Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

A Model Study on the Photochemical Isomerizations of Isothiazoles and Thiazoles

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Details of the present computational approach are as follows:

All the geometries were fully optimized at the CAS(10,7)/6-311G(d) level of theory. To correct the energetics for dynamic electron correlation, we have used the MP2-CAS-(10,7)/6-311++G(3df,3pd) level of theory. The CASSCF calculations were performed using the MCSCF program released in GAUSSIAN 09. See (1).

(1) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Zakrzewski, V. G.; Montgomery, Jr., J. A.; Stratmann, R. E.; Burant, J. C.; Dapprich, S.; Millam, J. M.; Daniels, A. D.; Kudin, K. N.; Strain, M. C.; Farkas, O.; Tomasi, J.; Barone, V.; Cossi, M.; Cammi, R.; Mennucci, B.; Pomelli, C.; Adamo, C.; Clifford, S.; Ochterski, J.; Petersson, G. A.; Ayala, P. Y.; Cui, Q.; Morokuma, K.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Cioslowski, J.; Ortiz, J. V.; Baboul, A. G.; Stefanov, B. B.; Liu, Liashenko, G.; Piskorz, A.; Komaromi, P.; I.; Gomperts, R.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Gonzalez, C.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Andres, J. L.; Gonzalez, C.; Head-Gordon, M.; Replogle, E. S. and Pople, J. A. Gaussian, Inc., Wallingford CT, 2013.

3-methylisothiazole (Rea-1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	0.032654	-0.174519	1.403115
6	1.064125	0.026560	0.034614
1	2.129506	0.083317	0.128270
6	0.311864	0.091055	-1.089612
7	-1.362769	-0.172982	0.493874
6	-1.093406	-0.030053	-0.767473
6	-2.195040	0.010521	-1.787401
1	-2.239428	0.983022	-2.267170
1	-3.146911	-0.183679	-1.314071
1	-2.032766	-0.731303	-2.562370
1	0.695623	0.213919	-2.083831

Hartree Fock Energies = -606.43657

MP2 Energies = -607.6832613

CI-1-A

Atomic Number	Coordinates (Angstroms) X	Y	Z
7	-0.014867	-1.166527	0.071267
6	-1.090199	-0.551890	-0.344702
16	1.243653	-0.417691	-0.840933
6	-0.843765	0.820910	0.182230
6	0.456257	1.072050	-0.156957
6	-1.805383	-0.778535	-1.653799
1	0.996456	1.993561	-0.034474
1	-1.530716	1.561114	0.547975
1	-1.267376	-1.516544	-2.237732
1	-1.931113	0.130067	-2.231575
1	-2.794589	-1.180290	-1.451608

Derivative.Coupling			
-1	-0.0310287131	-0.0202233166	-0.0554178334
-2	0.0597158069	0.0030484279	0.0208411261
-3	-0.0130175371	0.0065421395	0.0372905014
-4	-0.0016745249	0.0106968801	-0.0123703740
-5	0.0054888949	0.0118031498	-0.0022897606
-6	-0.0182238651	-0.0159063550	0.0104141795
-7	-0.0017296894	0.0006250330	-0.0010743947
-8	-0.0001339308	0.0010751756	-0.0011688505

-9	0.0007838073	0.0010017061	0.0030338442
-10	0.0019744088	0.0013203719	0.0049124434
-11	-0.0021546574	0.0000167876	-0.0041708815

Gradient.Difference

-1	0.0717501413	-0.0934716878	-0.0112427922
-2	-0.1021068283	0.0548981900	0.0145342509
-3	0.0099696717	0.0225789662	0.0245822083
-4	0.0311072882	0.0156426987	-0.0306303808
-5	-0.0099918824	0.0197276474	0.0012890850
-6	-0.0029512600	-0.0148657952	0.0068992320
-7	0.0016384801	-0.0033089314	-0.0001833584
-8	-0.0013411360	-0.0034124740	-0.0003934690
-9	-0.0021498061	0.0018561942	-0.0033947312
-10	0.0042725689	-0.0000299633	0.0014756992
-11	-0.0001972373	0.0003851553	-0.0029357436

Hartree Fock Energies = -606.2417858

MP2 Energies = -607.5008909

Int-1

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.811260
1	0.875909	0.000000	2.425260
6	-1.308120	-0.027576	2.047053
7	-1.485501	-1.093030	-0.126799
6	-1.866557	-0.073494	0.612284
6	-2.901029	0.935418	0.211146
1	-3.871094	0.497235	0.436187
1	-2.808036	1.876243	0.782420
1	-2.854191	1.128231	-0.850511
1	-1.861289	-0.111301	2.962512

Hartree Fock Energies = -606.28311

MP2 Energies = -607.562553496

TS-1

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.786853
1	0.867228	0.000000	2.414493
6	-1.306431	-0.138850	1.990376
7	-1.669572	-1.419898	-0.179419
6	-1.821272	-0.231739	0.537745
6	-2.849690	0.782081	0.098711
1	-3.817965	0.486084	0.494983

1	-2.620964	1.773499	0.470437
1	-2.919863	0.801101	-0.979782
1	-1.876631	-0.233067	2.895299

	1
	A
Frequencies --	-120.2037
Red. masses --	7.1009
Frc consts --	0.4842
IR Inten --	0.0000
-1	0.04 0.19 0.04
-2	0.02 0.14 0.03
-3	-0.01 0.31 0.06
-4	0.03 -0.16 -0.04
-5	-0.49 -0.35 0.02
-6	0.13 -0.11 -0.06
-7	0.23 0.02 -0.04
-8	0.18 0.20 -0.01
-9	0.41 -0.01 -0.08
-10	0.20 0.02 -0.04
-11	0.01 -0.27 -0.07

