358431
8	1.426839	2.279780	0.410503	6	-2.765475	0.326660	0.523103
6	1.697913	1.669889	-0.821117	6	-4.060906	0.558433	-0.277603
6	3.161167	1.979205	-1.239099	6	-3.162396	-0.673310	1.673951
7	1.828597	0.225749	-0.498940	8	-3.301038	-1.954749	1.027277
6	3.135841	-0.823451	1.471657	6	-0.914955	-0.559440	-1.021509
8	2.049071	-1.412158	1.889032	6	-0.330046	0.767800	-1.407859
6	1.245971	-0.836810	-1.022507	6	-1.925482	1.476839	1.125711
6	-0.147034	-0.752816	-1.341504	8	-0.742753	1.111501	1.541825
8	4.278397	-1.082247	1.800645	6	-0.120988	-1.740210	-1.138718
6	1.909200	-2.184047	-0.986431	6	0.718935	-1.693931	0.540788
6	-0.798640	-1.121528	0.330166	8	-0.082779	-1.233240	1.473003
6	-2.247083	-0.710236	0.202263	6	2.056179	-1.016072	0.311590
6	-3.182673	-1.553463	-0.412398	6	3.026684	-1.645615	-0.486242
6	-4.515050	-1.169909	-0.530310	6	4.280708	-1.079066	-0.674680
6	-4.896837	0.072265	-0.025760	6	4.562767	0.135262	-0.048158
6	-3.988163	0.929174	0.595375	6	3.630525	0.778000	0.761680
6	-2.660566	0.529908	0.707270	6	2.377987	0.193823	0.944626
7	-6.302104	0.488763	-0.149478	7	5.886547	0.746109	-0.243891
8	-6.613551	1.591569	0.299707	8	6.686688	0.153632	-0.968633
8	-0.122809	-0.488519	1.268136	8	6.114564	1.812672	0.325368
8	-7.083324	-0.288872	-0.698126	8	-2.426303	2.580005	1.233321
1	0.999219	-0.979531	1.581463	1	-0.414870	-0.020448	1.479414
1	1.490935	-2.807385	-0.188514	1	-4.106147	-0.372009	2.140821
1	2.986052	-2.113607	-0.835704	1	-2.374890	-0.748608	2.423104
1	1.716654	-2.685669	-1.941039	1	-2.853000	-2.593735	-0.875393
1	-0.544846	0.237312	-1.550221	1	-5.246319	-1.311462	-0.521143
1	-0.531808	-1.511581	-2.020491	1	-4.321717	-0.839730	-1.963980
1	-0.694713	-2.220539	0.313816	1	-4.867911	0.923921	0.354730
1	1.573171	1.160724	2.139299	17	-3.888426	1.790593	-1.601313
1	2.998229	2.193842	1.795230	1	0.565787	0.992373	-0.820398
1	0.924390	1.906216	-1.548659	1	-1.039014	1.587934	-1.304065
1	3.339401	1.732883	-2.288047	1	-0.022077	0.702193	-2.458009
1	3.376138	3.039518	-1.083603	1	-0.649254	-2.688901	-1.081282
17	4.994454	-0.122617	-1.262021	1	0.644860	-1.725043	-1.910001
1	4.709291	1.582138	0.335127	1	0.863349	-2.783764	0.602954
1	-2.870821	-2.523927	-0.791645	1	1.651603	0.678724	1.587179
1	-5.255692	-1.808776	-0.995166	1	3.892764	1.713673	1.240217
1	-4.331548	1.881151	0.981318	1	5.038497	-1.555281	-1.284406
1	-1.926902	1.160749	1.197190	1	2.800858	-2.599999	-0.956670
NImag = 1 (-828)				NImag = 1 (-897)			

69. **4**-C(β')Cl **t(s-*re*)** **Et** = -1640.815236 (-1641.1971536)				70. **4**-C(β')Cl **t(s-*si*)** **Et** = -1640.811900 (-1641.1940632)			
6	3.835002	-0.899631	0.200595	6	-3.881141	-0.801065	0.608115
6	2.807411	0.020645	-0.513450	6	-2.676177	-0.664017	-0.361638
7	1.533916	-0.598040	-0.005253	7	-2.338703	0.780729	-0.134335
6	1.814135	-1.956780	-0.544044	6	-3.674245	1.300676	-0.532728
6	3.170265	-2.299914	0.102197	6	-4.620537	0.553631	0.427710
8	2.000014	-1.717988	-1.919282	8	-3.839441	0.792776	-1.835842
6	2.712536	-0.466715	-1.991452	6	-3.263224	-0.527031	-1.800640
6	0.645032	-0.276421	0.928489	6	-1.394667	1.428614	0.542644
6	-0.271570	-1.369314	1.420682	6	-1.630547	2.895141	0.818223
6	3.193288	1.526995	-0.506527	6	-1.699391	-1.867771	-0.342121
8	4.366175	1.777994	-0.313216	8	-2.134339	-2.912510	0.097056
6	0.390046	1.065556	1.292729	6	-0.121433	0.881033	0.807893
8	2.290420	2.413557	-0.836118	8	-0.530795	-1.741965	-0.921504
6	-0.615323	1.719630	-0.203828	6	0.736424	1.137926	-0.904430
8	0.064922	1.484682	-1.280694	8	0.053391	0.488659	-1.786137
6	-1.990844	1.108087	-0.117036	6	2.140425	0.695841	-0.545222
6	-2.384027	0.159753	-1.071624	6	3.016511	1.601264	0.071989
6	-3.654587	-0.407426	-1.025168	6	4.319636	1.235114	0.387639
6	-4.528809	-0.011154	-0.014056	6	4.739621	-0.057347	0.074628
6	-4.170945	0.941592	0.940636	6	3.895388	-0.976940	-0.545706
6	-2.898221	1.498289	0.879134	6	2.594635	-0.592798	-0.857942
7	-5.870806	-0.609144	0.045433	7	6.115958	-0.456512	0.403351
8	-6.623761	-0.236841	0.945687	8	6.466376	-1.599498	0.111166
8	-6.160723	-1.450250	-0.805465	8	6.837201	0.376827	0.953401
1	-0.600970	2.747492	0.200420	1	0.684695	2.239649	-0.970361
1	1.319107	2.018943	-1.097004	1	-0.296951	-0.783515	-1.340374
1	2.130475	0.233168	-2.594490	1	-2.468991	-0.583328	-2.548310
1	3.705550	-0.608466	-2.430718	1	-4.023121	-1.290294	-1.998207
1	3.728753	-2.985333	-0.540655	1	-3.745643	2.384924	-0.554200
1	1.004665	-2.668619	-0.404689	1	-5.605841	0.436526	-0.030950
1	3.055416	-2.759110	1.086550	1	-4.737486	1.074728	1.380480
1	4.817906	-0.822406	-0.257914	1	-4.474351	-1.683138	0.378514
17	4.063445	-0.426919	1.942050	17	-3.337356	-1.004363	2.331167
1	1.212874	1.769001	1.228787	1	-1.759975	3.458019	-0.114259
1	-0.220149	1.192710	2.182505	1	-2.525400	3.046999	1.431836
1	-0.869642	-1.782625	0.599690	1	-0.778835	3.317208	1.353154
1	0.297689	-2.186303	1.877859	1	0.467844	1.424777	1.540015
1	-0.960628	-0.973189	2.166805	1	-0.026604	-0.195925	0.889357
1	-2.608365	2.251442	1.608366	1	1.928095	-1.292962	-1.347828
1	-4.886629	1.231013	1.700208	1	4.264698	-1.968460	-0.777202
1	-3.980831	-1.137512	-1.755917	1	5.010243	1.922683	0.859944
1	-1.682282	-0.100660	-1.856870	1	2.675082	2.608833	0.299827
NImag = 1 (-341)				NImag = 1 (-358)			

Optimized Cartesian coordinates for the lowest energy transition states of aldol reaction between (a) acetone and benzaldehyde with varying *p*-substituents catalyzed by **2 (**Table S6). **(**b**)** acetone and 2,6-dimethyl-benzaldehyde with varying *p*-substituents (Table S7). Computed gas phase electronic in energies at B3LYP/6-31G** are also provided.

(a) X=CF_3

71. **2t-cf3(s-*re*)** **Et** = -1317.2238574				72. **2t-cf3(s-*si*)** **Et** = -1317.2208962			
6	4.464539	0.716982	-0.234320	6	4.317912	-1.066432	-0.906482
6	3.378253	-0.245683	0.298114	6	3.058090	-0.990643	-0.012453
7	2.138546	0.515269	-0.125650	7	2.846990	0.506998	0.000354
6	2.460760	1.793184	0.567296	6	4.194836	0.878730	0.510528
6	3.855231	2.137155	-0.022507	6	5.129105	0.212539	-0.533785
6	2.612565	1.305639	2.019695	6	4.234022	0.090228	1.832329
6	3.287663	-0.084707	1.841574	6	3.482759	-1.222223	1.465951
6	1.167626	0.300248	-1.004471	6	1.890491	1.325603	-0.425000
6	0.205775	1.433508	-1.278339	6	2.166504	2.811776	-0.347528
6	3.612077	-1.709296	-0.155147	6	1.942414	-1.951832	-0.488730
8	4.567271	-1.956657	-0.867840	8	2.129254	-2.628958	-1.481280
6	3.793291	2.957733	-1.312726	6	5.426862	1.101875	-1.743073
6	0.865060	-0.979272	-1.523164	6	0.580979	0.914550	-0.749688
8	2.816898	-2.635645	0.335455	8	0.872469	-2.070950	0.272177
6	-0.077608	-1.831402	-0.019806	6	-0.217559	0.772813	1.066506
8	0.646057	-1.700797	1.040017	8	0.457091	-0.107424	1.716271
6	-1.457392	-1.227168	-0.003599	6	-1.651971	0.515062	0.667438
6	-1.840722	-0.404428	1.062483	6	-2.492569	1.597381	0.374264
6	-3.117768	0.150385	1.105582	6	-3.824409	1.394448	0.028704
6	-4.029402	-0.118118	0.080957	6	-4.333022	0.093395	-0.026895
6	-3.663062	-0.953646	-0.979367	6	-3.505229	-0.993015	0.268613
6	-2.386417	-1.506032	-1.014823	6	-2.173277	-0.783698	0.616514
6	-5.384370	0.533378	0.091364	6	-5.786322	-0.126890	-0.343153
1	-0.057664	-2.799592	-0.549381	1	-0.080995	1.825007	1.374600
1	1.916693	-2.260161	0.748142	1	0.721085	-1.286322	0.958155
1	2.675399	-0.873353	2.275652	1	2.607664	-1.356389	2.099629
1	4.286768	-0.137930	2.281171	1	4.109513	-2.114379	1.540399
1	4.422915	2.701361	0.725559	1	3.697418	0.632743	2.614626
1	3.205319	2.004218	2.616014	1	5.260494	-0.075389	2.169814
1	1.701389	2.558778	0.421320	1	4.327822	1.953408	0.617973
1	1.631678	1.199577	2.489437	1	6.074795	-0.048212	-0.046088
1	5.409264	0.565861	0.291721	1	4.864525	-1.995012	-0.729869
1	4.646076	0.506244	-1.290498	1	4.015603	-1.064132	-1.955849
1	1.666322	-1.701198	-1.618055	1	2.354320	3.125976	0.685208
1	0.179552	-0.981401	-2.364435	1	3.038734	3.091116	-0.945556
1	-0.320650	1.730155	-0.364762	1	1.306689	3.369145	-0.718766
1	0.722793	2.311697	-1.675393	1	-0.012887	1.650701	-1.280729
1	-0.543511	1.117344	-2.002788	1	0.405214	-0.101747	-1.077377
1	-2.110024	-2.167869	-1.832083	1	-1.531930	-1.627292	0.842124
1	-4.380921	-1.178213	-1.760717	1	-3.903427	-2.000662	0.220415
1	-3.415607	0.777817	1.939115	1	-4.468372	2.236704	-0.200432
1	-1.126493	-0.236235	1.861108	1	-2.098212	2.609966	0.421744

1	4.799224	3.119664	-1.713051	1	6.034260	0.562933	-2.477170
1	3.217744	2.438530	-2.087309	1	4.503006	1.405371	-2.248339
1	3.338056	3.940344	-1.146320	1	5.974884	2.006124	-1.455494
9	-5.839898	0.734473	1.348036	9	-6.260885	0.805089	-1.202186
9	-5.358408	1.747966	-0.511417	9	-6.006577	-1.338924	-0.898318
9	-6.307532	-0.205605	-0.563144	9	-6.558910	-0.058607	0.767925
NImag = 1 (-304)				NImag = 1 (-316)			

