

Promotion of oxygen atom transfer in Mo and W enzymes by bicyclic forms of the pterin cofactor[†]

Jonathan P. McNamara,^a John A. Joule,^a Ian H. Hillier*^a and C. David Garner^b

^a School of Chemistry, University of Manchester, Manchester, M13 9PL, UK.

Fax: +44 (0) 161 275 4734; Tel: +44 (0) 161 275 4686; E-mail: Ian.Hillier@man.ac.uk

^b School of Chemistry, University of Nottingham, University Park, Nottingham, NG7 2RD, UK.,

Table S1 Summary of important structural parameters of ring opened dihydropterin tautomers

Tautomer ^a	Structural Parameter		
	C–C (Å) ^b	Mo–OS(CH ₃) ₂ (Å)	Dihedral (deg) ^c
T1^d	R	1.515	-88.0
	TS2	1.518	-59.6
	P	1.517	-48.5
T2	R	1.469	-37.0
	TS2	1.471	-35.3
	P	1.474	-25.4
T3	R	1.460	-4.4
	TS2	1.462	2.3
	P	1.463	-1.1
T4	R	1.414	0.8
	TS2	1.412	4.1
	P	1.418	-0.1
T4 (x2)	R	1.426, 1.425	0.2, 1.2
	TS2	1.424, 1.424	2.9, 3.5

^a Reactants (R), transition state 2 (TS2) and products (P). ^b C–C bond between the metallo-dithiolene and the pyrazine ring. ^c Dihedral angle between the metallo-dithiolene and the pyrazine ring. ^d The pyrazine ring of T1 corresponds to that identified in a crystallographic study of *Escherichia coli* nitrate reductase A (M. G. Bertero, R. A. Rothery, M. Palak, C. Hou, D. Lim, F. Blasco, J. H. Weiner and N. C. J. Strynadka, *Nature. Struct. Biol.* 2003, **10**, 681).

Cartesian co-ordinates (Å), absolute energies (Hartrees) and transition state imaginary frequencies (cm⁻¹)

Note: All energies (*E*) are calculated at the B3LYP level with LANL2DZ on Mo and 6-31G(d) on all other atoms.

DMSO

E = -553.186944

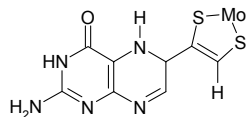
O	-.48628	2.74817	.97919
S	-1.04422	3.89987	.17527
C	-2.50304	3.27299	-.74992
H	-3.00677	4.10045	-1.25923
H	-2.13072	2.55680	-1.48642
H	-3.18337	2.76628	-.05899
C	-1.99964	4.96691	1.32676
H	-2.50911	5.75784	.76756
H	-1.28176	5.40874	2.02200
H	-2.71717	4.35539	1.88185

DMS

E = -478.013826

H	-1.64421	4.08826	-2.31630
C	-2.27998	3.97353	-1.43440
H	-2.64660	2.94277	-1.39673
H	-3.12692	4.66182	-1.51954
S	-1.25176	4.36455	.02335
C	-2.48850	4.11111	1.34298
H	-2.85381	3.07923	1.35211
H	-1.99017	4.31566	2.29421
H	-3.33314	4.79880	1.23342

Tautomer T1



Reactant Structure

E = -2511.052543

N	-6.82232	-3.38089	.48035
C	-5.65215	-2.78608	.06597
C	-5.20476	-2.81779	-1.24378
C	-5.98672	-3.48353	-2.26416
N	-7.14792	-4.07718	-1.74105
C	-7.51327	-4.01210	-.41607
N	-4.96052	-2.02631	1.01675
C	-3.76862	-1.65451	.71707
C	-3.01483	-2.04472	-.56161
N	-4.04055	-2.17556	-1.59596
C	-1.96063	-1.01771	-.92010
C	-2.19699	.05751	-1.69337
S	-.9333	1.22192	-2.09197
Mo	.94352	.66788	-.70385
O	-5.70491	-3.57386	-3.45933
N	-8.67040	-4.72106	-.06673
S	-.34653	-1.29948	-.23141
O	.94031	1.77444	.81807
C	1.99367	2.48554	1.43436
S	2.25489	1.79873	-2.33251
C	3.85896	1.06242	-2.27613
C	4.10798	-.01385	-1.51022