Hartree Fock Energies = -606.2643104

MP2 Energies = -607.540176496

Int-2

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.460998
6	1.459335	0.000000	1.318230
16	1.542664	-0.909789	-0.263189
1	-0.811082	0.158632	-0.681728
1	-0.719739	-0.016735	2.253679
6	2.529321	0.195672	2.339331
1	2.176701	0.867702	3.113768
1	2.799003	-0.748614	2.797936
1	3.412738	0.628857	1.887162
7	0.581603	1.151924	0.818742

Hartree Fock Energies = -606.3156775

MP2 Energies = -607.6003051

TS-2

Atomic	Coordinates (Angstroms)

Number	X	Y	Z
16	0.239388	-0.335732	0.142955
6	-0.343882	0.119499	1.769259
6	1.836193	0.091729	0.879402
6	1.634441	1.322815	1.773078
6	0.412662	1.334130	2.263556
1	2.451443	-0.717461	1.238349
1	2.414364	2.041595	1.944121
1	-0.482126	-0.689232	2.472776
6	-0.233519	2.323275	3.182826
1	0.446051	3.130071	3.430514
1	-0.546251	1.845075	4.107357
1	-1.122101	2.746957	2.723261

	1
	A
Frequencies --	-426.1162
Red. masses --	2.3817
Frc consts --	0.2548
IR Inten --	0.0000
-1	0.03 -0.05 0.06
-2	-0.19 0.12 -0.03
-3	0.12 0.12 -0.14
-4	0.00 -0.07 0.02
-5	-0.03 -0.05 0.00
-6	0.41 0.20 -0.47
-7	-0.01 -0.09 0.17
-8	-0.61 0.19 -0.04
-9	0.03 -0.02 0.02
-10	0.06 -0.04 0.02
-11	0.00 0.00 0.01
-12	0.05 0.02 0.01

Hartree Fock Energies = -606.2992933

MP2 Energies = -607.5504956

Int-3

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	0.109781	0.086736	1.435380
6	1.226924	0.006462	0.101628
1	2.286490	0.038722	0.218871
6	0.414870	-0.050093	-1.115882
7	-1.306516	-0.006413	0.582403
6	-1.001126	-0.083504	-0.792587
6	-2.121449	0.018474	-1.766962
1	-2.456498	1.049887	-1.873597
1	-2.970702	-0.563888	-1.427243
1	-1.822356	-0.338138	-2.746790

1	0.804327	-0.060193	-2.112062

Hartree Fock Energies = -606.22343521

MP2 Energies = -607.4693847

TS-3

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	0.000000	0.000000	0.000000
7	0.000000	0.000000	1.844594
6	1.142065	0.000000	2.365784
6	2.343151	0.005095	1.474255
6	1.987424	-0.082272	0.198613
1	3.338704	0.065825	1.877819
1	2.578313	-0.089712	-0.696267
6	1.324119	-0.007963	3.853489
1	1.888951	0.867624	4.160799
1	1.895022	-0.882245	4.153000
1	0.368727	-0.013201	4.355106

	1
	A
Frequencies --	-1144.8381
Red. masses --	7.6366
Frc consts --	1.7548
IR Inten --	0.0000
-1	0.24 -0.02 -0.17
-2	-0.01 0.00 0.35
-3	-0.04 0.02 0.11
-4	-0.09 -0.01 -0.07
-5	-0.50 0.06 -0.01
-6	-0.01 -0.21 -0.31
-7	-0.59 0.00 -0.07
-8	0.05 0.00 0.04
-9	0.03 0.00 0.08
-10	0.03 -0.01 0.08
-11	0.03 -0.01 -0.01

Hartree Fock Energies = -606.2108551

MP2 Energies = -607.4454028

CI-1-B

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	1.135152	0.090072	0.709603
6	0.263126	-0.206086	2.414214
1	0.788761	0.184582	3.268314
6	-0.989260	0.431593	1.981812

7	-1.361924	-0.059807	0.546717
6	-2.125504	-0.314506	1.491890
6	-3.446617	-0.928528	1.768503
1	-3.859327	-1.341852	0.857921
1	-4.126922	-0.185568	2.167557
1	-3.338528	-1.715431	2.504771
1	-1.056003	1.500859	2.114276

Derivative.Coupling

-1	-0.0056417401	0.0013959451	-0.0053486281
-2	0.0002657428	-0.0082626654	0.0115884699
-3	-0.0016352432	0.0046684545	-0.0015184410
-4	0.0022845778	-0.0011540443	-0.0017158515
-5	0.0021457845	0.0037381425	-0.0028624443
-6	0.0015297064	0.0001639875	0.0007519343
-7	0.0001976671	-0.0005825556	-0.0001374855
-8	0.0000141819	-0.0000135491	0.0000410774
-9	0.0001619579	0.0000766439	-0.0000641869
-10	-0.0000673964	0.0000250541	-0.0001033651
-11	0.0007447614	-0.0000554131	-0.0006310792

Gradient.Difference

-1	0.0197229133	-0.0143254056	0.0334825334
-2	0.0235974049	0.0202592187	-0.0404642010
-3	0.0006265095	-0.0041863556	0.0012173015
-4	-0.0204608759	-0.0072738433	-0.0096275327
-5	-0.0167871331	0.0112638465	0.0109705580
-6	-0.0072434530	-0.0014742860	0.0018507374
-7	0.0013380536	-0.0027117710	0.0012574759
-8	-0.0001954604	-0.0001204308	-0.0000454081
-9	0.0002125963	0.0001782404	-0.0000657384
-10	-0.0010872125	-0.0005334363	0.0002167299
-11	0.0002766573	-0.0010757769	0.0012075441

Hartree Fock Energies = -606.2492028

MP2 Energies = -607.5320806

Int-4

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.080153
6	1.336700	0.000000	1.703031
16	-1.409575	-0.005800	1.885654
1	1.373266	-0.296120	2.736828
6	2.432960	0.761248	1.125421
7	2.501568	-0.441934	0.831856
6	3.107002	2.069539	0.942198
1	4.030516	1.932054	0.395227
1	3.320169	2.520573	1.903398
1	2.465436	2.746812	0.391079