X= -F

73. **2t-f(s-*re*)** **Et** = -1079.4191856				74. **2t-f(s-*si*)** **Et** = -1079.41644806			
6	3.696644	0.422195	-0.247246	6	3.484989	-1.002906	-0.822068
6	2.512158	-0.419099	0.282200	6	2.180547	-0.969355	0.008165
7	1.364797	0.484404	-0.121179	7	1.937165	0.523260	0.033349
6	1.833993	1.706579	0.586910	6	3.248548	0.915237	0.616908
6	3.254838	1.899507	-0.009025	6	4.249268	0.285222	-0.387419
6	1.940595	1.185008	2.031116	6	3.238685	0.105721	1.926973
6	2.449794	-0.271050	1.828243	6	2.535275	-1.215806	1.502439
6	0.370451	0.395703	-0.995122	6	0.982194	1.327617	-0.420081
6	-0.459402	1.634776	-1.240612	6	1.217010	2.817969	-0.299532
6	2.576184	-1.895141	-0.189393	6	1.110119	-1.946447	-0.538556
8	3.503887	-2.239232	-0.899947	8	1.364173	-2.601157	-1.532439
6	3.279829	2.742707	-1.285877	6	4.592575	1.200521	-1.564794
6	-0.082743	-0.834018	-1.527267	6	-0.302453	0.892448	-0.811187
8	1.675990	-2.726310	0.283176	8	0.009136	-2.099100	0.165720
6	-1.106279	-1.589294	-0.050174	6	-1.186544	0.697511	0.937651
8	-0.361460	-1.569464	1.008166	8	-0.520300	-0.181357	1.607228
6	-2.409635	-0.838191	0.004170	6	-2.596109	0.415664	0.477766
6	-2.685597	-0.002327	1.093504	6	-3.453474	1.483127	0.178746
6	-3.893845	0.689501	1.177443	6	-4.768794	1.261916	-0.222981
6	-4.825421	0.529769	0.158192	6	-5.216879	-0.050901	-0.320691
6	-4.590794	-0.303346	-0.931606	6	-4.395619	-1.134088	-0.027729
6	-3.378823	-0.987285	-0.997385	6	-3.083345	-0.894552	0.374598
9	-5.997986	1.195664	0.230156	9	-6.490484	-0.278570	-0.706805
1	-1.205634	-2.545883	-0.592044	1	-1.090557	1.743698	1.279573
1	0.811122	-2.251792	0.701183	1	-0.201728	-1.317166	0.857767
1	1.752730	-0.990311	2.254600	1	1.631945	-1.378777	2.087810
1	3.438757	-0.445959	2.259095	1	3.176881	-2.095699	1.595031
1	3.888074	2.382413	0.743300	1	2.652744	0.623751	2.690308
1	2.615580	1.802885	2.629287	1	4.250648	-0.043997	2.312590
1	1.165194	2.555258	0.457558	1	3.352211	1.990629	0.747333
1	0.958550	1.186282	2.510383	1	5.173320	0.034827	0.145179
1	4.622758	0.156488	0.266338	1	4.041887	-1.923166	-0.634279
1	3.843689	0.208193	-1.308099	1	3.234892	-0.988092	-1.885053
1	0.632740	-1.638666	-1.642097	1	1.342108	3.114701	0.747897
1	-0.765203	-0.742975	-2.366358	1	2.112168	3.131017	-0.844552
1	-0.954532	1.959291	-0.318761	1	0.363983	3.362016	-0.704656
1	0.151193	2.462464	-1.612295	1	-0.885386	1.624889	-1.359487
1	-1.236191	1.422669	-1.974045	1	-0.434370	-0.119769	-1.170798
1	-3.187444	-1.651284	-1.837189	1	-2.430193	-1.727606	0.606291
1	-5.351680	-0.411013	-1.697003	1	-4.788622	-2.141361	-0.113255
1	-4.127112	1.334128	2.018259	1	-5.444782	2.078862	-0.450823
1	-1.943997	0.071242	1.881679	1	-3.089070	2.504145	0.269273
1	4.295260	2.793688	-1.691735	1	5.246400	0.684749	-2.275295

1	2.643243	2.306602	-2.064042	1	3.690772	1.497425	-2.112061
1	2.942184	3.768571	-1.100752	1	5.108931	2.108763	-1.234310
NImag = 1 (-333)				NImag = 1 (343 nm^{-1})			

X= -NH_2

75. **2t-nh2(s-*re*)** **Et** = -1035.545956				76. **2t-nh2(s-*si*)** **Et** = -1035.5435891			
6	3.710109	0.434088	-0.237466	6	3.482314	-1.021550	-0.831621
6	2.525312	-0.407716	0.289651	6	2.186295	-0.971899	0.010474
7	1.378133	0.489638	-0.129447	7	1.956819	0.523522	0.027810
6	1.836944	1.718875	0.571888	6	3.276493	0.908674	0.595565
6	3.260933	1.911983	-0.016120	6	4.261171	0.264093	-0.415314
6	1.935348	1.209780	2.021269	6	3.274066	0.107892	1.911089
6	2.449423	-0.246712	1.833424	6	2.553037	-1.209323	1.502925
6	0.383881	0.386492	-1.000923	6	1.001138	1.331864	-0.415702
6	-0.458313	1.615661	-1.252835	6	1.243505	2.821134	-0.297719
6	2.594193	-1.890130	-0.168910	6	1.098523	-1.944124	-0.517540
8	3.531596	-2.231938	-0.871493	8	1.341766	-2.603209	-1.514062
6	3.289352	2.742582	-1.301159	6	4.595892	1.169022	-1.603171
6	-0.062899	-0.851784	-1.522134	6	-0.290989	0.901547	-0.792595
8	1.691859	-2.711273	0.302434	8	0.010324	-2.079393	0.199840
6	-1.087248	-1.597355	-0.064220	6	-1.173355	0.710084	0.935675
8	-0.338013	-1.580577	0.999981	8	-0.496209	-0.167994	1.610710
6	-2.391538	-0.859107	-0.000382	6	-2.581612	0.426570	0.492854
6	-2.678103	-0.016743	1.081233	6	-3.449073	1.486442	0.196535
6	-3.889996	0.661816	1.165079	6	-4.761884	1.262031	-0.200212
6	-4.864472	0.514366	0.162377	6	-5.253343	-0.050645	-0.313399
6	-4.583574	-0.338676	-0.921114	6	-4.386359	-1.116879	-0.013361
6	-3.370062	-1.012591	-0.991803	6	-3.075875	-0.880947	0.382789
7	-6.104221	1.142750	0.270819	7	-6.583955	-0.288049	-0.654925
1	-1.183327	-2.557462	-0.599894	1	-1.076611	1.752906	1.285312
1	0.789439	-2.226619	0.710857	1	-0.208160	-1.263589	0.897199
1	1.750137	-0.964818	2.257913	1	1.652820	-1.358736	2.096509
1	3.434905	-0.416219	2.274503	1	3.186443	-2.095110	1.596885
1	3.887432	2.405250	0.735264	1	2.702033	0.637020	2.677484
1	2.604779	1.834747	2.618575	1	4.288992	-0.048656	2.286385
1	1.165933	2.564113	0.431065	1	3.390735	1.984110	0.717515
1	0.949972	1.212734	2.493860	1	5.190008	0.011458	0.108014
1	4.633173	0.176928	0.285912	1	4.034290	-1.944414	-0.641766
1	3.866767	0.210403	-1.294925	1	3.221449	-1.014203	-1.892055
1	0.661338	-1.649174	-1.633619	1	1.382732	3.117080	0.748208
1	-0.742101	-0.768991	-2.364901	1	2.133078	3.131155	-0.853724
1	-0.970763	1.925315	-0.335168	1	0.387343	3.368465	-0.691724
1	0.144805	2.454015	-1.612482	1	-0.872440	1.636419	-1.339417
1	-1.223251	1.395024	-1.996076	1	-0.425056	-0.108713	-1.157114
1	-3.182045	-1.675485	-1.834064	1	-2.423784	-1.718592	0.602480
1	-5.331406	-0.480943	-1.697559	1	-4.752166	-2.138157	-0.087834
1	-4.098284	1.299186	2.021444	1	-5.419319	2.101571	-0.413025
1	-1.937238	0.074814	1.868848	1	-3.090689	2.510606	0.283776
1	4.306219	2.791869	-1.703751	1	5.237077	0.644156	-2.318613
1	2.656603	2.296776	-2.076984	1	3.688788	1.467977	-2.140476
1	2.948329	3.769561	-1.128036	1	5.122211	2.076310	-1.285688
1	-6.124741	1.968447	0.852707	1	-7.033404	0.446473	-1.183821

1 -6.603342 1.275149 -0.597604	1 -6.773112 -1.203013 -1.040246
NImag = 1 (-408)	NImag = (-421)

X=OMe

77. **2t-ome(s-*re*)** **Et** = -1094.7127593				78. **2t-ome(s-*re*)** **Et** = -1094.7101899		
6	3.964349	.623163	-.171575	6	3.732922	-1.163536	-.824403
6	2.822390	-.267056	.370501	6	2.459914	-1.016019	.040552
7	1.632695	.497786	-.173826	7	2.296112	.487158	-.008233
6	1.958666	1.811822	.443978	6	3.643801	.838374	.514162
6	3.393247	2.072639	-.087846	6	4.576623	.103529	-.484860
6	2.014158	1.426488	1.932859	6	3.634421	.101118	1.866111
6	2.657311	.010188	1.891560	6	2.850332	-1.201407	1.534575
6	.688897	.243757	-1.070511	6	1.369386	1.316746	-.474174
6	-.227766	1.378850	-1.463563	6	1.684225	2.796751	-.439429
6	3.029851	-1.768808	.037825	6	1.321278	-1.963058	-.418136
8	4.019085	-2.089799	-.598502	8	1.512499	-2.681536	-1.383357
6	3.428367	2.806492	-1.430293	6	4.924330	.936229	-1.720823
6	0.359331	-1.064939	-1.496547	6	.051681	.930117	-.803796
8	2.175739	-2.625482	.542123	8	.241213	-2.017437	.325781
6	-.670612	-1.757743	-.005481	6	-.794939	.863877	.960528
8	0.030985	-1.595789	1.074821	8	-.148074	-.013181	1.659724
6	-2.023300	-1.106114	-.056254	6	-2.225564	.629940	.553299
6	-2.412520	-.217208	.948023	6	-3.046673	1.722456	.230929
6	-3.673130	.386197	.937574	6	-4.373900	1.544710	-.130455
6	-4.569237	.095344	-.097544	6	-4.916667	.251329	-.178804
6	-4.194365	-.805679	-1.107859	6	-4.112566	-.849059	.143315
6	-2.940314	-1.397732	-1.079211	6	-2.779554	-.652559	.506669
8	-5.823352	.622541	-.213648	8	-6.229533	.174478	-.544021
1	-0.681067	-2.762917	-.461796	1	-.640908	1.917273	1.254480
1	1.239529	-2.187265	.877017	1	.079669	-1.172005	.982495
1	2.001912	-.729914	2.347270	1	1.959080	-1.286014	2.153993
1	3.631054	-.034501	2.385869	1	3.448922	-2.107910	1.655013
1	3.939394	2.667896	.652311	1	3.100227	.689755	2.616205
1	2.592212	2.151346	2.512394	1	4.649146	-.081347	2.230016
1	1.233788	2.586566	.201830	1	3.808138	1.912049	.582133
1	1.005222	1.378352	2.349823	1	5.504557	-.166194	.031460
1	4.877665	.481433	.409591	1	4.247477	-2.100698	-.602438
1	4.188523	.333150	-1.200380	1	3.449891	-1.192830	-1.878731
1	1.141793	-1.813411	-1.504620	1	1.861117	3.139481	.586270
1	-.285372	-1.109112	-2.368735	1	2.574642	3.033887	-1.029034
1	-.804884	1.724519	-.598615	1	.846432	3.363871	-.844683
1	0.329695	2.227897	-1.868641	1	-.508930	1.663496	-1.373762
1	-.937968	1.039519	-2.216410	1	-.139348	-.089868	-1.111292
1	-2.668049	-2.105147	-1.859590	1	-2.162900	-1.510088	.750553
1	-4.909416	-1.029217	-1.892779	1	-4.510429	-1.856499	.117505
1	-3.947651	1.062635	1.738437	1	-5.014580	2.386097	-.373189
1	-1.716786	-.025803	1.758356	1	-2.637552	2.730039	.273171
1	4.458573	2.905610	-1.787140	1	5.523125	.349447	-2.424826
1	2.872229	2.257213	-2.198332	1	4.019387	1.252749	-2.251730
1	3.003292	3.813570	-1.352987	1	5.499618	1.831115	-1.457910
6	-6.270724	1.518276	.791604	6	-6.833715	-1.108365	-.608474
1	-7.283837	1.807305	.508578	1	-7.867199	-.939124	-.914194