S	2.84661	-.74859	-.51667
H	-7.67100	-4.64884	-2.39424
H	-8.89125	-4.53045	.90577
H	-9.47144	-4.51363	-.65762
H	-3.72269	-2.32919	-2.54521
H	-3.23634	-1.01351	1.42063
H	-2.50509	-3.01065	-.37192
H	5.07816	-.50734	-1.50305
H	4.61414	1.49526	-2.92965
H	2.45740	3.18181	.72364
H	2.76189	1.79374	1.80380
H	1.58187	3.05285	2.28054
H	-3.17461	.23424	-2.13590

Transition Structure

$E = -3064.209669$; Imaginary Frequency = -464

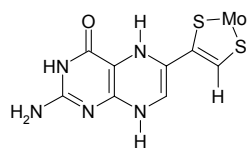
C	-3.07339	-2.29786	.12760
N	-3.83319	-2.09642	-1.10859
C	-5.01175	-2.77888	-1.25215
C	-5.74261	-3.15030	-.13424
N	-5.32651	-2.72697	1.13199
C	-4.12277	-2.29068	1.24486
C	-5.52143	-3.05645	-2.58061
N	-6.73508	-3.76297	-2.54551
C	-7.38466	-4.11971	-1.38518
N	-6.94396	-3.82134	-.20435
N	-8.55014	-4.88264	-1.55212
O	-4.98647	-2.75697	-3.64725
C	-2.00864	-1.22883	.29049
S	-.34453	-1.77555	.39069
Mo	1.12101	.22299	.39989
O	1.69107	1.96554	1.23687
C	1.53384	3.29138	.82067
C	-2.32013	.08788	.33212
S	-1.09287	1.31958	.42218
S	1.41628	1.13997	-1.83177
C	2.52031	.10569	-2.70731
C	3.10666	-.95554	-2.11530
S	2.80879	-1.34177	-.44049
O	1.93159	-.34678	2.06243
S	2.47638	.90786	3.29153
C	.97521	1.67545	3.97663
C	2.67612	-.43531	4.50907
H	-7.07163	-4.08426	-3.44581
H	-8.98746	-5.01340	-.64514
H	-9.21372	-4.47194	-2.20443
H	-3.31307	-1.89081	-1.95247
H	-3.81228	-1.88778	2.20991
H	-2.57445	-3.28558	.13321
H	3.78926	-1.60841	-2.65719
H	2.71168	.36596	-3.74696
H	1.76109	-1.03090	4.55737
H	3.48994	-1.06675	4.14729
H	2.93094	-.01902	5.48930
H	.93019	1.52969	5.06034
H	.11292	1.21560	3.48237
H	.99672	2.73665	3.72818
H	1.89571	3.42932	-.20912
H	2.11235	3.95245	1.48920
H	.47947	3.60979	.85448
H	-3.35133	.42858	.25845