Hartree Fock Energies = -606.37895

MP2 Energies = -607.638803

TS-4

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.697948
1	0.954272	0.000000	2.207428
6	-1.010307	0.043117	2.577708
7	-2.544660	-0.194563	2.079715
6	-2.519069	0.822113	1.498838
6	-2.657424	2.111869	0.821028
1	-3.134240	1.947519	-0.135109
1	-3.239391	2.784822	1.434571
1	-1.665322	2.499722	0.642432
1	-1.044323	0.143050	3.636972

	1
	A
Frequencies --	-479.5189
Red. masses --	3.3823
Frc consts --	0.0046
IR Inten --	0.0000
-1	0.02 -0.02 0.00
-2	-0.03 0.03 -0.08
-3	-0.06 -0.03 -0.02
-4	-0.21 0.33 -0.18
-5	-0.20 -0.23 -0.06
-6	0.34 -0.01 0.24
-7	0.10 -0.05 0.10
-8	-0.04 -0.24 0.20
-9	0.08 -0.07 0.10
-10	-0.01 0.12 -0.11
-11	-0.16 0.55 -0.20

Hartree Fock Energies -606.3320194

MP2 Energies = -607.5846164

CI-1-C

Atomic Number	Coordinates (Angstroms) X	Y	Z

16	0.461010	-0.116097	1.668663
6	1.372068	-0.165819	0.221620
1	2.423352	0.009132	0.133831
6	0.311082	0.168106	-0.770672
7	-0.909068	0.233599	0.675628
6	-0.866572	-0.571439	-0.518586
6	-2.072970	-0.695470	-1.385346
1	-1.847777	-1.314171	-2.246280
1	-2.410770	0.275312	-1.741115
1	-2.885910	-1.153758	-0.836026
1	0.441221	0.917735	-1.535508

Derivative.Coupling

-1	0.0081684591	-0.0020044611	-0.0060812511
-2	0.0158774750	-0.0138568891	0.0365607521
-2	0.0005634909	-0.0045702583	-0.0014681057
-4	-0.0801350652	0.0178983312	0.0188993811
-5	0.0408887290	0.0413099507	-0.0183577571
-6	0.0152862371	-0.0469518235	-0.0347101491
-7	0.0023291149	-0.0001595366	-0.0002896617
-8	-0.0002259922	-0.0000796171	0.0000405935
-9	-0.0006840508	0.0005488208	-0.0003059272
-10	-0.0002315401	-0.0001468844	-0.0000053493
-11	-0.0018368577	0.0080123673	0.0057174745

Gradient.Difference

-1	0.0205064668	-0.0334898987	0.0424744202
-2	0.0015703130	0.0022967464	-0.0187507420
-3	0.0008496831	0.0045888287	0.0018206007
-4	0.0250456859	0.0578372982	0.0375625333
-5	0.0308646654	0.0548824238	-0.1171533842
-6	-0.0696983195	-0.1040782057	0.0395446824
-7	0.0022200063	0.0097764041	0.0018326058
-8	0.0004026849	-0.0001017252	0.0000033350
-9	-0.0028937246	0.0015524337	-0.0012752512
-10	0.0005493611	-0.0001338007	0.0000306457
-11	-0.0094168226	0.0068694954	0.0139105544
-1	0.0205064668	-0.0334898987	0.0424744202
-2	0.0015703130	0.0022967464	-0.0187507420
-3	0.0008496831	0.0045888287	0.0018206007
-4	0.0250456859	0.0578372982	0.0375625333
-5	0.0308646654	0.0548824238	-0.1171533842
-6	-0.0696983195	-0.1040782057	0.0395446824
-7	0.0022200063	0.0097764041	0.0018326058
-8	0.0004026849	-0.0001017252	0.0000033350
-9	-0.0028937246	0.0015524337	-0.0012752512
-10	0.0005493611	-0.0001338007	0.0000306457
-11	-0.0094168226	0.0068694954	0.0139105544

Hartree Fock Energies = -606.2077217

MP2 Energies = -607.510863

Pro-1

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	-0.013255	-0.149951	0.080561
6	-0.112445	-0.055836	1.840236
6	1.136769	0.069858	2.340467
1	-1.045244	-0.093118	2.362847
1	1.381302	0.150574	3.380435
7	2.159406	0.097250	1.411998
6	1.724292	-0.000047	0.223612
6	2.604202	-0.022466	-0.990074
1	2.633738	-1.017051	-1.422491
1	3.606197	0.259203	-0.698352
1	2.248345	0.662428	-1.751125

Hartree Fock Energies = -606.44094117

MP2 Energies = -607.7278863

4-methylisothiazole (Rea-2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	-0.098094	0.049277	1.512757
6	1.191003	0.085992	0.364524
1	2.214999	0.161818	0.670927
6	0.697648	0.006952	-0.897675
7	-1.282241	-0.067279	0.348118
6	-0.742983	-0.080216	-0.829691
1	-1.383700	-0.151438	-1.691106
6	1.484228	-0.004735	-2.178625
1	1.419978	-0.970438	-2.668386
1	2.530168	0.206250	-1.997953
1	1.111052	0.739810	-2.873009

Hartree Fock Energies = -606.43657

MP2 Energies = -607.6832613

CI-2-A

Atomic Number	Coordinates (Angstroms) X	Y	Z
7	0.109397	-1.298837	0.100425

6	-0.870966	-0.500663	-0.299741
16	1.204572	-0.362753	-1.068362
6	-0.681626	0.929641	0.138156
6	0.535100	1.189567	-0.339169
1	-1.400665	-0.681129	-1.236087
1	1.122909	2.087518	-0.303832
6	-1.739123	1.808113	0.720346
1	-2.503592	1.988993	-0.032965
1	-1.348143	2.768481	1.029397
1	-2.229897	1.338532	1.564352