1	-6.294417	1.040137	1.779094	1	-6.339608	-1.752267	-1.346950
1	-5.641558	2.416248	.844448	1	-6.823605	-1.610154	.367343
NImag = 1 (-364)				NImag = 1 (-384)			

(b) X=NO_2

79. **2t-no2(s-*re*)** **Et** = -1263.3188277				80. **2t-no2(s-*si*)** **Et** = -1263.314959			
6	-4.427675	-0.259286	-0.532284	6	4.439182	-0.737658	-0.839377
6	-3.256186	0.317425	0.296516	6	3.100464	-0.920560	-0.084562
7	-2.122624	-0.532851	-0.246807	7	2.651428	0.522800	-0.015410
6	-2.725835	-1.861657	0.055176	6	3.871763	1.061184	0.651668
6	-4.080996	-1.771745	-0.696407	6	4.995231	0.623015	-0.320964
6	-2.967321	-1.743887	1.571699	6	3.911422	0.192229	1.924642
6	-3.340240	-0.242412	1.741720	6	3.402380	-1.188126	1.415342
6	-1.057053	-0.286155	-0.991596	6	1.603564	1.209905	-0.452328
6	-0.262409	-1.463545	-1.511059	6	1.681297	2.718358	-0.341722
6	-3.197101	1.868684	0.238632	6	2.208791	-1.994075	-0.747996
8	-4.022046	2.452766	-0.442498	8	2.605443	-2.557253	-1.749763
6	-4.007503	-2.210254	-2.160648	6	5.262677	1.625473	-1.446105
6	-0.533085	1.020274	-1.180426	6	0.363752	0.637359	-0.837158
8	-2.322585	2.473163	1.004761	8	1.090345	-2.323466	-0.135583
6	0.400025	1.429454	0.461500	6	-0.467170	0.304104	0.912972
8	-0.360928	1.104004	1.463571	8	0.203347	-0.657297	1.456207
6	1.771536	0.802551	0.332237	6	-1.931849	0.165331	0.521158
6	2.128091	-0.379130	1.033588	6	-2.682995	1.360886	0.338402
6	3.406486	-0.915285	0.852333	6	-4.033347	1.292071	-0.000395
6	4.316620	-0.285838	0.014504	6	-4.641468	0.051955	-0.138687
6	4.001886	0.895686	-0.643525	6	-3.940463	-1.124940	0.074007
6	2.733945	1.455474	-0.484588	6	-2.582680	-1.092825	0.411714
7	5.649254	-0.876198	-0.170581	7	-6.065220	-0.011150	-0.496979
1	0.428940	2.499082	0.209107	1	-0.297595	1.294071	1.364657
1	-1.489767	1.854489	1.322400	1	0.737109	-1.645989	0.593508
1	-2.627043	0.267280	2.388080	1	2.493804	-1.480536	1.939441
1	-4.344276	-0.089560	2.144643	1	4.141953	-1.986226	1.514952
1	-4.810626	-2.402437	-0.177170	1	3.236425	0.594443	2.684320
1	-3.756904	-2.425870	1.897574	1	4.918837	0.155293	2.347262
1	-2.091323	-2.693494	-0.244778	1	3.818129	2.131939	0.836997
1	-2.060205	-1.987238	2.130261	1	5.919174	0.480095	0.249794
1	-5.380100	-0.083763	-0.028327	1	5.105829	-1.581280	-0.649863
1	-4.473257	0.254159	-1.494839	1	4.245888	-0.714357	-1.913716
1	-1.239394	1.842078	-1.173188	1	1.658636	3.041971	0.705476
1	0.184482	1.088280	-1.991510	1	2.598000	3.107175	-0.791562
1	0.054168	-2.129783	-0.703280	1	0.833810	3.174705	-0.851652
1	-0.852507	-2.052962	-2.219685	1	-0.281019	1.305189	-1.398167
1	0.631290	-1.109513	-2.023198	1	0.341698	-0.379838	-1.205481
6	2.460563	2.775217	-1.177433	6	-1.915227	-2.426501	0.657532
1	4.750071	1.370814	-1.265681	1	-4.460168	-2.070318	-0.019722
1	3.705113	-1.821045	1.365562	1	-4.620831	2.189554	-0.147928
6	1.216307	-1.090319	2.011411	6	-2.092869	2.743583	0.521694
1	-4.977686	-2.075267	-2.649317	1	6.022897	1.239185	-2.132437
1	-3.279885	-1.612085	-2.720650	1	4.358630	1.809898	-2.037286
1	-3.730711	-3.266196	-2.254732	1	5.621674	2.584711	-1.056670
1	1.689353	-2.014664	2.354786	1	-2.668630	-3.218247	0.669320
1	1.005636	-0.456014	2.875417	1	-1.183574	-2.672130	-0.116047

1	0.243575	-1.326794	1.579919	1	-1.378537	-2.429596	1.607371
1	3.339120	3.091302	-1.744389	1	-2.857794	3.503842	0.348419
1	1.619797	2.728067	-1.875971	1	-1.704250	2.892823	1.535318
1	2.231205	3.568197	-0.457094	1	-1.269766	2.945060	-0.169978
8	5.900675	-1.925274	0.424028	8	-6.659617	1.053916	-0.672946
8	6.437910	-0.290311	-0.913652	8	-6.583082	-1.123098	-0.602742
NImag = 1 (-351)				NImag = 1(-387)			

(b)X=CF_3

81. **2t-cf3(s-*re*)** **Et** = -1395.8543769				82. **2t-cf3(s-*si*)** **Et** = -1395.8503034			
6	2.397306	1.563108	-0.534706	6	-2.259510	-1.088050	0.448055
6	1.447499	0.929456	0.307694	6	-1.606812	0.167067	0.550439
6	1.837091	-0.196855	1.075359	6	-2.361494	1.358765	0.369961
6	3.137076	-0.694938	0.934197	6	-3.715522	1.282592	0.043301
6	4.054615	-0.097912	0.074918	6	-4.347009	0.049246	-0.091491
6	3.684772	1.033443	-0.646633	6	-3.622170	-1.116334	0.123198
6	0.057019	1.518964	0.391183	6	-0.138307	0.307467	0.925736
8	-0.702290	1.226165	1.407112	8	0.539446	-0.654697	1.466286
6	0.939943	-0.882044	2.085108	6	-1.771106	2.743256	0.539060
6	5.417748	-0.703355	-0.109646	6	-5.818868	-0.008878	-0.389252
6	2.090166	2.832091	-1.304116	6	-1.590571	-2.422297	0.686912
6	-0.859557	0.996166	-1.226716	6	0.681123	0.639714	-0.818103
6	-1.338739	-0.315318	-0.972366	6	1.925304	1.211439	-0.445925
6	-0.498495	-1.489622	-1.422417	6	2.004308	2.719631	-0.333386
7	-2.398223	-0.560776	-0.217297	7	2.977370	0.523831	-0.019656
6	-3.563237	0.276302	0.276986	6	3.422101	-0.920711	-0.089041
6	-4.709330	-0.380865	-0.526422	6	4.755692	-0.742896	-0.853892
6	-4.310672	-1.887081	-0.611312	6	5.318413	0.618092	-0.343457
6	-2.956882	-1.892442	0.149349	6	4.203463	1.060882	0.636924
6	-3.211285	-1.706616	1.657097	6	4.251264	0.194752	1.911594
6	-3.637700	-0.212849	1.748011	6	3.734449	-1.185256	1.409233
6	-3.556126	1.825064	0.144130	6	2.522072	-1.994532	-0.742372
8	-2.702838	2.493138	0.877422	8	1.408709	-2.317219	-0.121457
6	-4.214107	-2.397823	-2.050501	6	5.577706	1.617362	-1.473323
8	-4.402310	2.344875	-0.564075	8	2.913003	-2.561269	-1.745449
1	0.052758	2.573531	0.081089	1	0.033709	1.295298	1.381294
1	-1.837005	1.916391	1.225399	1	1.054481	-1.630000	0.611495
1	-2.947502	0.354799	2.370449	1	2.828388	-1.473525	1.939884
1	-4.649187	-0.075340	2.137677	1	4.472408	-1.985322	1.505584
1	-5.021530	-2.514910	-0.063174	1	3.583277	0.600556	2.675583
1	-3.978641	-2.398450	2.014212	1	5.261971	0.156214	2.326356
1	-2.292347	-2.716205	-0.104800	1	4.154017	2.132256	0.820067
1	-2.299303	-1.889008	2.230830	1	6.246901	0.475185	0.219987
1	-5.670112	-0.212624	-0.035952	1	5.421989	-1.587317	-0.666627
1	-4.766715	0.081797	-1.513852	1	4.554715	-0.722598	-1.926886
1	-1.593114	1.793033	-1.261913	1	1.995592	3.040867	0.714787
1	-0.140120	1.048058	-2.037232	1	2.914849	3.109763	-0.794692
1	-0.138505	-2.077401	-0.572761	1	1.149522	3.176617	-0.830309
1	-1.069286	-2.156618	-2.075662	1	0.032110	1.308803	-1.372651
1	0.370664	-1.133008	-1.973423	1	0.656355	-0.376117	-1.190154
1	4.409952	1.519604	-1.290668	1	-4.120245	-2.075876	0.034814
1	3.440035	-1.556959	1.519596	1	-4.282888	2.195715	-0.105246
1	-5.185708	-2.321873	-2.549056	1	6.330380	1.227728	-2.166118

1	-3.504404	-1.804600	-2.638011	1	4.668289	1.802442	-2.056006
1	-3.900636	-3.447008	-2.088286	1	5.942508	2.576778	-1.089631
1	1.435796	-1.774382	2.478537	1	-2.343894	-3.214479	0.706222
1	0.706967	-0.211118	2.915267	1	-0.865735	-2.669397	-0.092686
1	-0.024011	-1.167853	1.663229	1	-1.045003	-2.426784	1.631848
1	2.961942	3.141296	-1.885742	1	-2.540137	3.502435	0.377591
1	1.254915	2.720048	-2.002016	1	-1.364464	2.897179	1.545002
1	1.833492	3.659320	-0.632911	1	-0.960665	2.946216	-0.167513
9	6.341140	0.218922	-0.462189	9	-6.178645	-1.181338	-0.956356
9	5.859378	-1.310488	1.014888	9	-6.565152	0.129568	0.733580
9	5.416818	-1.646183	-1.084766	9	-6.200251	0.981564	-1.229943
NImag = 1 (-385)				NImag = 1 (-359)			