Product Structure

$E = -2586.259567$

C	-2.80108	-3.27434	-.33396
C	-1.33370	-3.44694	-.74424
N	-1.38339	-3.96358	-2.11507
C	-2.27958	-4.97316	-2.36090
C	-3.44618	-5.06224	-1.61692
N	-3.75459	-4.05438	-.69670
N	-4.40144	-6.03369	-1.81838
C	-4.16735	-6.90573	-2.74787
N	-3.04705	-6.87373	-3.54858
C	-2.03017	-5.90987	-3.43924
C	-.52354	-2.16706	-.66606
S	1.05458	-2.30064	.10303
Mo	2.12405	-.03519	-.03100
O	2.02175	.37835	1.63285
O	-1.05103	-5.92531	-4.18394
N	-5.03775	-7.98282	-2.96260
S	4.11318	-1.25775	.67763
C	4.77886	-2.13400	-.65563
C	4.39609	-1.92124	-1.94676
S	3.15086	-.82712	-2.39985
O	2.49935	1.75283	-.70315
C	2.58861	2.34321	-1.96267
S	-.02002	.46698	-1.13964
C	-.96103	-1.00550	-1.19171
H	5.54200	-2.87077	-.41070
H	4.88788	-2.47738	-2.74559
H	3.38477	1.86397	-2.55822
H	2.80836	3.41373	-1.83466
H	1.64777	2.24155	-2.52564
H	-.87646	-4.18745	-.05880
H	-.51547	-3.98588	-2.63798
H	-2.86179	-7.62038	-4.20863
H	-5.30101	-8.10762	-3.93707
H	-5.86522	-7.85736	-2.38722
H	-3.04158	-2.43781	.32370
H	-1.92824	-.93460	-1.68628

Tautomer T2



Reactant Structure

$E = -2511.051645$

N	-3.70670	-2.34308	-.10904
C	-4.91790	-3.05179	-.26678
C	-6.07193	-2.61596	.35627
N	-6.02181	-1.45501	1.11004
C	-4.96443	-.53411	.79731
C	-3.84630	-.95224	.17094
N	-7.28680	-3.24585	.27733
C	-7.32098	-4.36050	-.40204
N	-6.23420	-4.86926	-1.04108
C	-4.95169	-4.24089	-1.05629
O	-4.03213	-4.75063	-1.70007
N	-8.49676	-5.10879	-.45016
C	-2.74743	-.05573	-.21100
S	-1.07679	-.69006	-.14886

Mo	.38126	1.16755	-.53208
C	-2.96250	1.20961	-.63907
S	-1.65820	2.29890	-1.08374
O	.99315	1.79349	1.13505
C	2.28669	2.15039	1.57192
S	1.95183	-.45070	-1.29882
C	3.00513	.38456	-2.44234
C	2.76308	1.65127	-2.82245
S	1.37821	2.54871	-2.19584
H	2.51020	1.60932	2.50197
H	2.31551	3.23027	1.77393
H	3.05027	1.90583	.82444
H	3.82569	-.19765	-2.85796
H	3.37490	2.16083	-3.56472
H	-3.97123	1.58631	-.79243
H	-6.93444	-1.05186	1.28102
H	-5.09802	.48020	1.14285
H	-3.00470	-2.57500	-.80412
H	-9.26910	-4.56946	-.07465
H	-8.71908	-5.48963	-1.36434
H	-6.26817	-5.76793	-1.50726

Transition Structure

$E = -3064.209677$; *Imaginary Frequency* = -459

C	-5.09182	-3.86864	-1.73641
C	-4.83430	-3.12128	-.54692
C	-5.86029	-2.90249	.35326
N	-7.14563	-3.35276	.19599
C	-7.38305	-4.07822	-.86319
N	-6.43454	-4.35231	-1.79734
N	-5.59711	-2.17228	1.50059
C	-4.45676	-1.29814	1.45647
C	-3.46366	-1.49674	.56655
N	-3.53544	-2.63390	-.28739
C	-2.28799	-.61941	.45827
C	-2.38557	.72054	.66255
S	-1.00560	1.77497	.60193
Mo	1.00956	.42116	.16566
S	-.72674	-1.35527	.08255
N	-8.64191	-4.65196	-1.04448
O	-4.30969	-4.13036	-2.65255
O	1.91404	1.86291	1.24673
C	1.90903	3.25514	1.12736
O	1.85980	-.57428	1.57877
S	2.58094	.30931	3.04134
C	1.19416	1.11318	3.90086
S	2.32199	-1.16605	-1.15035
C	2.59422	-.46157	-2.72315
C	2.17076	.78443	-3.02034
S	1.29700	1.75183	-1.85553
C	2.56360	-1.28152	3.93296
H	2.60599	3.68408	1.86844
H	.90889	3.67999	1.31327
H	2.22876	3.57028	.12269
H	3.28222	-1.93218	3.43094
H	2.85555	-1.13315	4.97780
H	1.56967	-1.72964	3.85692
H	1.11987	.74684	4.92939
H	1.36383	2.18992	3.88347
H	.28013	.89221	3.33851
H	3.12695	-1.07346	-3.44954
H	2.35301	1.23937	-3.99255
H	-3.35169	1.19463	.82051
H	-6.43345	-1.79908	1.93230
H	-4.41854	-.52956	2.21390