Derivative.Coupling

-1	0.0223245274	-0.0060349581	0.0189251739
-2	-0.0461154519	0.0183362788	0.0035545342
-3	0.0148215545	-0.0082963901	-0.0252697595
-4	-0.0005089053	-0.0129179984	-0.0042775129
-5	-0.0019149370	-0.0070596010	0.0086491128
-6	0.0153094457	0.0111454832	0.0012275660
-7	-0.0001705219	0.0014701146	-0.0003080998
-8	-0.0029993069	0.0047031572	-0.0016426822
-9	-0.0000212407	-0.0003150868	-0.0004392833
-10	-0.0008259907	-0.0004996291	-0.0001236778
-11	0.0001008267	-0.0005313703	-0.0002953714

Gradient.Difference

-1	0.0068522220	-0.0356401950	-0.0352821348
-2	-0.0749871914	0.0243358617	0.0420908091
-3	0.0656585547	0.0432248620	0.0257638442
-4	0.0392007712	-0.0063610796	-0.0653286447
-5	-0.0208273114	-0.0199430745	0.0181974119
-6	-0.0089923946	-0.0071007209	0.0230726918
-7	0.0000179035	-0.0003143086	-0.0000017211
-8	-0.0067441279	0.0038725724	-0.0062313704
-9	0.0000337712	-0.0004884110	-0.0011055358
-10	-0.0000683948	-0.0010204506	-0.0005242807
-11	-0.0001438027	-0.0005650559	-0.0006510695

Hartree Fock Energies = -606.2074039
MP2 Energies = -607.4554095

Int-5

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.530220
6	1.314824	0.000000	-0.217408
16	1.904293	-0.039520	1.495807
7	0.529675	1.082105	2.144482
1	1.933972	0.070834	-1.088335
6	-1.187396	0.131738	-0.897392
1	-1.722568	1.051409	-0.684650

1	-0.891527	0.143845	-1.939107
1	-1.878322	-0.692673	-0.751377
1	-0.486067	-0.807886	2.067633

Hartree Fock Energies = -606.2706739

MP2 Energies = -607.5584267

TS-5

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.490485
6	1.462162	0.000000	1.512085
16	1.774687	-0.481330	-0.194189
1	-0.458341	0.724744	-0.648433
7	0.650843	1.229902	1.489485
1	2.112145	-0.173806	2.348610
6	-1.060378	-0.469429	2.434798
1	-0.759348	-0.271071	3.456631
1	-1.986775	0.065023	2.250852
1	-1.245274	-1.530721	2.317650

1

Frequencies -- -186.6819

Red. masses -- 7.8835

Frc consts -- 0.4265

IR Inten -- 0.0000

Atom AN	X	Y	Z
-1	0.25	0.54	0.27
-2	-0.02	-0.20	0.12
-3	-0.02	-0.04	0.02
-4	0.02	-0.03	0.00
-5	-0.30	0.02	0.14
-6	0.13	-0.15	-0.47
-7	0.01	0.20	0.05
-8	-0.07	-0.07	0.11
-9	-0.08	0.00	0.10
-10	-0.02	-0.01	0.04
-11	-0.03	-0.06	0.01

Hartree Fock Energies = -606.2479881

MP2 Energies = -607.526432

Int-6

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.465292
6	1.456450	0.000000	1.297720
16	1.586748	-0.933307	-0.255352
1	-0.798921	0.185103	-0.690219
7	0.626058	1.124926	0.832525
1	2.220336	0.143890	2.036447
6	-0.993108	-0.038854	2.575378
1	-0.588483	0.444400	3.457022
1	-1.897572	0.484764	2.287320
1	-1.250591	-1.060394	2.828563

Hartree Fock Energies = -606.3063101

MP2 Energies = -607.557932

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TS-6

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.814132
1	1.002826	0.000000	2.209839
6	-1.003544	0.005324	2.681343
7	-2.236687	-0.003098	2.035066
6	-2.035076	-0.006401	0.835718
1	-2.773859	-0.014965	0.057285
6	-0.936767	0.006451	4.173280
1	-1.427725	-0.873556	4.574830
1	0.088722	0.015977	4.518097
1	-1.443595	0.877591	4.574351

	1
Frequencies --	--189.9222
Red. masses --	3.7221
Frc consts --	0.8034
IR Inten --	0.0000

Atom AN	X	Y	Z
-1	0.28	0.34	0.00

-2	0.08	-0.18	0.00
-3	-0.03	-0.19	0.00
-4	-0.03	-0.05	0.00
-5	-0.30	-0.16	0.00
-6	-0.40	-0.46	0.00
-7	-0.30	-0.39	-0.01
-8	-0.01	0.03	0.00
-9	-0.02	0.04	0.00
-10	0.03	0.03	0.00
-11	-0.02	0.04	0.00

Hartree Fock Energies = -606.3612884
MP2 Energies = -607.6188083

Pro-2

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.735107
6	1.244755	0.000000	2.219483
1	-0.916465	0.001223	2.287870
6	1.653783	0.001837	3.659200
7	2.256057	-0.000109	1.253184
6	1.733081	-0.000777	0.061082
1	2.324390	0.004108	-0.833289
1	2.245196	0.882883	3.883613
1	2.264628	-0.866591	3.879739
1	0.790989	-0.008309	4.313336

Hartree Fock Energies = --606.452517
MP2 Energies = -607.7277401

Int-7

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	-0.089614	-0.111615	1.509275
6	1.246139	-0.254918	0.393237
1	2.220981	0.067220	0.710936
6	0.688164	0.029689	-0.936875
7	-1.329957	0.085922	0.417958
6	-0.758854	0.142896	-0.862709
1	-1.419424	0.081581	-1.698792
6	1.484722	-0.008161	-2.196958