(b) X = -CN

83. **2t-cn(s-*re*)**				84. **2t-cn(s-*si*)**			
Et = -1151.0602586				**Et** = -1151.0564888			
6	3.078156	1.283045	-0.569160	6	-2.914037	-1.090932	0.339207
6	2.098790	0.700518	0.278244	6	-2.264397	0.166118	0.456454
6	2.420512	-0.463581	1.022986	6	-3.014601	1.358680	0.259941
6	3.677722	-1.050166	0.854725	6	-4.359334	1.286105	-0.098271
6	4.627815	-0.503429	-0.014700	6	-4.992606	0.047829	-0.250430
6	4.322967	0.670602	-0.712704	6	-4.266058	-1.123011	-0.018053
6	0.751645	1.381029	0.391871	6	-0.805823	0.306482	0.868708
8	-0.012387	1.119801	1.411489	8	-0.143078	-0.654194	1.425859
6	1.492002	-1.102874	2.034310	6	-2.428606	2.742611	0.448320
6	5.904507	-1.133877	-0.179834	6	-6.375810	-0.015448	-0.621238
6	2.847628	2.582774	-1.313489	6	-2.249489	-2.423860	0.597305
6	-0.214173	0.951233	-1.223049	6	0.054201	0.636123	-0.862987
6	-0.773020	-0.332884	-0.988158	6	1.288547	1.209102	-0.461255
6	-0.015193	-1.547415	-1.476275	6	1.364564	2.717642	-0.351054
7	-1.837915	-0.526213	-0.226841	7	2.329844	0.522703	-0.007902
6	-2.941528	0.372163	0.300363	6	2.778164	-0.921276	-0.066089
6	-4.137722	-0.198040	-0.497030	6	4.128213	-0.741638	-0.801106
6	-3.834584	-1.723865	-0.616264	6	4.678236	0.619348	-0.277293
6	-2.474081	-1.827328	0.123717	6	3.540243	1.061810	0.676242
6	-2.696033	-1.654727	1.638200	6	3.559094	0.196692	1.952386
6	-3.024378	-0.138589	1.763603	6	3.056967	-1.184715	1.439035
6	-2.841379	1.918926	0.192702	6	1.895153	-1.996142	-0.739486
8	-1.939254	2.522767	0.925391	8	0.768126	-2.322227	-0.142745
6	-3.789683	-2.210825	-2.066268	6	4.965245	1.618823	-1.400343
8	-3.662061	2.502720	-0.494367	8	2.307058	-2.562298	-1.733770
1	0.817531	2.439529	0.101549	1	-0.643947	1.296492	1.323077
1	-1.114734	1.891500	1.253999	1	0.400779	-1.639232	0.579286
1	-2.289025	0.370917	2.384699	1	2.140197	-1.475259	1.949725
1	-4.018713	0.056086	2.172488	1	3.794418	-1.983011	1.552235
1	-4.575349	-2.317198	-0.069435	1	2.872394	0.601781	2.699974
1	-3.501147	-2.303110	1.993416	1	4.559616	0.160216	2.391160
1	-1.865986	-2.685605	-0.155867	1	3.485077	2.133208	0.857425
1	-1.790391	-1.905835	2.195652	1	5.592831	0.476421	0.308367
1	-5.079191	0.019796	0.011036	1	4.791055	-1.585664	-0.600291
1	-4.180519	0.285965	-1.474928	1	3.950667	-0.720156	-1.878204
1	-0.896008	1.793436	-1.233527	1	1.326995	3.042125	0.695465
1	0.495486	0.973103	-2.043579	1	2.287519	3.106245	-0.788204
1	0.288109	-2.197789	-0.650670	1	0.524211	3.173349	-0.873224

1	-0.625598	-2.140965	-2.164050	1	-0.581382	1.303461	-1.435039
1	0.885274	-1.233815	-2.002697	1	0.038290	-0.381057	-1.231786
1	5.069495	1.111829	-1.365011	1	-4.765131	-2.081875	-0.111880
1	3.927689	-1.945363	1.415089	1	-4.927539	2.197804	-0.251338
1	-4.761084	-2.064191	-2.549149	1	5.734917	1.229371	-2.074261
1	-3.051818	-1.651765	-2.652654	1	4.070734	1.804316	-2.005565
1	-3.543431	-3.276638	-2.128918	1	5.320548	2.578023	-1.007389
1	1.939879	-2.022648	2.421708	1	-3.001495	-3.217370	0.599038
1	1.298986	-0.422777	2.866686	1	-1.505282	-2.670011	-0.164001
1	0.513096	-1.335221	1.614315	1	-1.727826	-2.424879	1.555497
1	3.734693	2.848560	-1.893252	1	-3.191454	3.502863	0.264795
1	2.004789	2.535358	-2.009546	1	-2.052569	2.893963	1.466328
1	2.644793	3.410728	-0.625278	1	-1.597343	2.944291	-0.233563
7	6.938339	-1.649834	-0.318149	7	-7.498462	-0.062378	-0.923862
NImag = 1 (-361)				NImag = 1 (-347)			

(b) X= F

85. **2t-f(s-*re*)** **Et** = -1158.0496515				86. **2t-f(s-*si*)** **Et** = -1158.0458557			
6	3.313254	1.076718	-0.585908	6	-3.106209	-1.098518	0.238007
6	2.312853	0.511523	0.247701	6	-2.459699	0.159579	0.366792
6	2.588967	-0.690494	0.948912	6	-3.211930	1.347755	0.155873
6	3.825171	-1.321992	0.764715	6	-4.554969	1.273919	-0.221615
6	4.770543	-0.766504	-0.080533	6	-5.152004	0.033638	-0.371304
6	4.538157	0.423222	-0.750191	6	-4.455524	-1.137810	-0.137489
6	1.003620	1.247145	0.394328	6	-1.010601	0.305263	0.799891
8	0.238544	0.993933	1.420936	8	-0.351805	-0.656565	1.374956
6	1.634332	-1.328850	1.936279	6	-2.633858	2.734824	0.347728
9	5.954364	-1.395054	-0.247078	9	-6.450797	-0.030735	-0.736124
6	3.130704	2.401991	-1.298127	6	-2.442268	-2.430002	0.505334
6	-0.020691	0.924215	-1.214343	6	-0.108047	0.640264	-0.887641
6	-0.652441	-0.328702	-1.007371	6	1.118632	1.213311	-0.460629
6	0.027046	-1.572180	-1.535728	6	1.189040	2.721250	-0.340277
7	-1.719836	-0.480777	-0.238818	7	2.151689	0.526883	0.010652
6	-2.751006	0.469768	0.340363	6	2.596616	-0.918486	-0.035537
6	-3.994118	0.012734	-0.456399	6	3.964343	-0.741968	-0.737143
6	-3.800631	-1.525573	-0.629294	6	4.506262	0.616031	-0.197609
6	-2.435815	-1.748333	0.076253	6	3.344987	1.063422	0.724921
6	-2.614479	-1.619232	1.600449	6	3.327597	0.199995	2.002378
6	-2.846384	-0.091006	1.785208	6	2.838160	-1.181157	1.476275
6	-2.540476	2.010631	0.289811	6	1.724916	-1.992397	-0.728407
8	-1.594993	2.513238	1.035898	8	0.586001	-2.309878	-0.158831
6	-3.816356	-1.967814	-2.094329	6	4.828030	1.615622	-1.311202
8	-3.323149	2.672907	-0.373633	8	2.163862	-2.558988	-1.712870
1	1.109254	2.309735	0.136021	1	-0.862530	1.290162	1.269328
1	-0.777610	1.801742	1.319404	1	0.187552	-1.610807	0.561290
1	-2.074372	0.350253	2.414051	1	1.908744	-1.471977	1.963192
1	-3.821961	0.148305	2.215355	1	3.572845	-1.979359	1.607749
1	-4.570513	-2.083985	-0.085670	1	2.620045	0.607030	2.729267
1	-3.449121	-2.230764	1.953305	1	4.315198	0.163124	2.469767
1	-1.894212	-2.634567	-0.249468	1	3.288795	2.135358	0.903019
1	-1.712707	-1.943737	2.125623	1	5.404199	0.468725	0.412423
1	-4.912144	0.279041	0.071336	1	4.619790	-1.588474	-0.522788
1	-4.013590	0.531180	-1.417302	1	3.811974	-0.717842	-1.818061

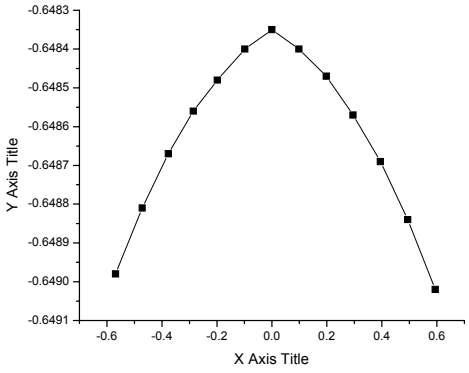
1	-0.651215	1.805339	-1.193149	1.128747	3.038941	0.707373
1	0.683286	0.926596	-2.040006	2.119957	3.114969	-0.755733
1	0.266416	-2.277729	-0.735116	0.357879	3.177908	-0.876141
1	-0.609977	-2.089570	-2.260495	-0.730534	1.310725	-1.470439
1	0.958471	-1.300307	-2.030664	-0.111931	-0.373035	-1.267628
1	5.314272	0.839651	-1.383460	-4.969183	-2.087689	-0.240730
1	4.059990	-2.242995	1.287992	-5.140936	2.171872	-0.386498
1	-4.780899	-1.732172	-2.555235	5.611838	1.222489	-1.966536
1	-3.046330	-1.447829	-2.675382	3.950064	1.808376	-1.938094
1	-3.652746	-3.046670	-2.194453	5.179409	2.571925	-0.907565
1	2.029961	-2.292974	2.269068	-3.191322	-3.226345	0.494004
1	1.490708	-0.684593	2.806920	-1.683358	-2.672612	-0.242589
1	0.638649	-1.478724	1.518039	-1.936037	-2.430036	1.471964
1	4.026267	2.649713	-1.872886	-3.399876	3.491931	0.163938
1	2.285808	2.401146	-1.993973	-2.259332	2.886881	1.366298
1	2.957175	3.220606	-0.590819	-1.801952	2.942428	-0.332370
NImag = 1 (-461)				NImag = 1 (-393)		

(b) X = -NH_2

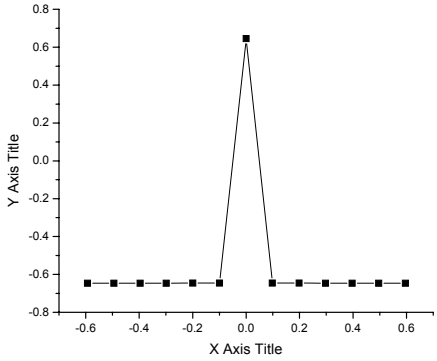
85. **2t-nh2(s-*re*)** **Et** =-1114.1766469			86. **2t-nh2(s-*si*)** **Et**=-1114.1728772		
6	3.315456	1.095416 -0.572543	6	-3.100952	-1.090691 0.257558
6	2.318993	0.517002 0.257069	6	-2.446382	0.163509 0.387536
6	2.618192	-0.691762 0.937925	6	-3.207188	1.345143 0.171006
6	3.860640	-1.298227 0.747718	6	-4.545508	1.266476 -0.208448
6	4.839129	-0.744848 -0.088551	6	-5.186278	0.032045 -0.371223
6	545070	0.461167 -0.738554	6	-4.445595	-1.127277 -0.118584
6	1.014522	1.230145 0.409353	6	-1.002732	0.312470 0.809831
8	0.248194	0.965341 1.437238	8	-0.330423	-0.650774 1.382903
6	1.667253	-1.359180 1.909601	6	-2.633106	2.734748 0.360384
7	6.090077	-1.340774 -0.217317	7	-6.538627	-0.036072 -0.700586
6	3.110489	2.419142 -1.281774	6	-2.438824	-2.422830 0.528607
6	-0.052323	0.888677 -1.227700	6	-0.095993	0.654488 -0.869550
6	-0.686762	-0.352317 -0.995433	6	1.135664	1.219918 -0.446931
6	-0.014966	-1.607542 -1.506996	6	1.211198	2.726515 -0.313648
7	-1.758775	-0.490949 -0.225572	7	2.170440	0.526506 0.011103
6	-2.776420	0.478974 0.343906	6	2.603684	-0.922069 -0.044273
6	-4.017885	0.052400 -0.470082	6	3.964716	-0.753565 -0.760131
6	-3.856482	-1.490082 -0.642285	6	4.521400	0.600759 -0.225596
6	-2.502240	-1.744076 0.075683	6	3.374397	1.053178 0.712760
6	-2.692198	-1.618548 1.598640	6	3.367950	0.186183 1.988089
6	-2.903502	-0.087260 1.784009	6	2.859824	-1.189019 1.464058
6	-2.512305	2.015421 0.303253	6	1.710875	-1.987534 -0.727949
8	-1.575483	2.471717 1.075204	8	0.579918	-2.287912 -0.145533
6	-3.866760	-1.931122 -2.107680	6	4.832290	1.600799 -1.341852
8	-3.252516	2.696629 -0.395852	8	2.138590	-2.553190 -1.720717
1	1.077197	2.289071 0.136184	1	-0.851883	1.292265 1.286960
1	-0.698137	1.710919 1.357361	1	0.168569	-1.563490 0.594828
1	-2.138460	0.344071 2.428232	1	1.932524	-1.472883 1.959041
1	-3.882562	0.164561 2.199170	1	3.588177	-1.994521 1.586570
1	-4.643801	-2.032347 -0.106886	1	2.674382	0.597236 2.726243
1	-3.537788	-2.219415 1.944248	1	4.361859	0.140036 2.441389
1	-1.978026	-2.640954 -0.250103	1	3.328068	2.125144 0.894254
1	-1.798047	-1.957454 2.128535	1	5.427002	0.448281 0.371900