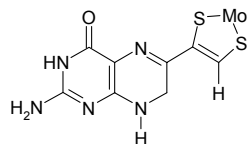
H	-2.93393	-2.60118	-1.10376
H	-9.29921	-4.26380	-.37672
H	-8.99957	-4.59362	-1.99272
H	-6.62358	-4.97104	-2.57674

Product Structure

$$E = -2586.258171$$

N	-3.46721	-4.40608	-1.19657
C	-2.76614	-5.46618	-1.75134
C	-1.38897	-5.47950	-1.65424
N	-.70056	-4.44036	-.99514
C	-1.38470	-3.19952	-.88902
C	-2.73174	-3.19613	-.95716
C	-.65422	-6.57731	-2.19763
N	-1.50450	-7.57568	-2.76140
C	-2.85749	-7.46692	-2.83272
N	-3.51243	-6.43786	-2.36537
O	.56760	-6.73667	-2.21509
N	-3.55311	-8.53963	-3.38761
C	-.56373	-1.99550	-.66900
S	1.03969	-2.23733	.03481
Mo	2.22093	-.02940	-.05111
O	2.62546	1.81008	-.54774
C	2.52009	2.56933	-1.71087
C	-.98582	-.75133	-1.00203
S	-.03896	.68627	-.71777
S	4.17956	-1.47040	.04607
C	4.35621	-2.28858	-1.46891
C	3.72607	-1.88544	-2.60805
S	2.62212	-.56911	-2.67182
O	2.47214	.15387	1.63900
H	2.83167	3.60110	-1.48759
H	3.15771	2.14981	-2.50728
H	1.48623	2.58679	-2.08908
H	3.90743	-2.43070	-3.53470
H	5.00926	-3.15875	-1.46751
H	-1.94784	-.58934	-1.48238
H	-3.32721	-2.31658	-.76277
H	-4.39649	-4.29823	-1.58405
H	-4.52608	-8.29197	-3.52917
H	-3.13877	-8.92410	-4.23053
H	-1.02416	-8.41360	-3.06697
H	.28493	-4.37840	-1.23042

Tautomer T3



Reactant Structure

$$E = -2511.063752$$

N	-7.20580	-3.18141	-.18914
C	-6.07462	-2.43504	-.40760
C	-4.78773	-2.93045	-.62377
C	-4.59802	-4.36137	-.63897
N	-5.83799	-5.06891	-.42792
C	-7.03672	-4.47710	-.19452
N	-6.23439	-1.08138	-.36561
C	-5.25803	-.21418	-1.01022
C	-3.85190	-.81483	-.83935

N	-3.68345	-2.09238	-.70341
C	-2.71216	.09597	-.89725
C	-2.85281	1.42055	-1.18208
S	-1.50578	2.52317	-1.31554
Mo	.41962	1.29167	-.55267
O	-3.58660	-5.02953	-.79536
N	-8.11537	-5.30845	.08882
S	-1.06720	-.56693	-.66412
O	.75905	1.72371	1.24815
C	1.97205	2.04336	1.89616
S	1.67944	2.82565	-1.87616
C	3.15465	1.97570	-2.34312
C	3.34039	.67927	-2.04029
S	2.11179	-.25036	-1.17797
H	-5.72166	-6.07177	-.34283
H	-8.98589	-4.79010	.06271
H	-8.15994	-6.16013	-.45959
H	-7.19151	-.76280	-.29862
H	-5.31783	.77036	-.54052
H	4.22585	.13146	-2.35775
H	3.87977	2.54479	-2.92218
H	2.71048	1.24489	1.74818
H	1.77334	2.15753	2.97100
H	2.38399	2.98263	1.50404
H	-3.82135	1.86679	-1.39336
H	-5.47305	-.07893	-2.08752