1	1.874785	-1.006968	-2.386610
1	2.339044	0.662511	-2.137417
1	0.886074	0.287834	-3.052162

Hartree Fock Energies = -606.224+D1108

MP2 Energies = -607.4693847

TS-7

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.717022
1	0.965973	0.000000	2.192665
6	-1.103646	-0.042678	2.514973
7	-2.832856	0.058192	0.790425
6	-2.489611	-0.008650	1.975714
1	-3.289697	-0.017895	2.711094
6	-0.950661	-0.110387	4.018744
1	-0.399461	-0.996719	4.311483
1	-1.911867	-0.151531	4.514737
1	-0.421053	0.755310	4.399193

1

A

Frequencies -- -173.2358

Red. masses -- 7.6915

Frc consts -- 0.0665

IR Inten -- 0.0000

-1	0.07	-0.05	0.00
-2	0.00	0.39	0.00
-3	-0.01	0.11	0.02
-4	-0.01	0.48	-0.03
-5	-0.01	0.33	0.01
-6	-0.06	-0.58	0.00
-7	-0.03	-0.26	0.01
-8	-0.01	0.04	0.00
-9	-0.06	-0.17	-0.01
-10	-0.04	0.40	-0.01
-11	-0.01	0.02	-0.01

Hartree Fock Energies = -606.20359112

MP2 Energies = -607.4393847

CI-2-B

Atomic Coordinates (Angstroms)

Number	X	Y	Z
16	-0.036197	1.365744	0.885219
6	0.133967	-0.448453	1.554265
1	1.120411	-0.715773	1.893521
6	-0.968155	-0.307715	2.527423
7	-2.127832	0.468435	1.813838
6	-2.291982	-0.721163	2.143893
1	-3.087777	-1.438858	2.169349
6	-0.629664	0.058451	3.952052
1	-0.340096	-0.833139	4.500825
1	-1.485039	0.499153	4.449202
1	0.184690	0.769671	3.987456

Derivative.Coupling			
-1	-0.0106415051	0.0050784046	0.0022561558
-2	0.0043989080	-0.0170293904	-0.0026482516
-3	-0.0010091059	0.0029916963	0.0044331909
-4	0.0009858006	0.0017406894	-0.0024505356
-5	0.0037850241	0.0064574610	-0.0009145668
-6	0.0019234445	-0.0005668877	-0.0000917846
-7	-0.0000066587	0.0005855168	-0.0005099438
-8	0.0008113463	0.0010995661	-0.0000208859
-9	-0.0001536584	-0.0000486961	-0.0003161247
-10	-0.0001540245	-0.0000247297	0.0000190499
-11	0.0000604290	-0.0002836303	0.0002436963
Gradient.Difference			
-1	-0.0288973129	0.0248519047	0.0104082625
-2	-0.0029628360	-0.0459659912	0.0062469632
-3	0.0003294207	0.0018745444	0.0018394437
-4	0.0244072174	0.0028712123	0.0036380889
-5	0.0050784386	0.0078141924	-0.0240775664
-6	0.0047775504	0.0059963129	-0.0011172033
-7	-0.0006096861	0.0022059755	0.0030018443
-8	-0.0009671527	0.0008351681	0.0010534198
-9	-0.0005627227	-0.0007153215	-0.0006973730
-10	0.0004130287	0.0004028438	0.0007312806
-11	-0.0010059455	-0.0001708413	-0.0010271604

Hartree Fock Energies = -606.2382353957

MP2 Energies = -607.4863219

Int-8

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.624005
1	0.948533	0.000000	2.138886
6	-1.195612	0.018117	2.512219
7	-2.285742	1.011604	2.138456

6	-2.512516	-0.194765	1.949704
1	-3.275851	-0.851368	1.584538
6	-0.912635	-0.156321	3.988989
1	-1.831529	-0.147233	4.560750
1	-0.281433	0.646293	4.358080
1	-0.405436	-1.096797	4.181829

Hartree Fock Energies = -606.36582

MP2 Energies = -607.631414

TS-8

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	-1.825689	-0.444276	-0.001151
6	-0.058981	-0.856342	0.003254
1	0.098590	-1.922831	0.007317
6	1.013523	-0.076036	-0.003068
7	0.664234	1.271694	-0.000030
6	-0.549563	1.347789	0.000984
1	-1.139847	2.244103	0.005372
6	2.451292	-0.479953	-0.000367
1	2.952402	-0.089904	0.879090
1	2.554171	-1.556987	-0.005882
1	2.958451	-0.080580	-0.872093

	1		
	A		
Frequencies --	-89.9222		
Red. masses --	7.6915		
Frc consts --	0.0665		
IR Inten --	0.0000		
-1	0.28	0.34	0.00
-2	0.08	-0.18	0.00
-3	-0.03	-0.19	0.00
-4	-0.03	-0.05	0.00
-5	-0.30	-0.16	0.00
-6	-0.40	-0.46	0.00
-7	-0.30	-0.39	-0.01
-8	-0.01	0.03	0.00
-9	-0.02	0.04	0.00
-10	0.03	0.03	0.00
-11	-0.02	0.04	0.00

Hartree Fock Energies = - -606.3612884

MP2 Energies = -607.6188083

CI-2-C

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	0.106489	0.580884	1.412231
6	1.210511	-0.353822	0.490228
1	2.263909	-0.412758	0.674360
6	0.561554	-0.288169	-0.853917
7	-0.811828	0.753765	-0.050610
6	-0.838554	-0.494052	-0.743971
1	-1.501345	-0.578329	-1.585807
6	1.353961	0.001045	-2.091729
1	2.052162	-0.814020	-2.266919
1	1.932845	0.910766	-1.981407
1	0.716042	0.097273	-2.960043