1	-4.937749	0.338118	0.044545	1	4.617268	-1.604232	-0.553292
1	-4.010669	0.573746	-1.429664	1	3.800565	-0.728493	-1.839301
1	-0.668499	1.779387	-1.206975	1	1.169946	3.034553	0.737880
1	0.665395	0.875275	-2.040751	1	2.135656	3.122717	-0.741437
1	0.161304	-2.333605	-0.708949	1	0.371228	3.189577	-0.830010
1	-0.627697	-2.093247	-2.274028	1	-0.719434	1.332302	-1.442463
1	0.948357	-1.353617	-1.948032	1	-0.104834	-0.355570	-1.257799
1	5.299841	0.921646	-1.371794	1	-4.935536	-2.094293	-0.206763
1	4.082193	-2.221467	1.278651	1	-5.110017	2.183359	-0.363055
1	-4.820382	-1.672777	-2.579222	1	5.604189	1.204891	-2.009647
1	-3.078389	-1.428197	-2.679081	1	3.945811	1.798886	-1.954938
1	-3.726552	-3.013454	-2.207586	1	5.194299	2.554810	-0.941929
1	2.061027	-2.334221	2.212070	1	-3.187763	-3.219784	0.516139
1	1.530045	-0.743367	2.802260	1	-1.674780	-2.667125	-0.213473
1	0.668638	-1.493376	1.492249	1	-1.937812	-2.422698	1.498333
1	3.997842	2.681106	-1.863365	1	-3.402501	3.490382	0.182924
1	2.259804	2.406852	-1.970929	1	-2.252572	2.887330	1.376781
1	2.931099	3.235009	-0.572589	1	-1.805513	2.947522	-0.324045
1	6.129014	-2.328156	-0.007694	1	-6.903439	0.764689	-1.197495
1	6.606932	-1.101827	-1.051693	1	-6.837471	-0.908392	-1.114292
NImag = 1 (-665)				NImag = 1 (-505)			

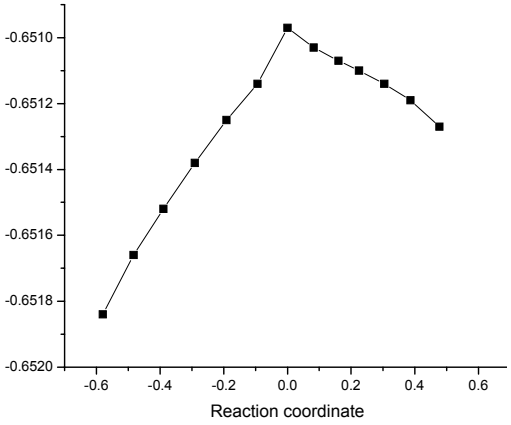
TABLE S9. IRC profiles for the Lowest Energy Transition States for Catalysts **1 - 11**



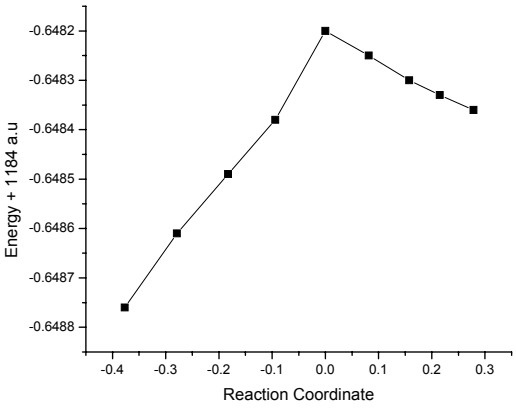
1t(s-*re*)



1t(s-*si*)



2t(s-*re*)



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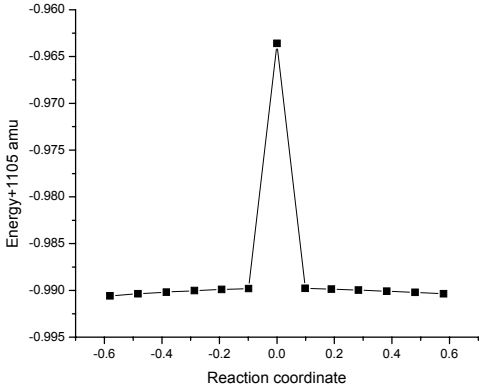
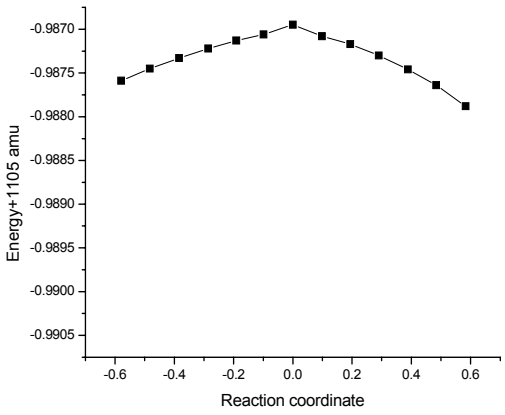
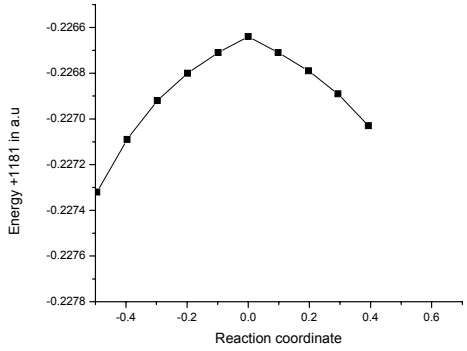


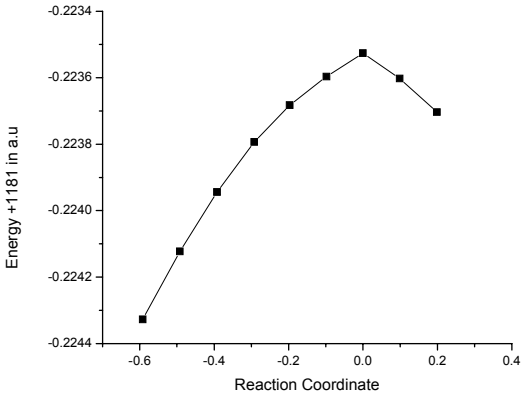
3t(s-*re*)



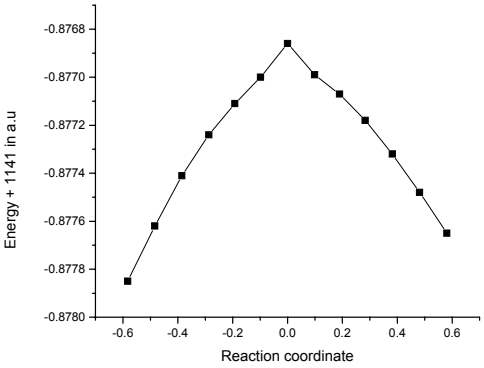
3t(s-*si*)



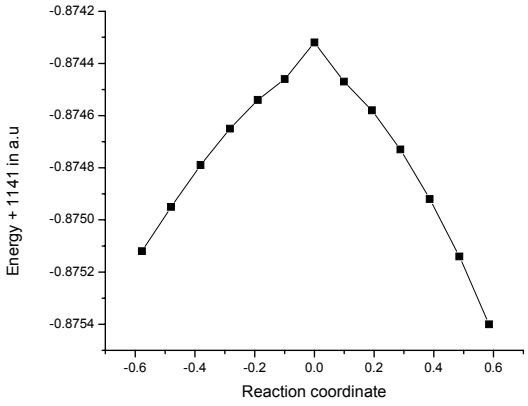
4t(s-*re*)



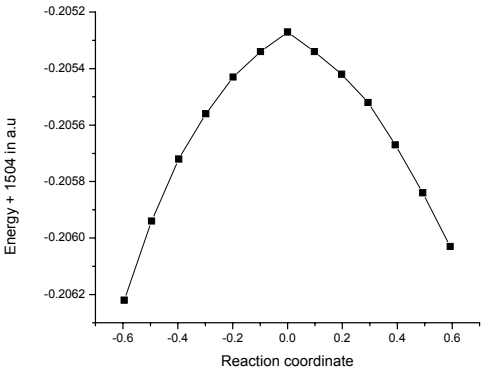
4t(s-*si*)



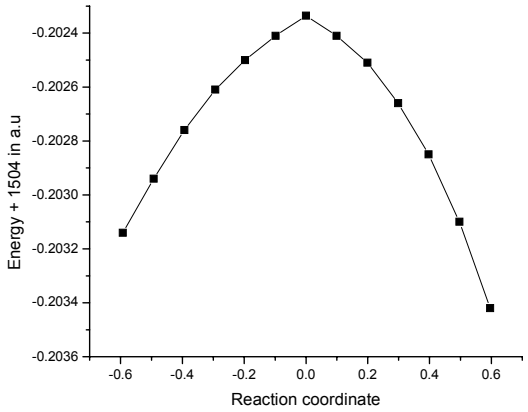
5t(s-*re*)



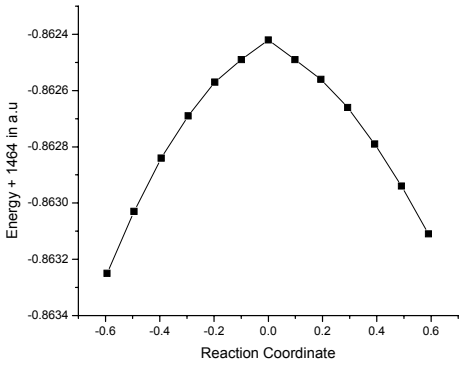
5t(s-*si*)



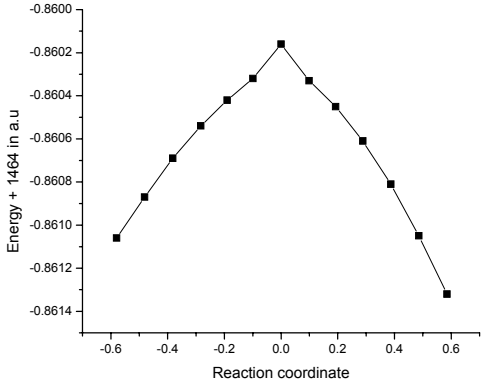
6t(s-*re*)



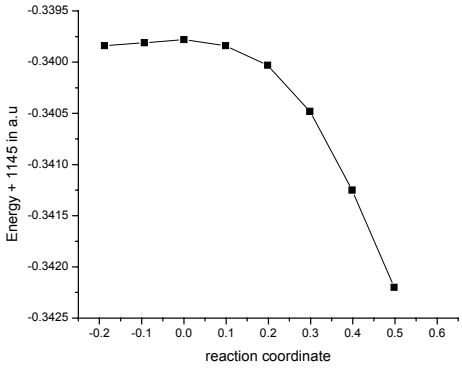
6t(s-*si*)



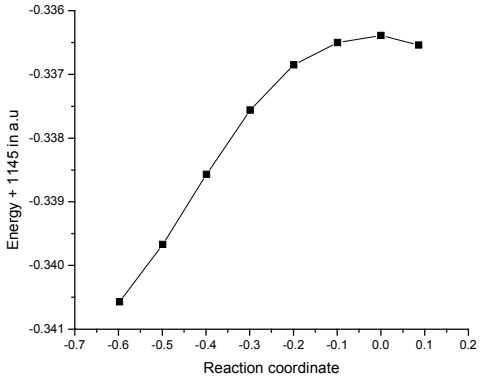
7t(s-*re*)



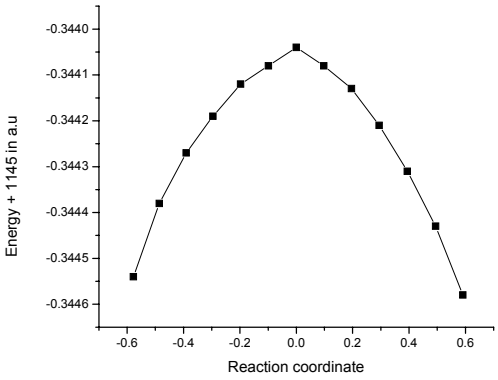
7t(s-*si*)