Transition Structure

$E = -3064.221064$; Imaginary Frequency = -462

C	-3.57754	-1.12559	-.19391
N	-3.52895	-2.37033	-.55417
C	-4.70526	-3.07402	-.77455
C	-5.94759	-2.58230	-.37355
N	-5.98530	-1.33947	.19094
C	-4.92230	-.38402	-.09424
C	-4.64434	-4.40486	-1.33213
N	-5.94889	-5.01813	-1.40032
C	-7.09721	-4.44783	-.95580
N	-7.14849	-3.24352	-.45242
N	-8.25644	-5.21732	-1.01238
O	-3.69263	-5.05884	-1.73275
C	-2.35652	-.35707	.04179
S	-.79412	-1.15891	-.16098
Mo	1.00512	.48697	.20125
O	1.87247	1.81504	1.45175
C	1.95213	3.21004	1.41779
C	-2.39327	.96779	.38657
S	-.97519	1.92472	.60290
S	1.46376	1.93481	-1.70075
C	2.38051	1.01477	-2.87235
C	2.75948	-.25550	-2.62391
S	2.36940	-1.04929	-1.11954
O	1.72430	-.63725	1.59534
S	2.42109	.11113	3.13092
C	1.04563	.90016	4.02287
C	2.32862	-1.53714	3.90631
H	-5.92599	-5.98368	-1.70632
H	-9.07345	-4.64416	-.83477
H	-8.35931	-5.77438	-1.85370
H	-6.91442	-.97900	.36243
H	-4.90808	.34860	.71569
H	3.32836	-.83515	-3.34934
H	2.63185	1.52178	-3.80241
H	1.32218	-1.94394	3.77973
H	3.03567	-2.17553	3.37323

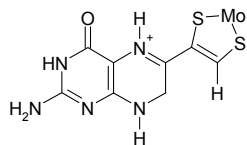
H	2.60243	-1.47265	4.96457
H	.95630	.48489	5.03159
H	.13069	.72569	3.44655
H	1.23864	1.97226	4.05882
H	2.37552	3.56233	.46524
H	2.60229	3.55604	2.24047
H	.96423	3.68229	1.54388
H	-3.32771	1.50620	.51887
H	-5.10374	.17081	-1.03433

Product Structure

$$E = -2586.271880$$

Mo	2.28998	-.26804	-.04925
O	2.51928	1.67505	-.05165
C	2.39777	2.68363	-1.00453
H	1.39456	2.70094	-1.45930
H	2.57561	3.65430	-.51684
H	3.12719	2.53674	-1.81985
S	3.01864	-.02010	-2.64179
C	4.28568	-1.16702	-2.80041
H	4.66599	-1.35730	-3.80427
C	4.82426	-1.84504	-1.74670
H	5.59704	-2.59572	-1.89875
S	4.35136	-1.56251	-.10989
S	1.28901	-2.46675	-.67280
C	-.43171	-2.19638	-.99505
C	-.94853	-.93671	-.94373
H	-1.99506	-.73258	-1.15334
S	-.01560	.47011	-.55322
O	2.42079	-.47938	1.64860
C	-1.24959	-3.35118	-1.36450
C	-2.73578	-3.10647	-1.67307
H	-2.83546	-2.68772	-2.69235
H	-3.15962	-2.37460	-.98032
N	-3.47659	-4.35090	-1.52090
H	-4.48355	-4.32547	-1.60613
C	-2.89761	-5.54515	-1.83040
N	-3.76044	-6.58699	-2.06076
C	-3.19879	-7.73940	-2.31632
N	-3.99780	-8.86235	-2.49504
H	-4.96920	-8.60054	-2.61640
H	-3.68148	-9.51178	-3.20627
N	-1.85473	-7.91311	-2.38116
H	-1.44826	-8.83385	-2.49763
C	-.87853	-6.87984	-2.13147
O	.30134	-7.19253	-2.18656
C	-1.50359	-5.61048	-1.84662
N	-.71525	-4.52320	-1.49582