Derivative.Coupling

-1	0.0031036085	-0.0097866393	0.0199395200
-2	0.0062665440	0.0001912451	0.0235628975
-3	0.0004052663	-0.0012530092	0.0002177896
-4	-0.0379521352	0.0521583937	-0.0056883308
-5	0.0675659386	0.0032486343	-0.0513338167
-6	-0.0397641658	-0.0574469126	0.0100308926
-7	0.0022960257	0.0017828261	-0.0004373623
-8	-0.0019562099	0.0131226713	0.0023119419
-9	-0.0016069474	-0.0014393531	0.0024425715
-10	0.0016376535	-0.0002952955	-0.0016266430
-11	0.0000044218	-0.0002825607	0.0005805398

Gradient.Difference

-1	-0.0141288398	-0.0237089412	0.0337656679
-2	0.0360380727	-0.0132667567	-0.0506998379
-3	0.0025479519	0.0029638511	-0.0031418920
-4	-0.0503431875	0.0217865067	-0.0386032248
-5	-0.0000411734	0.0059662223	-0.0007935087
-6	-0.0430729052	-0.0133087090	0.0903200272
-7	0.0508354303	0.0396090641	-0.0137012460
-8	0.0027063731	-0.0043864403	-0.0122908012
-9	0.0220604363	-0.0172385333	-0.0085737466
-10	-0.0066021585	0.0015837365	0.0037185620

Hartree Fock Energies = -606.241228435

MP2 Energies = -607.4914385

5-methylisothiazole (Rea-3)

Atomic Number	Coordinates (Angstroms) X	Y	Z

16	-0.120769	0.000053	1.428459
6	1.139912	-0.000006	0.240997
6	2.599064	-0.000004	0.605049
6	0.564747	-0.000009	-0.990972
7	-1.358938	-0.000040	0.318123
6	-0.867966	0.000011	-0.882836
1	-1.543481	0.000026	-1.718870
1	1.101345	-0.000036	-1.920414
1	2.742019	-0.000043	1.678431
1	3.094061	0.877677	0.206365
1	3.094099	-0.877629	0.206290

Hartree Fock Energies = -606.4334332
MP2 Energies = -607.6728378

CI-3-A

Atomic Number	Coordinates (Angstroms) X	Y	Z
7	-1.113751	-1.554550	0.078114
6	-0.693266	-0.507087	-0.753713
16	1.150052	-0.325861	-0.600486
6	-0.838457	0.868724	-0.123695
6	0.446160	1.176870	0.084376
1	-0.999502	-0.588979	-1.789941
6	1.178044	2.325099	0.687680
1	-1.743755	1.388687	0.126166
1	1.851675	2.776554	-0.032506
1	1.768125	1.998331	1.536905
1	0.480309	3.082374	1.025324

Derivative.Coupling

-1	0.0005630029	0.0012591380	0.0014648463
-2	-0.0004759385	-0.0017552069	-0.0021937780
-3	-0.0006242183	0.0000901783	0.0000967466
-4	-0.0003991374	-0.0000655960	0.0007314564
-5	0.0001445030	-0.0003345254	0.0001464750
-6	0.0007944053	0.0009097715	-0.0001866503
-7	-0.0000104580	0.0000372640	-0.0000443210
-8	0.0000653950	-0.0000997586	-0.0000122182
-9	-0.0000153819	-0.0000016254	0.0000012247
-10	-0.0000324423	-0.0000405522	-0.0000072465
-11	-0.0000097299	0.0000009127	0.0000034650

Gradient.Difference

-1	-0.0036086154	0.0041959266	-0.0015086848
-2	0.0001441418	-0.0050986359	0.0011373752
-3	0.0045276501	0.0031959255	-0.0013015743
-4	-0.0013034310	-0.0007570257	0.0016865405
-5	0.0012035100	-0.0017111087	-0.0000604341

-6	-0.0002546684	-0.0000731664	0.0005173060
-7	-0.0005724140	0.0004632679	-0.0002173722
-8	-0.0001001395	-0.0001033487	-0.0002123487
-9	-0.0000118944	-0.0001025874	-0.0000145043
-10	-0.0000824755	-0.0001474207	-0.0001109150
-11	0.0000583362	0.0001381735	0.0000846117

Hartree Fock Energies = -606.1977846
MP2 Energies = -607.4533379

Int-9

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.522888
6	1.309530	0.000000	-0.247312
16	1.912898	-0.061430	1.472697
7	0.549441	1.066862	2.141915
1	-0.485952	-0.807837	2.058923
1	-0.838681	0.105696	-0.661281
6	2.170043	0.074816	-1.461587
1	2.838186	-0.777160	-1.523732
1	1.558479	0.091207	-2.355725
1	2.776990	0.973609	-1.441126

Hartree Fock Energies = -606.27221

MP2 Energies = -607.5533122

TS-9

Atomic Number	Coordinates (Angstroms) X	Y	Z
7	0.000000	0.000000	0.000000
16	0.000000	0.000000	1.698105
6	1.954107	0.000000	1.956882
6	2.032564	-1.035408	1.079714
6	0.701310	-1.216664	0.355686
6	3.056337	0.425584	2.879886
1	2.848612	-1.746946	1.016376
1	0.327103	-2.151600	-0.025381
1	2.757603	0.316416	3.920309
1	3.973931	-0.144982	2.747192
1	3.304343	1.473558	2.743274

	1
	A
Frequencies --	-113.9180
Red. masses --	4.0007
Frc consts --	0.2548

IR Inten	--	0.0000	
-1	-0.07	-0.03	0.01
-2	0.12	-0.05	0.03
-3	-0.02	0.18	-0.08
-4	-0.18	-0.01	0.07
-5	0.04	0.04	-0.16
-6	-0.04	-0.01	0.03
-7	-0.39	-0.28	0.45
-8	0.05	0.00	-0.06
-9	-0.24	0.25	0.00
-10	-0.20	-0.31	0.27
-11	0.30	-0.11	-0.10