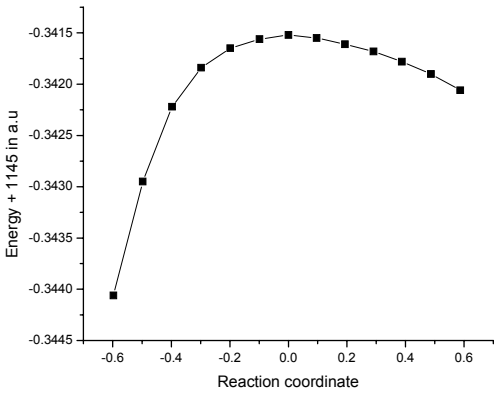
8t(a-*re*)



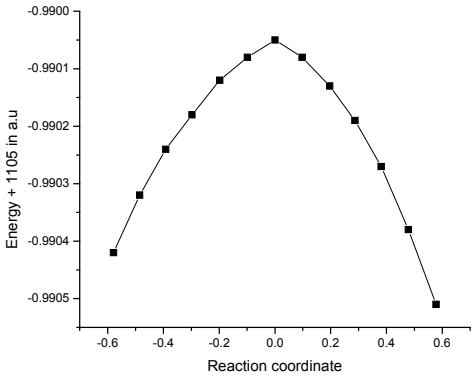
8t(a-*si*)



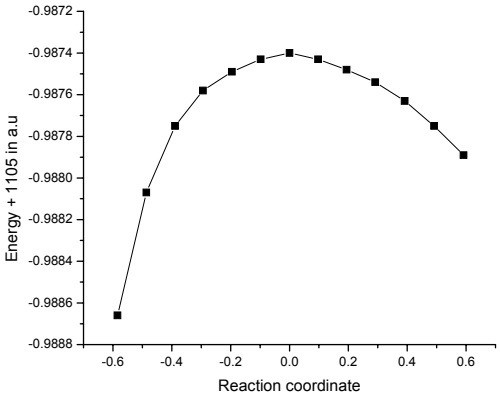
9t(a-*re*)



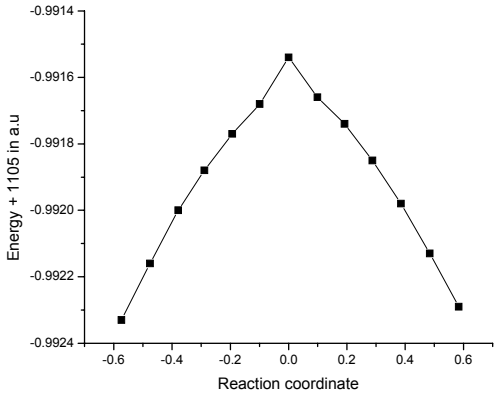
9t(a-*si*)



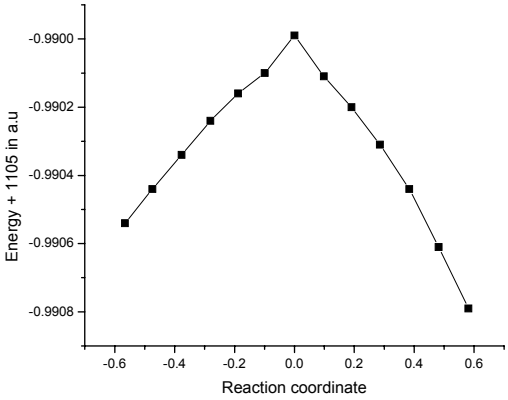
10t(a-*re*)



10t(a-*si*)



11(s-*re*)



11(s-*si*)

TABLE S10. Total electronic energies (a.u.) of Reactants (*anti*-enamine, *syn*-enamine), and Transition states (t-a-*re*, t-a-*si*, t-s-*re*, t-s-*si*) Obtained for the Enamine Addition on the Prochiral Faces of *p*-Nitrobenzaldehyde for Catalysts **1-11**

Catalyst 1	0.980600					
File name	*syn*-enamine	*anti*-enamine	1t -a-*re*	1t -a-*si*	1t-s-*re*	1t -s-*si*
B3LYP/6-31G* (g)	-634.580854	-634.579513	-1184.642142	-1184.638223	-1184.648346	-1184.645612
B3LYP/6-311+G** (g)	-634.772051	-634.769726	-1184.991894	-1184.987340	-1184.997590	-1184.995101
B3LYP/6-311+G** (sol)	-634.779896	-634.777182	-1185.013198	-1185.008615	-1185.016539	-1185.013986
ZPE (raw)	0.270607	0.271028	0.382792	0.382701	0.384763	0.384664
Thermal Corr H	0.284778	0.285019	0.405538	0.405479	0.407756	0.407788
Thermal Corr G	0.232020	0.232843	0.332023	0.331924	0.333071	0.332489
H (raw)	-634.296076	-634.294494	-1184.236604	-1184.232744	-1184.240591	-1184.237824
G (raw)	-634.348834	-634.346670	-1184.310119	-1184.306300	-1184.315276	-1184.313123
Scaled ZPE	0.265357	0.265770	0.375366	0.375277	0.377299	0.377202
H(298)	-634.301326	-634.299752	-1184.244030	-1184.240168	-1184.248055	-1184.245286
G(298)	-634.354084	-634.351928	-1184.317545	-1184.313724	-1184.322740	-1184.320585
H(0)	-634.315497	-634.313743	-1184.266776	-1184.262946	-1184.271047	-1184.268411
NImag	0	0	1	1	1	1
Del E (BW) at B3LYP/6-31G*			5.475773	7.935046	2.424006	4.139366
Del H(0) at B3LYP/6-31G*			4.915818	7.319095	3.335934	4.990376
Del H(298) at B3LYP/6-31G*			4.285673	6.708967	2.747393	4.484917
Del G(298) at B3LYP/6-31G*			18.908527	22.658899	17.001271	18.353504
H(0) at B3LYP/6-311+G**(g)	-634.506693	-634.503956	-1184.616528	-1184.612063	-1184.620292	-1184.617899
H(298) at B3LYP/6-311+G** (g)	-634.492522	-634.489965	-1184.593782	-1184.589285	-1184.597299	-1184.594775
G(298) at B3LYP/6-311+G** (g)	-634.545280	-634.542141	-1184.667297	-1184.662840	-1184.671984	-1184.670074
Del E (BW) at B3LYP/6-311+G** (g)			5.475773	7.935046	2.424006	7.406495
Del H(0) at B3LYP/6-311+G**(g)			7.399940	10.201999	6.755986	8.257504
Del H(298) at B3LYP/6-311+G** (g)			6.769920	9.592060	6.168010	7.751731
Del G(298) at B3LYP/6-311+G**(g)			21.392774	24.189813	20.421888	21.620319
Relative ΔH_{298K} in kcal/mol (g)			**2.206661**	**5.028800**	**0.000000**	**1.583721**
Relative ΔE in kcal/mol (sol)			**2.096886**	**4.972887**	**0.000000**	**1.602408**

Catalyst 2	0.980600					
File name	*anti*-enamine	*syn*-enamine	2t -a-*re*	2t -a-*si*	2t -s-*re*	2t -s-*si*
B3LYP/6-31G* (g)	-634.575509	-634.584035	-1184.643134	-1184.639278	-1184.651120	-1184.648361
B3LYP/6-311+G** (g)	-634.766267	-634.775580	-1184.993560	-1184.989120	-1185.000854	-1184.998340
B3LYP/6-311+G** (sol)	-634.773222	-634.783938	-1185.015507	-1185.010769	-1185.019303	-1185.016913
ZPE (raw)	0.269768	0.270331	0.382246	0.382401	0.384920	0.384621
Thermal Corr H	0.284172	0.284582	0.405170	0.405272	0.407984	0.407889
Thermal Corr G	0.230538	0.231691	0.330963	0.331391	0.333070	0.332072
H (raw)	-634.291337	-634.299453	-1184.237963	-1184.234006	-1184.243136	-1184.240472
G (raw)	-634.344971	-634.352344	-1184.312171	-1184.307887	-1184.318050	-1184.316289
Scaled ZPE	0.264373	0.264924	0.374830	0.374982	0.377453	0.377159
H(298)	-634.296732	-634.304860	-1184.245379	-1184.241425	-1184.250603	-1184.247934
G(298)	-634.350366	-634.357751	-1184.319587	-1184.315306	-1184.325517	-1184.323751
H(0)	-634.311136	-634.319110	-1184.268303	-1184.264296	-1184.273667	-1184.271201
NImag	0	0	1	1	1	1
Del E (BW) at B3LYP/6-31G*			2.340799	4.760099	2.679277	4.410702
Del H(0) at B3LYP/6-31G*			2.321762	4.836439	3.959427	5.506865
Del H(298) at B3LYP/6-31G*			1.544717	4.025885	3.365991	5.041316
Del G(298) at B3LYP/6-31G*			16.647616	19.333979	17.559628	18.668312
H(0) at B3LYP/6-311+G**(g)	-634.501894	-634.510655	-1184.618729	-1184.614137	-1184.623402	-1184.621181
H(298) at B3LYP/6-311+G** (g)	-634.487490	-634.496404	-1184.595805	-1184.591266	-1184.600338	-1184.597913
G(298) at B3LYP/6-311+G** (g)	-634.541124	-634.549295	-1184.670012	-1184.665147	-1184.675252	-1184.673730
Del E (BW) at B3LYP/6-311+G** (g)			4.743784	7.530051	6.010600	7.588159
Del H(0) at B3LYP/6-311+G**(g)			4.724747	7.606392	7.290749	8.684322
Del H(298) at B3LYP/6-311+G** (g)			3.947263	6.795649	6.697125	8.218710
Del G(298) at B3LYP/6-311+G**(g)			19.050789	22.103744	20.890762	21.845707
Relative ΔH_{298K} in kcal/mol (g)			**2.843983**	**5.692370**	**0.000000**	**1.521585**
Relative ΔE in kcal/mol (sol)			**2.382277**	**5.355103**	**0.000000**	**1.500187**

Catalyst 3	0.980600					
File name	*anti*-enamine	*syn*-enamine	3t -a-*re*	3t -a-*si*	3t-s-*re*	3t -s-*si*
B3LYP/6-31G* (g)	-555.912376	-555.914571	-1105.961853	-1105.957877	-1105.989682	-1105.986949
B3LYP/6-311+G** (g)	-556.082876	-556.091551	-1106.291272	-1106.286659	-1106.317720	-1106.315023
B3LYP/6-311+G** (sol)	-556.091878	-556.094132	-1106.315630	-1106.310747	-1106.336422	-1106.334234
ZPE (raw)	0.211562	0.211359	0.323494	0.323571	0.326333	0.326078
Thermal Corr H	0.223703	0.223599	0.344141	0.344139	0.347422	0.347275
Thermal Corr G	0.174343	0.174296	0.274778	0.275233	0.276077	0.275600
H (raw)	-555.688673	-555.690972	-1105.617712	-1105.613738	-1105.642261	-1105.639673
G (raw)	-555.738033	-555.740274	-1105.687075	-1105.682644	-1105.713605	-1105.711348
Scaled ZPE	0.207458	0.207259	0.317218	0.317294	0.320002	0.319752
H(298)	-555.692777	-555.695072	-1105.623988	-1105.620015	-1105.648592	-1105.645999
G(298)	-555.742137	-555.744374	-1105.693351	-1105.688921	-1105.719936	-1105.717674
H(0)	-555.704918	-555.707312	-1105.644635	-1105.640583	-1105.669680	-1105.667196
NImag	0	0	1	1	1	1
Del E (BW) at B3LYP/6-31G*			13.728590	16.223882	-2.357302	-0.642005
Del H(0) at B3LYP/6-31G*			13.272011	15.814683	-0.942030	0.616357
Del H(298) at B3LYP/6-31G*			12.485804	14.978590	-1.513314	0.113784
Del G(298) at B3LYP/6-31G*			27.947011	30.726568	12.668400	14.087793
H(0) at B3LYP/6-311+G**(g)	-555.875418	-555.884292	-1105.974054	-1105.969365	-1105.997718	-1105.995271
H(298) at B3LYP/6-311+G** (g)	-555.863277	-555.872052	-1105.953407	-1105.948797	-1105.976629	-1105.974074
G(298) at B3LYP/6-311+G** (g)	-555.912637	-555.921355	-1106.022770	-1106.017703	-1106.047974	-1106.045749
Del E (BW) at B3LYP/6-311+G** (g)		0.000000	16.601454	19.496469	5.448790	7.141184
Del H(0) at B3LYP/6-311+G**(g)			16.144875	19.087271	6.864063	8.399545
Del H(298) at B3LYP/6-311+G** (g)			15.358606	18.251428	6.293029	7.896283
Del G(298) at B3LYP/6-311+G**(g)			30.819812	33.999407	20.474744	21.870919
Relative ΔH_{298K} in kcal/mol (g)			**14.571948**	**15.861517**	**0.000000**	**1.603254**
Relative ΔE in kcal/mol (sol)			**13.046613**	**16.111181**	**0.000000**	**1.372865**