Tautomer T4



Reactant Structure

$$E = -2511.594944$$

H	12.76249	-3.67882	-1.42268
N	12.43145	-2.90289	-1.98049
H	12.79551	-2.85867	-2.92230
C	11.12704	-2.56229	-1.75328

N	10.50379	-3.07575	-.71480
N	10.54887	-1.66682	-2.60677
H	11.07787	-1.23485	-3.35628
C	9.22768	-1.16005	-2.44910
O	8.78489	-.31379	-3.21592
C	8.57025	-1.74529	-1.32417
C	9.23117	-2.64711	-.50346
N	8.57483	-3.10398	.60137
H	9.05509	-3.82024	1.13085
C	7.11469	-3.09067	.64542
H	6.80781	-3.15608	1.68952
H	6.68354	-3.95850	.11570
C	6.55947	-1.82019	.01591
N	7.29537	-1.29807	-.96676
H	6.91655	-.50306	-1.48692
C	5.30556	-1.26181	.35360
C	4.49041	-1.84034	1.31308
H	4.80776	-2.72933	1.85356
S	2.93085	-1.27162	1.70345
S	4.73859	.17314	-.54787
S	.39029	.39729	.59955
C	-.35145	1.22324	-.76878
H	-1.43397	1.15947	-.84308
C	.40400	1.85251	-1.68425
H	-.01787	2.34319	-2.55772
S	2.16229	1.84901	-1.56513
Mo	2.69383	.87681	.50304
O	2.98343	2.29572	1.66541
C	2.30257	3.50876	1.94789
H	2.89044	4.06608	2.68573
H	2.20294	4.09952	1.03048
H	1.30775	3.29254	2.35326

Transition Structure

$E = -3064.761924$ Imaginary Frequency = -451

Mo	1.03261	.31814	.47808
O	1.79193	1.98100	1.27722
C	1.81781	3.31312	.82714
H	2.38912	3.91864	1.54706
H	.80615	3.73889	.74879
H	2.29467	3.38764	-.15955
O	1.97775	-.37771	1.97582
S	2.79356	.75904	3.23305
C	3.07456	-.68926	4.29815
H	3.78157	-1.33315	3.77179
H	3.49987	-.36849	5.25378
H	2.13765	-1.23177	4.44541
H	1.68318	1.52426	5.24220
H	1.35321	2.56727	3.81326
H	.52387	.99967	3.97191
S	2.42695	-1.35085	-.59399
C	2.54432	-.93578	-2.27773
H	3.11434	-1.61550	-2.90724
H	2.07637	.48165	-3.81250
C	1.98227	.18976	-2.76953
S	1.11659	1.27920	-1.72070
S	-1.09568	1.64155	.83530
S	-.64809	-1.53250	.52716
C	-2.40216	.57433	.76830
H	-3.38609	1.02636	.86886
C	-2.25850	-.80131	.60067
C	-3.38598	-1.63773	.45304
C	-4.81671	-1.12522	.37172
N	-5.76221	-2.14021	.83364
H	-6.72510	-1.85572	.96091