Hartree Fock Energies = -606.29406846

MP2 Energies = -607.5287031

Int-10

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.466092
6	1.454113	0.000000	1.324049
16	1.565238	-0.910550	-0.236910
1	-0.718665	-0.017040	2.259738
7	0.584930	1.151948	0.826748
1	2.210741	0.155028	2.066631
6	-1.119098	0.199593	-0.966267
1	-1.604382	-0.743140	-1.190942
1	-1.853928	0.873289	-0.539813
1	-0.753237	0.632576	-1.888847

Hartree Fock Energies = -606.3157116

MP2 Energies = -607.5990554

TS-10

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.722796
6	1.368780	0.000000	2.103113
6	-1.022069	0.754710	2.520952
1	1.688513	0.457132	3.019797
6	1.556802	0.853324	0.285189
7	2.178896	-1.014602	1.770797
1	2.334322	0.276321	-0.223033
1	-1.084170	1.792488	2.209597
1	-0.799472	0.713158	3.580439
1	-2.000099	0.310858	2.367229

	1		
	A		
Frequencies --	-1097.4349		
Red. masses --	9.9430		
Frc consts --	0.2548		
IR Inten --	0.0000		
-1	-0.01	-0.04	-0.03
-2	0.19	0.19	0.03
-3	-0.21	-0.31	0.46
-4	0.02	0.01	0.00
-5	-0.11	-0.34	0.42
-6	0.01	0.21	-0.36
-7	0.03	0.06	-0.07
-8	-0.10	-0.21	-0.07
-9	-0.08	-0.02	-0.03
-10	-0.01	0.03	0.00
-11	0.08	-0.10	-0.04

Hartree Fock Energies = -606.2902766

MP2 Energies = -607.5414563

Int-11

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	0.061966	-0.014480	0.118191
7	0.013884	-0.065196	1.774642
6	1.337804	-0.095617	2.236792
1	1.494524	-0.315156	3.273364
6	1.807108	-0.132906	-0.140941
6	2.372628	-0.097455	1.220260
1	3.421268	-0.130062	1.434960
6	2.434999	0.555062	-1.317632
1	3.453309	0.208447	-1.454194
1	2.462595	1.635371	-1.184742
1	1.891954	0.346208	-2.232431

Hartree Fock Energies = -606.22425

MP2 Energies = -607.4840608

TS-11

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	0.000000	0.000000	0.000000
7	0.000000	0.000000	2.253609
6	1.227243	0.000000	2.457105
1	1.595230	0.027124	3.477215
6	1.708183	-0.002435	-0.070340

6	2.145556	-0.007782	1.320292
1	3.207852	-0.024470	1.484771
6	2.706731	-0.017365	-1.200223
1	2.582956	-0.903880	-1.809949
1	3.720390	-0.003902	-0.819682
1	2.573599	0.843821	-1.843208

	1
	A
Frequencies --	-168.5835
Red. masses --	11.0167
Frc consts --	0.0382
IR Inten --	0.0000

Atom AN	X	Y	Z
-1	0.02	-0.02	0.00
-2	-0.03	0.03	-0.08
-3	-0.06	-0.03	-0.02
-4	-0.21	0.33	-0.18
-5	-0.20	-0.23	-0.06
-6	0.34	-0.01	0.24
-7	0.10	-0.05	0.10
-8	-0.04	-0.24	0.20
-9	0.08	-0.07	0.10
-10	-0.01	0.02	-0.01
-11	-0.16	0.05	-0.02

Hartree Fock Energies = -606.2076883

MP2 Energies = -607.4243268

CI-3-B

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	-0.798907	0.046686	0.424071
6	0.205353	0.689216	1.940837
6	1.449590	-0.099113	2.183628
6	-0.891731	0.659134	2.927631
7	-2.241111	1.042944	2.386528
6	-2.038576	-0.181823	2.608318
1	-2.613095	-1.081122	2.688499
1	-0.686930	0.971398	3.938838
1	1.910537	0.201766	3.119710
1	2.179136	0.063245	1.397235
1	1.232713	-1.165950	2.227144

Derivative.Coupling			
-1	0.0225249043	0.0082924191	-0.0026069813
-2	-0.0175312675	-0.0183777633	-0.0211869606
-3	0.0044493750	0.0024661985	0.0009218763
-4	-0.0034924048	0.0021539653	0.0040279261
-5	-0.0020967351	-0.0042280255	0.0077687034
-6	-0.0047105933	0.0100528895	0.0109352112
-7	0.0013604549	-0.0012842813	-0.0010827281
-8	-0.0000995784	0.0001340843	0.0000809183
-9	0.0002376070	-0.0003079544	0.0004689790
-10	-0.0006432984	-0.0002587586	0.0003312337
-11	0.0000015365	0.0013572265	0.0003418222
Gradient.Difference			
-1	-0.0130258416	0.0045751240	0.0094349447
-2	0.0186442955	0.0084261759	0.0029048793
-3	-0.0073789181	-0.0037796965	0.0035975925
-4	0.0032759703	0.0034381648	-0.0074181645
-5	-0.0046050935	0.0050257142	-0.0071103692
-6	0.0061326298	-0.0181693257	-0.0054895610
-7	-0.0020143006	0.0007427148	0.0044298515
-8	-0.0006954852	0.0007616760	-0.0002420696
-9	0.0010847190	0.0003924490	0.0004783833
-10	-0.0004078115	0.0002436671	0.0008157935
-11	-0.0010101642	-0.0016566636	-0.0014012805