Catalyst 4	0.980600					
File name	*anti*-enamine	*syn*-enamine	4t-a-*re*	4t-a-*si*	4t -s-*re*	4t -s-*si*
B3LYP/6-31G* (g)	-631.161090	-631.163928	-1181.217009	-1181.212615	-1181.226644	-1181.223526
B3LYP/6-311+G** (g)	-631.354912	-631.358745	-1181.570785	-1181.565796	-1181.579524	-1181.576534
B3LYP/6-311+G** (sol)	-631.364446	-631.368683	-1181.594513	-1181.589788	-1181.600497	-1181.597590
ZPE (raw)	0.218110	0.217798	0.329189	0.334978	0.331598	0.331551
Thermal Corr H	0.230549	0.230401	0.350670	0.356580	0.353036	0.353125
Thermal Corr G	0.181186	0.180649	0.278978	0.284833	0.281179	0.280570
H (raw)	-630.930540	-630.933527	-1180.866339	-1180.866982	-1180.873608	-1180.870401
G (raw)	-630.979904	-630.983279	-1180.938031	-1180.938729	-1180.945466	-1180.942956
Scaled ZPE	0.213879	0.213573	0.322803	0.328479	0.325165	0.325119
H(298)	-630.934771	-630.937752	-1180.872725	-1180.873481	-1180.880041	-1180.876833
G(298)	-630.984135	-630.987504	-1180.944417	-1180.945228	-1180.951899	-1180.949388
H(0)	-630.947211	-630.950355	-1180.894206	-1180.884136	-1180.901479	-1180.898407
NImag	0	0	1	1	1	1
Del E (BW) at B3LYP/6-31G*			9.686048	12.443137	5.420678	7.377441
Del H(0) at B3LYP/6-31G*			8.704588	15.023855	6.113546	8.041388
Del H(298) at B3LYP/6-31G*			8.254224	7.780262	5.534104	7.547099
Del G(298) at B3LYP/6-31G*			22.256471	21.747996	19.675658	21.251279
H(0) at B3LYP/6-311+G**(g)	-631.141033	-631.145172	-1181.247982	-1181.237317	-1181.254359	-1181.251415
H(298) at B3LYP/6-311+G** (g)	-631.128594	-631.132569	-1181.226501	-1181.215715	-1181.232921	-1181.229841
G(298) at B3LYP/6-311+G** (g)	-631.177957	-631.182321	-1181.298193	-1181.287462	-1181.304778	-1181.302396
Del E (BW) at B3LYP/6-311+G** (g)			11.910068	15.040650	8.831506	10.708010
Del H(0) at B3LYP/6-311+G**(g)			10.928607	17.621368	9.524374	11.371958
Del H(298) at B3LYP/6-311+G** (g)			10.478683	17.247372	8.944555	10.877480
Del G(298) at B3LYP/6-311+G**(g)			24.480302	31.214479	23.086737	24.581660
Relative ΔH_{298K} in kcal/mol (g)			**4.028507**	**10.797197**	**0.000000**	**1.932925**
Relative ΔE in kcal/mol (sol)			**3.755080**	**6.719685**	**0.000000**	**1.824170**

Catalyst 5	0.980600					
File name	*anti*-enamine	*syn*-enamine	5t-a-*re*	5t -a-*si*	5t-s-*re*	5t-s-*si*
B3LYP/6-31G* (g)	-591.801011	-591.811220	-1141.850182	-1141.846004	-1141.876864	-1141.874315
B3LYP/6-311+G** (g)	-591.985699	-591.994204	-1142.193258	-1142.214657	-1142.219296	-1142.216602
B3LYP/6-311+G** (sol)	-591.995856	-592.002891	-1142.219716	-1142.189167	-1142.240943	-1142.237855
ZPE (raw)	0.187084	0.187270	0.298412	0.298351	0.301449	0.301547
Thermal Corr H	0.198989	0.199052	0.319110	0.319030	0.322450	0.322502
Thermal Corr G	0.150073	0.150550	0.249219	0.249349	0.250438	0.251121
H (raw)	-591.602022	-591.612168	-1141.531072	-1141.526973	-1141.554414	-1141.551813
G (raw)	-591.650938	-591.660669	-1141.600962	-1141.596654	-1141.626426	-1141.623194
Scaled ZPE	0.183455	0.183637	0.292623	0.292563	0.295601	0.295697
H(298)	-591.605651	-591.615801	-1141.536861	-1141.532761	-1141.560262	-1141.557663
G(298)	-591.654567	-591.664302	-1141.606751	-1141.602442	-1141.632274	-1141.629044
H(0)	-591.617556	-591.627583	-1141.557559	-1141.553441	-1141.581263	-1141.578618
NImag	0	0	1	1	1	1
Del E (BW) at B3LYP/6-31G*			13.920922	16.542656	3.583581	5.182789
Del H(0) at B3LYP/6-31G*			13.092680	15.676879	4.509662	6.169173
Del H(298) at B3LYP/6-31G*			12.486255	15.059159	4.170932	5.801891
Del G(298) at B3LYP/6-31G*			27.338149	30.042203	17.430835	19.457753
H(0) at B3LYP/6-311+G**(g)	-591.802245	-591.810567	-1141.900635	-1141.922094	-1141.923695	-1141.920905
H(298) at B3LYP/6-311+G** (g)	-591.790340	-591.798785	-1141.879937	-1141.901415	-1141.902694	-1141.899950
G(298) at B3LYP/6-311+G** (g)	-591.839256	-591.847287	-1141.949828	-1141.971096	-1141.974706	-1141.971331
Del E (BW) at B3LYP/6-311+G** (g)			17.127119	3.699482	6.124932	7.815819
Del H(0) at B3LYP/6-311+G**(g)			16.298877	2.833705	7.051012	8.802202
Del H(298) at B3LYP/6-311+G** (g)			15.692703	2.215608	6.712157	8.434482
Del G(298) at B3LYP/6-311+G**(g)			30.543970	17.198652	19.972688	22.090971
Relative ΔH_{298K} in kcal/mol (g)			**14.280182**	**2.911456**	**0.000000**	**1.722325**
Relative ΔE in kcal/mol (sol)			**13.319705**	**32.489744**	**0.000000**	**1.937498**

Catalyst 6	0.980600					
File name	*anti*-enamine	*syn*-enamine	6t -a-*re*	6t-a-*si*	6t -s-*re*	6t-s-*si*
B3LYP/6-31G* (g)	-954.135755	-954.141231	-1504.193860	-1504.189431	-1504.205271	-1504.202335
B3LYP/6-311+G** (g)	-954.332675	-954.338373	-1504.525388	-1504.545209	-1504.560968	-1504.558062
B3LYP/6-311+G** (sol)	-954.340425	-954.354299	-1504.547134	-1504.567438	-1504.579962	-1504.577105
ZPE (raw)	0.214276	0.214666	0.325901	0.325958	0.328954	0.328800
Thermal Corr H	0.226617	0.227794	0.347927	0.347911	0.350850	0.350838
Thermal Corr G	0.177526	0.176757	0.275151	0.275707	0.277760	0.276997
H (raw)	-953.909138	-953.913437	-1503.845933	-1503.841520	-1503.854421	-1503.851498
G (raw)	-953.958229	-953.964474	-1503.918709	-1503.913725	-1503.927511	-1503.925338
Scaled ZPE	0.210119	0.210501	0.319579	0.319634	0.322572	0.322421
H(298)	-953.913295	-953.917602	-1503.852255	-1503.847844	-1503.860803	-1503.857877
G(298)	-953.962386	-953.968639	-1503.925031	-1503.920049	-1503.933893	-1503.931717
H(0)	-953.925636	-953.930729	-1503.874281	-1503.869797	-1503.882698	-1503.879914
NImag	0	0	1	1	1	1
Del E (BW) at B3LYP/6-31G*			8.314815	11.093740	4.590295	6.432223
Del H(0) at B3LYP/6-31G*			7.669327	10.483327	5.583447	7.330614
Del H(298) at B3LYP/6-31G*			7.622578	10.391083	4.961522	6.797607
Del G(298) at B3LYP/6-31G*			20.773294	23.900108	19.136334	20.501787
H(0) at B3LYP/6-311+G**(g)		-954.127872	-1504.205810	-1504.225574	-1504.238396	-1504.235641
H(298) at B3LYP/6-311+G** (g)	-954.122555	-954.114744	-1504.183784	-1504.203621	-1504.216500	-1504.213603
G(298) at B3LYP/6-311+G** (g)	-954.110214	-954.165781	-1504.256560	-1504.275825	-1504.289590	-1504.287444
Del E (BW) at B3LYP/6-311+G** (g)	-954.159305		26.442748	14.005196	7.692262	9.515805
Del H(0) at B3LYP/6-311+G**(g)			25.797261	13.394783	8.685414	10.414195
Del H(298) at B3LYP/6-311+G** (g)			25.750825	13.302539	8.063553	9.881440
Del G(298) at B3LYP/6-311+G**(g)			38.901542	26.812191	22.238365	23.584992
Relative ΔH_{298K} in kcal/mol (g)			**20.529493**	**8.081207**	**0.000000**	**1.817887**
Relative ΔE in kcal/mol (sol)			**20.599631**	**7.859117**	**0.000000**	**1.792544**

Catalyst 7	0.980600					
File name	*anti*-enamine	*syn*-enamine	7t-a-*re*	7t -a-*si*	7t -s-*re*	7t -s-*si*
B3LYP/6-31G* (g)	-914.794098	-914.785627	-1464.831377	-1464.827188	-1464.862421	-1464.860160
B3LYP/6-311+G** (g)	-914.980619	-914.972675	-1465.177618	-1465.172659	-1465.207105	-1465.204588
B3LYP/6-311+G** (sol)	-914.992419	-914.982001	-1465.201127	-1465.196008	-1465.226795	-1465.224447
ZPE (raw)	0.183802	0.183659	0.295212	0.295330	0.298899	0.298646
Thermal Corr H	0.196338	0.196234	0.316484	0.316465	0.320148	0.320027
Thermal Corr G	0.145661	0.145864	0.245141	0.245960	0.248410	0.247656
H (raw)	-914.597759	-914.589393	-1464.514893	-1464.510723	-1464.542273	-1464.540133
G (raw)	-914.648437	-914.639764	-1464.586236	-1464.581228	-1464.614011	-1464.612504
Scaled ZPE	0.180236	0.180096	0.289485	0.289601	0.293100	0.292852
H(298)	-914.601325	-914.592956	-1464.520620	-1464.516452	-1464.548072	-1464.545927
G(298)	-914.652003	-914.643327	-1464.591963	-1464.586957	-1464.619810	-1464.618298
H(0)	-914.613862	-914.605531	-1464.541893	-1464.537587	-1464.569320	-1464.567308
NImag	0	0	1	1	1	1
Del E (BW) at B3LYP/6-31G*			21.382574	24.011651	-3.412899	-1.994351
Del H(0) at B3LYP/6-31G*			20.604790	23.306476	-1.833947	-0.571079
Del H(298) at B3LYP/6-31G*			19.962660	22.577938	-2.514920	-1.168970
Del G(298) at B3LYP/6-31G*			35.008455	38.149586	12.090363	13.039100
H(0) at B3LYP/6-311+G**(g)	-914.800383	-914.792579	-1464.888133	-1464.883058	-1464.914004	-1464.911736
H(298) at B3LYP/6-311+G** (g)	-914.787847	-914.780004	-1464.866861	-1464.861923	-1464.892755	-1464.890355
G(298) at B3LYP/6-311+G** (g)	-914.838524	-914.830374	-1464.938204	-1464.932428	-1464.964493	-1464.962726
Del E (BW)atB3LYP/6-311+G** (g)	0.000000		23.753807	26.865752	0.265562	1.844752
Del H(0) at B3LYP/6-311+G**(g)			22.976023	26.160578	1.844514	3.268024
Del H(298) at B3LYP/6-311+G**						
(g)			22.334081	25.432667	1.163666	2.670008
Del G(298) at B3LYP/6-311+G**(g)			37.379248	41.003687	15.768322	16.877450
Relative ΔH_{298K} in kcal/mol			**16.248999**	**19.347585**	**0.000000**	**1.506342**
Relative ΔE in kcal/mol			**16.106663**	**19.319009**	**0.000000**	**1.472953**