H	-5.02111	-.82479	-.67115
H	-4.93986	-.24173	.99821
H	-2.29115	-3.32540	.17040
C	-4.29987	-3.85636	.14505
N	-3.23987	-2.95248	.24874
C	-5.58339	-3.44438	.46736
N	-6.66938	-4.26492	.47186
C	-6.44726	-5.52614	.17803
N	-7.48584	-6.41921	.23268
H	-8.39459	-5.98218	.31450
H	-7.45717	-7.22984	-.37119
N	-5.21312	-6.01351	-.14374
H	-5.06022	-7.00464	-.29288
C	-4.02799	-5.22465	-.16400
O	-2.94126	-5.73488	-.40885
C	1.45216	1.54407	4.17297

Product Structure

$$E = -2586.797454$$

Mo	2.30152	-.27587	-.02662
O	2.54521	1.63817	-.03351
C	2.54785	2.67462	-.97446
H	2.83912	3.60139	-.46396
H	3.25287	2.45092	-1.79077
H	1.55185	2.81510	-1.41969
S	2.77206	-.08616	-2.65854
C	4.07270	-1.16816	-2.90329
H	4.38016	-1.36207	-3.92976
C	4.73199	-1.78755	-1.87772
H	5.54802	-2.48047	-2.06749
S	4.35292	-1.51495	-.22402
S	-.06839	.51100	-.49029
C	-.99051	-.86588	-.85728
H	-2.04091	-.67010	-1.05986
C	-.48666	-2.15442	-.91688
S	1.21413	-2.49118	-.56153
O	2.49439	-.54262	1.64970
C	-1.31091	-3.22970	-1.33497
C	-2.77023	-3.07125	-1.73905
H	-3.24713	-2.30167	-1.13149
H	-2.80864	-2.73823	-2.79123
N	-3.50451	-4.31849	-1.54201
H	-4.51324	-4.28784	-1.61627
C	-2.92455	-5.51238	-1.85371
N	-3.73508	-6.57391	-2.10298
C	-3.13659	-7.72204	-2.33904
N	-3.89831	-8.83920	-2.53286
H	-4.88526	-8.65734	-2.65722
H	-3.52404	-9.60746	-3.07221
N	-1.77897	-7.86833	-2.36541
H	-1.34826	-8.77899	-2.48128
C	-.86235	-6.81128	-2.10311
O	.34494	-7.01631	-2.08682
C	-1.53871	-5.57630	-1.86335
N	-.79769	-4.44847	-1.50251
H	.20479	-4.58061	-1.34842

Tautomer T4 (x2)

Reactant Structure

$$E = -3092.679857$$

C	-1.73714	2.39355	-3.23583
C	-.23440	2.36452	-2.98797

N	.51554	2.89517	-3.94123
C	.02366	3.59176	-5.04492
C	-1.31836	3.95977	-5.07590
N	-2.10960	3.54668	-4.04969
C	.35373	1.73576	-1.85083
S	2.13637	1.72615	-1.70763
Mo	2.65824	.78118	.38020
S	.29491	.26080	.44188
C	-.39551	1.08363	-.90081
C	.94443	4.06832	-6.02746
O	2.15193	3.87089	-6.06135
N	-1.85940	4.73850	-6.03790
C	-1.03582	5.17245	-6.97777
S	4.66700	.04661	-.64380
C	5.24988	-1.34720	.31352
C	4.42370	-1.90547	1.25874
S	2.84284	-1.31641	1.59081
C	6.54014	-1.87748	.02387
N	7.28435	-1.37082	-.94797
C	8.58169	-1.78313	-1.25334
C	9.25300	-2.62763	-.37448
N	8.57254	-3.07569	.71455
C	7.11308	-3.10195	.72600
N	10.54809	-2.98577	-.52068
C	11.18767	-2.47247	-1.55767
N	10.59806	-1.63468	-2.46390
C	9.25186	-1.19070	-2.36666
N	12.49786	-2.76853	-1.72396
O	8.78755	-.38494	-3.16290
O	3.01471	2.16281	1.52968
C	2.82837	3.54765	1.78489
H	12.88607	-3.46662	-1.10526
H	12.97625	-2.59745	-2.59581
H	11.12852	-1.21539	-3.22013
H	9.06728	-3.72024	1.31828
H	6.78256	-3.12468	1.76518
H	6.71504	-4.00431	.22936
H	6.91405	-.60232	-1.51335
H	4.71782	-2.77856	1.83527
H	-1.47884	1.02471	-.96605
H	3.77240	3.95508	2.15887
H	2.53783	4.06039	.86248
H	2.04835	3.66330	2.54407
H	1.53465	2.82247	-3.87615
H	-3.08983	3.79184	-4.11206
H	-2.27032	2.46105	-2.28660
H	-2.02746	1.44151	-3.71415
N	-1.52380	5.98580	-7.94154
N	.29480	4.85740	-7.01420
H	.91169	5.24562	-7.71982
H	-1.00965	6.18483	-8.78657
H	-2.52348	6.13149	-7.95191