Hartree Fock Energies = -606.2480603

MP2 Energies = -607.5043702

Int-12

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	-0.798907	0.046686	0.424071
6	0.205353	0.689216	1.940837
6	1.449590	-0.099113	2.183628
6	-0.891731	0.659134	2.927631
7	-2.241111	1.042944	2.386528
6	-2.038576	-0.181823	2.608318
1	-2.613095	-1.081122	2.688499
1	-0.686930	0.971398	3.938838
1	1.910537	0.201766	3.119710
1	2.179136	0.063245	1.397235
1	1.232713	-1.165950	2.227144

Hartree Fock Energies = -606.36849

MP2 Energies = -607.6345502

TS-12

Atomic Number	Coordinates (Angstroms) X	Y	Z

16	0.000000	0.000000	0.000000
7	0.000000	0.000000	2.253609
6	1.227243	0.000000	2.457105
1	1.595230	0.027124	3.477215
6	1.708183	-0.002435	-0.070340
6	2.145556	-0.007782	1.320292
1	3.207852	-0.024470	1.484771
6	2.706731	-0.017365	-1.200223
1	2.582956	-0.903880	-1.809949
1	3.720390	-0.003902	-0.819682
1	2.573599	0.843821	-1.843208

1

A

Frequencies -- -168.5835

Red. masses -- 11.0167

Frc consts -- 0.0382

IR Inten -- 0.0000

Atom AN	X	Y	Z
-1	0.02	-0.02	0.00
-2	-0.03	0.03	-0.08
-3	-0.06	-0.03	-0.02
-4	-0.21	0.33	-0.18
-5	-0.20	-0.23	-0.06
-6	0.34	-0.01	0.24
-7	0.10	-0.05	0.10
-8	-0.04	-0.24	0.20
-9	0.08	-0.07	0.10
-10	-0.01	0.02	-0.01
-11	-0.16	0.05	-0.02

Hartree Fock Energies = -606.2076883

MP2 Energies = -607.4243268

CI-3-C

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	2.53943517	0.06296386	1.47388399
6	1.17816443	0.30940437	1.91409328
6	0.07314800	0.29824800	1.07481200
1	1.08825443	0.45704537	2.97840328
1	-0.80169200	0.58955400	1.64182900

16	1.06871680	0.05755876	-1.51544462
6	-0.03300100	-0.05780700	-0.29908700
1	3.21824110	-0.27619635	2.24033340
6	-1.35118400	-0.08704400	-0.94570200
6	-2.55147600	-0.35205400	-0.27708600
6	-3.75013400	-0.39314000	-0.96525200
6	-3.77583200	-0.14373400	-2.32970500
6	-2.59745100	0.12208400	-3.00913400
6	-1.39490000	0.12639500	-2.32498000
1	-2.54773400	-0.54790900	0.77977400
1	-4.66306900	-0.61208700	-0.44079400
1	-4.71047900	-0.16552700	-2.86142700
1	-2.61514800	0.30715200	-4.06811000
1	-0.47181700	0.30155100	-2.84613600

Derivative.Coupling

-1	-0.0246967984	0.0158850843	0.0625683365
-2	-0.0116408539	-0.0090099147	-0.0598697420
-3	0.0547842495	-0.0044948845	0.0169057367
-4	-0.0004941651	-0.0008817539	-0.0077533578
-5	0.0000553318	-0.0043088158	0.0002679771
-6	0.0021603923	-0.0003592425	-0.0148242559
-7	-0.0259784698	0.0031482695	0.0220516658
-8	0.0003991612	0.0031516410	0.0006388459
-9	0.0027564968	-0.0032766864	-0.0210974834
-10	0.0039026445	-0.0014353270	0.0026337290
-11	0.0017541850	0.0026346603	-0.0019960725
-12	-0.0010247150	-0.0000265318	-0.0009344947
-13	-0.0007014218	-0.0013987908	0.0007038031
-14	-0.0016989549	0.0005629016	0.0017974440
-15	0.0001651310	-0.0008269073	-0.0004594334
-16	0.0003624622	0.0000935067	0.0003076520
-17	0.0000571577	-0.0000434781	-0.0000229469
-18	0.0000412309	-0.0000268242	-0.0000194734
-19	-0.0002030639	0.0006130935	-0.0008979300

Gradient.Difference

-1	-0.0030925511	-0.0526171809	0.0014928103
-2	0.0123883600	0.0286907175	0.0041948971
-3	-0.0068435448	0.0128271439	-0.0027081839
-4	-0.0035470402	-0.0225536781	0.0060334945
-5	-0.0004832348	-0.0002559451	-0.0003360741

-6	-0.0094408400	-0.0011892424	0.0033796404
-7	0.0063877682	0.0070574888	-0.0030588281
-8	-0.0013988727	-0.0047112655	-0.0010664250
-9	0.0029804494	0.0348801168	-0.0094600145
-10	0.0040144353	0.0021192897	0.0050891086
-11	0.0026078957	-0.0021831475	-0.0042887070
-12	-0.0028679629	0.0001342860	-0.0002996784
-13	0.0006595267	-0.0000647098	0.0025236518
-14	-0.0012231593	-0.0019199726	-0.0011824050
-15	-0.0005483758	0.0002433813	0.0003490370
-16	0.0003512122	-0.0001960344	0.0003017639
-17	0.0000032312	-0.0000512551	0.0000046717
-18	0.0001336644	0.0000870729	-0.0000408295
-19	-0.0000809615	-0.0002970655	-0.0009279296

Hartree Fock Energies = -780.75501

MP2 Energies = -782.50942

Pro-3

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.744683
6	1.282889	0.000000	2.180617
6	-1.261862	-0.011667	2.553555
1	1.580078	-0.001987	3.211074
7	2.269609	0.025738	1.207742
6	1.740622	0.026709	0.039521
1	2.314327	0.052146	-0.865818
1	-1.880081	0.852688	2.338760
1	-1.022207	0.005270	3.609734
1	-1.849901	-0.901141	2.357394

Hartree Fock Energies = -606.4449188

MP2 Energies = -607.6914034