Catalyst 8

File name	*anti*-enamine	*syn*-enamine	8t-a-*re*	8t-a-*si*	8t-s-*re*	8t-s-*si*
B3LYP/6-31G* (g)	-595.272613	-595.273117	-1145.339784	-1145.336393	-1145.325553	-1145.328359
B3LYP/6-311+G** (g)	-595.453001	-595.453921	-1145.679261	-1145.675554	-1145.664874	-1145.667378
B3LYP/6-311+G** (sol)	-595.467796	-595.468809	-1145.700586	-1145.697194	-1145.687586	-1145.688977
ZPE (raw)	0.242780	0.242261	0.355139	0.355044	0.354265	0.353862
Thermal Corr H	0.255325	0.255014	0.376435	0.376239	0.375762	0.375526
Thermal Corr G	0.205950	0.205027	0.305451	0.305786	0.304363	0.303465
H (raw)	-595.017289	-595.018103	-1144.963349	-1144.960154	-1144.949791	-1144.952833
G (raw)	-595.066664	-595.068090	-1145.034333	-1145.030608	-1145.021190	-1145.024894
Scaled ZPE	0.238070	0.237561	0.348249	0.348156	0.347392	0.346997
H(298)	-595.021999	-595.022803	-1144.970239	-1144.967042	-1144.956664	-1144.959698
G(298)	-595.071374	-595.072790	-1145.041223	-1145.037496	-1145.028063	-1145.031759
H(0)	-595.034543	-595.035556	-1144.991535	-1144.988237	-1144.978161	-1144.981362
NImag	0	0	1	1	1	1
Del E (BW) at B3LYP/6-31G*			2.625500	4.753573	11.871727	10.110998
Del H(0) at B3LYP/6-31G*			2.431669	4.501285	11.459452	9.450742
Del H(298) at B3LYP/6-31G*			1.799767	3.805816	10.822655	8.918677
Del G(298) at B3LYP/6-31G*			16.253193	18.591823	11.459452	23.080312
H(0) at B3LYP/6-311+G**(g)	-595.214930	-595.216360	-1145.331012	-1145.327398	-1145.317482	-1145.320381
H(298) at B3LYP/6-311+G** (g)	-595.202385	-595.203607	-1145.309716	-1145.306203	-1145.295985	-1145.298717
G(298) at B3LYP/6-311+G** (g)	-595.251760	-595.253594	-1145.380700	-1145.376656	-1145.367384	-1145.370778
Del E(BW)atB3LYP/6-311+G** (g)			5.391813	7.717739	14.997603	13.426382
Del H(0) at B3LYP/6-311+G**(g)			5.197982	7.465452	14.585328	12.766126
DelH(298) at B3LYP/6-311+G** (g)			4.565452	6.769544	13.948405	12.233998
Del G(298) at B3LYP/6-11+G**(g)			19.018879	21.556177	28.525451	26.395633
Relative ΔH_{298K} in kcal/mol (g)			**0.000000**	**2.204091**	**8.616242**	**6.901835**
Relative ΔE in kcal/mol (sol)			**0.000000**	**2.128136**	**8.157372**	**7.284319**

Catalyst 9	0.980600					
File name	*anti*-enamine	syn-enamine	9t -a-*re*	9t-a-*si*	9t -s-*re*	9t -s-*si*
B3LYP/6-31G* (g)	-595.278257	-595.278607	-1145.344040	-1145.341517	-1145.337110	-1145.336435
B3LYP/6-311+G** (g)	-595.458687	-595.465475	-1145.683959	-1145.680922	-1145.678273	-1145.677349
B3LYP/6-311+G** (sol)	-595.467258	-595.469648	-1145.704812	-1145.703016	-1145.688101	-1145.700248
ZPE (raw)	0.242968	0.242801	0.356404	0.356213	0.355113	0.355575
Thermal Corr H	0.255463	0.255383	0.377824	0.377438	0.376532	0.377010
Thermal Corr G	0.205764	0.205312	0.306097	0.306403	0.304456	0.305151
H (raw)	-595.022794	-595.023225	-1144.966217	-1144.964079	-1144.960578	-1144.959424
G (raw)	-595.072493	-595.073295	-1145.037943	-1145.035114	-1145.032654	-1145.031283
Scaled ZPE	0.238254	0.238091	0.349490	0.349302	0.348224	0.348677
H(298)	-595.027508	-595.027935	-1144.973131	-1144.970990	-1144.967467	-1144.966322
G(298)	-595.077207	-595.078005	-1145.044857	-1145.042025	-1145.039543	-1145.038181
H(0)	-595.040003	-595.040517	-1144.994550	-1144.992215	-1144.988887	-1144.987758
NImag	0	0	1	1	1	1
Del E (BW) at B3LYP/6-31G*			3.496357	5.079564	8.064627	8.488447
Del H(0) at B3LYP/6-31G*			3.965243	5.430921	7.841875	8.549980
Del H(298) at B3LYP/6-31G*			3.441398	4.785339	7.264064	7.982586
Del G(298) at B3LYP/6-31G*			17.632526	19.410075	21.468369	22.323061
H(0) at B3LYP/6-311+G**(g)	-595.220432	-595.227384	-1145.334469	-1145.331619	-1145.330049	-1145.328672
H(298) at B3LYP/6-311+G** (g)	-595.207937	-595.214802	-1145.313049	-1145.310394	-1145.308630	-1145.307237
G(298) at B3LYP/6-311+G** (g)	-595.257636	-595.264873	-1145.384776	-1145.381429	-1145.380706	-1145.379096
DelE (BW)at B3LYP/6-311+G** (g)			6.012043	7.917789	13.839408	14.419415
Del H(0) at B3LYP/6-311+G**(g)			6.480929	8.269146	13.616657	14.480949
Del H(298)at B3LYP/6-311+G** (g)			5.957586	7.623439	13.038093	13.912425
Del G(298) at B3LYP/6-311+G**(g)			20.148086	22.248175	27.243025	28.253527
Relative ΔH_{298K} in kcal/mol			**0.000000**	**1.665853**	**2.772993**	**3.647325**
Relative ΔE in kcal/mol			**0.000000**	**1.127195**	**10.486562**	**2.864142**

Catalyst 10	0.980600					
File name	*anti*-enamine	syn-enamine	10t -a-*re*	10t-a-*si*	10t-s-*re*	10t-s-*si*
B3LYP/6-31G* (g)	-555.925346	-555.925030	-1105.990047	-1105.987399	-1105.985249	-1105.984315
B3LYP/6-311+G** (g)	-556.095023	-556.095795	-1106.319199	-1106.315966	-1106.315111	-1106.313931
B3LYP/6-311+G** (sol)	-556.110742	-556.105285	-1106.341380	-1106.339285	-1106.339481	-1106.338085
ZPE (raw)	0.212616	0.212653	0.326295	0.326247	0.325395	0.325505
Thermal Corr H	0.224286	0.224316	0.346818	0.346571	0.345934	0.346073
Thermal Corr G	0.176216	0.176113	0.276944	0.277452	0.275790	0.275978
H (raw)	-555.701060	-555.700714	-1105.643229	-1105.640828	-1105.639315	-1105.638242
G (raw)	-555.749131	-555.748917	-1105.713103	-1105.709947	-1105.709459	-1105.708337
Scaled ZPE	0.208491	0.208528	0.319965	0.319918	0.319082	0.319190
H(298)	-555.705185	-555.704839	-1105.649559	-1105.647157	-1105.645628	-1105.644557
G(298)	-555.753256	-555.753042	-1105.719433	-1105.716276	-1105.715772	-1105.714652
H(0)	-555.716855	-555.716502	-1105.670082	-1105.667481	-1105.666166	-1105.665125
NImag	0	0	1	1	1	1
Del E (BW) at B3LYP/6-31G*			4.175636	5.837533	6.987946	7.573851
Del H(0) at B3LYP/6-31G*			4.794049	6.426409	7.029789	7.683381
Del H(298) at B3LYP/6-31G*			4.225337	5.732572	6.475698	7.147676
Del G(298) at B3LYP/6-31G*			18.557027	20.538031	20.720791	21.423517
H(0) at B3LYP/6-311+G**(g)	-555.886532	-555.887267	-1105.999234	-1105.996048	-1105.996029	-1105.994740
H(298) at B3LYP/6-311+G** (g)	-555.874862	-555.875604	-1105.978711	-1105.975724	-1105.975490	-1105.974172
G(298) at B3LYP/6-311+G** (g)	-555.922932	-555.923807	-1106.048585	-1106.044843	-1106.045634	-1106.044267
Del E (BW) at B3LYP/6-311+G** (g)			6.700044	8.728657	9.748988	10.489888
Del H(0) at B3LYP/6-311+G**(g)			7.318457	9.317534	9.790830	10.599418
Del H(298) at B3LYP/6-311+G** (g)			6.749933	8.624136	9.236740	10.063525
Del G(298) at B3LYP/6-311+G**(g)			21.080995	23.428967	23.481833	24.339366
Relative ΔH_{298K} in kcal/mol (g)			**0.000000**	**1.874202**	**2.020932**	**2.847717**
Relative ΔE in kcal/mol (sol)			**0.000000**	**1.314821**	**1.191578**	**2.067895**

Catalyst 11	0.980600					
File name	*anti*-enamine	*syn*-enamine	11t -s-*re*	11t -s-*si*	11t -a-*re*	11t -a-*si*
B3LYP/6-31G* (g)	-555.925226	-555.924992	-1105.991543	-1105.989990	-1105.978979	-1105.978918
B3LYP/6-311+G** (g)	-556.095608	-556.095073	-1106.321334	-1106.319877	-1106.309186	-1106.309690
B3LYP/6-311+G** (sol)	-556.107266	-556.106603	-1106.342974	-1106.343073	-1106.337298	-1106.336181
ZPE (raw)	0.213296	0.213017	0.326779	0.326995	0.327002	0.326486
Thermal Corr H	0.224790	0.224610	0.347600	0.347622	0.347529	0.347359
Thermal Corr G	0.177033	0.176674	0.276498	0.277562	0.277381	0.275373
H (raw)	-555.700437	-555.700383	-1105.643943	-1105.642368	-1105.631449	-1105.631560
G (raw)	-555.748194	-555.748318	-1105.715045	-1105.712428	-1105.701598	-1105.703545
Scaled ZPE	0.209158	0.208884	0.320439	0.320651	0.320658	0.320152
H(298)	-555.704575	-555.704516	-1105.650283	-1105.648712	-1105.637793	-1105.637894
G(298)	-555.752332	-555.752451	-1105.721385	-1105.718772	-1105.707942	-1105.709879
H(0)	-555.716069	-555.716108	-1105.671104	-1105.669339	-1105.658320	-1105.658766
NImag	0.000000	0.000000	1	1.000000	1.000000	1.000000
Del E (BW) at B3LYP/6-31G*			3.161769	4.136292	10.898962	10.936738
Del H(0) at B3LYP/6-31G*			3.659576	4.767011	11.681139	11.425930
Del H(298) at B3LYP/6-31G*			3.388743	4.374441	11.226132	11.125478
Del G(298) at B3LYP/6-31G*			16.752813	18.392376	25.188218	24.047154
H(0) at B3LYP/6-311+G**(g)	-555.886450	-555.88618	-1106.000894	-1105.999226	-1105.988528	-1105.989537
H(298) at B3LYP/6-311+G** (g)	-555.874956	-555.87459	-1105.980073	-1105.978599	-1105.968001	-1105.968664
G(298) at B3LYP/6-311+G** (g)	-555.922713	-555.92253	-1106.051175	-1106.048659	-1106.038149	-1106.040650
DelE (BW)at B3LYP/6-311+G** (g)			5.727530	6.641435	13.014171	12.698470
Del H(0) at B3LYP/6-311+G**(g)			6.225337	7.272154	13.820876	13.187662
DelH(298) at B3LYP/6-311+G** (g)			5.954253	6.879333	13.303180	12.887085
Del G(298) at B3LYP/6-311+G**(g)			19.318323	20.897268	27.378219	25.808761
Relative ΔH_{298K} in kcal/mol (g)			**0.000000**	**0.925081**	**7.575341**	**7.159246**
Relative ΔE in kcal/mol (sol)			**0.061810**	**0.000000**	**3.623365**	**4.324356**