Transition State

$E = -3645.856829$; Imaginary Frequency = -407

C	5.922593	-4.247736	-2.751195
C	5.193783	-3.202781	-3.395630
C	5.195759	-3.071906	-4.779292
N	5.887343	-3.884890	-5.610487
C	6.596215	-4.842787	-5.040391
N	6.644310	-5.036279	-3.687693
N	4.353605	-2.390825	-2.631905
C	3.683458	-1.345168	-3.098612
C	4.006024	-.943306	-4.531886
N	4.410195	-2.101689	-5.323658

C	2.811182	-.597120	-2.257036
C	2.137064	.519370	-2.717509
S	1.129298	1.472007	-1.731551
Mo	1.087990	.432191	.537822
S	2.649481	-1.081935	-.565776
N	7.346396	-5.653606	-5.826325
O	5.957988	-4.493569	-1.551856
S	-1.029186	1.724206	.775292
C	-2.332764	.643838	.623322
C	-2.162956	-.719816	.468145
S	-.538253	-1.412722	.505087
C	-3.273754	-1.591774	.281387
C	-4.712720	-1.104042	.172822
N	-5.645923	-2.142581	.599192
C	-5.430908	-3.443568	.260658
C	-4.128061	-3.823854	-.041652
N	-3.096456	-2.892092	.086681
N	-6.479782	-4.297979	.278108
C	-6.212142	-5.562505	.006318
N	-4.958733	-6.014126	-.302263
C	-3.803392	-5.186306	-.320196
O	-2.692089	-5.652102	-.539450
N	-7.219470	-6.468282	.059255
O	1.835936	2.047214	1.369637
C	1.752569	3.418904	1.038892
O	1.955615	-.338648	2.012849
S	2.801761	.741380	3.375903
C	3.191638	-.782457	4.284488
C	1.397409	1.334217	4.359588
H	2.466735	3.964943	1.668497
H	.745975	3.817535	1.226465
H	2.001889	3.587154	-.016317
H	3.957951	-1.305891	3.709292
H	3.581257	-.526263	5.273768
H	2.301927	-1.411439	4.361716
H	1.703291	1.451299	5.403316
H	1.090854	2.292242	3.940728
H	.577249	.614938	4.280091
H	2.228564	.851720	-3.748210
H	-3.319510	1.097261	.658295
H	-6.608703	-1.878684	.766630
H	-4.895761	-.790865	-.870194
H	-4.864937	-.232162	.809450
H	-2.142613	-3.261270	.054942
H	-8.150946	-6.094326	.175908
H	-7.135956	-7.375309	-.375452
H	-4.774316	-7.000102	-.452904
H	3.128363	-.501173	-5.004675
H	4.475670	-1.989596	-6.327607
H	4.243095	-2.653723	-1.649544
H	4.793748	-.169798	-4.504866
H	7.213286	-5.768293	-3.276389
H	7.709924	-6.530851	-5.484500
H	7.205060	-5.566292	-6.82301