

How Reliable are DFT Transition Structures?

Comparison of GGA, Hybrid-GGA and Meta-GGA functionals

Luis Simón^{a} and Jonathan M. Goodman^{b*}*

Facultad de Ciencias Químicas, Universidad de Salamanca, Plaza de los Caídos 1-5, Salamanca, E37004, Spain.

Unilever Centre For Molecular Science Informatics, Department of Chemistry, Lensfield Road, Cambridge, CB2 1EW, UK.

- Page S-2: Full list of authors in Gaussian03 reference.
- Page S-3: Relative computational cost of each method.
- Page S-4: Cartesian coordinates of the structures optimized by M05(-2X) functional (ultrafine grid).
- Page S-37: Frequencies at which the RMSD differences were higher than 0.2 Å, 0.3 Å and 0.4 Å. Frequencies at which the maximum deviations distances of bonds forming (or breaking) in the TS were higher than 0.1 Å, 0.2 Å and 0.4 Å. Times that maximum dihedral angle deviations were higher than 30°, 60° and 90°.
- Page S-40: Comparison with experimental data.

Full list of authors in Gaussian03 reference:

Gaussian 03, R. D., 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.

Relative computational cost of each method

HF.....	0.22
BLYP.....	0.27
HCTH.....	0.28
B3LYP.....	0.35
B3LYP-UF.....	0.63
B3P86.....	0.35
B3PW91.....	0.35
O3LYP.....	0.35
PBE1PBE.....	0.36
BHandHLYP.....	0.38
BMK.....	0.51
MPWB1K.....	0.51
M05(-2X).....	0.54
M05(-2X)-UF.....	1.00

**Cartesian coordinates of the structures optimized by M05(-2X) functional
(ultrafine grid)**

an02-ts9maj

C	2.69838	1.80796	-2.37024
N	1.75432	0.77217	-1.80292
C	2.58029	-0.39991	-1.33722
C	1.79498	-0.99966	-0.15499
O	1.24098	0.14654	0.48241
B	0.84192	1.15024	-0.45955
C	3.90708	0.26284	-0.98304
C	0.66542	-1.94868	-0.57405
C	2.74703	-1.71806	0.78742
C	0.99371	2.64816	0.05282
C	4.57510	-3.02810	2.43931
C	3.33571	-2.91597	0.37491
C	3.06909	-1.18472	2.03176
C	3.97943	-1.84345	2.85655
C	4.25115	-3.56438	1.19440
H	3.06623	-3.34857	-0.58270
H	2.59984	-0.26454	2.35098
H	4.22190	-1.42728	3.82598
H	4.70484	-4.49090	0.86710
H	5.28362	-3.53583	3.08065
C	-1.47876	-3.66319	-1.15875
C	-0.05159	-2.57495	0.45236
C	0.28755	-2.19126	-1.89297
C	-0.78065	-3.04082	-2.18541
C	-1.11156	-3.42475	0.16618
H	0.24939	-2.40313	1.47936
H	0.82367	-1.74434	-2.72153
H	-1.04720	-3.22922	-3.21761
H	-1.63711	-3.92034	0.97327
H	-2.28720	-4.34645	-1.38714
H	1.08348	0.48188	-2.51049
H	2.72429	-1.10968	-2.15210
H	4.70801	-0.46632	-0.88138
H	3.80379	0.79834	-0.03608
C	4.10358	1.23774	-2.14385
H	2.54293	2.73408	-1.82528
H	2.46136	1.97016	-3.41941
H	4.44872	0.70295	-3.03056
H	4.82217	2.02436	-1.92139
C	1.31222	5.29716	0.94537
C	1.78081	2.94248	1.17076
C	0.37073	3.71634	-0.61029
C	0.52590	5.02839	-0.17351
C	1.93908	4.25263	1.61776
H	2.26789	2.13087	1.69859

H	-0.24891	3.51546	-1.47943
H	0.03827	5.83897	-0.70046
H	2.54880	4.45849	2.48848
H	1.43498	6.31615	1.28943
O	-0.56222	0.90950	-1.02105
C	-1.45878	0.35679	-0.26080
C	-2.73049	0.02392	-0.74192
H	-1.13326	0.00742	0.71369
C	-3.57453	-0.74176	0.09017
C	-4.64251	-1.66861	-0.44753
H	-3.10631	-1.11325	0.99699
C	-5.72076	-1.80324	0.62309
H	-4.17462	-2.62888	-0.67997
H	-5.06598	-1.27106	-1.37223
C	-6.15817	-0.36915	0.96911
H	-6.55750	-2.41791	0.29289
H	-5.28986	-2.27942	1.50800
C	-4.95019	0.54273	0.85355
H	-6.92428	-0.03487	0.26851
H	-6.58477	-0.31697	1.97165
C	-4.24478	0.97185	1.97621
H	-4.93215	1.18544	-0.01999
C	-3.10203	1.78808	1.90927
H	-4.48986	0.51595	2.93110
C	-2.62084	2.29869	0.73023
H	-2.50348	1.89952	2.80552
H	-1.67926	2.83372	0.70841
H	-3.24858	2.41252	-0.14334
C	-3.14174	0.44886	-2.12256
H	-2.48750	1.23609	-2.49230
H	-3.08309	-0.39510	-2.81464
H	-4.17238	0.81307	-2.13975

an02-ts9min

C	2.03428	2.19467	-2.54284
N	1.49552	0.95403	-1.87414
C	2.67093	0.17494	-1.35145
C	2.09984	-0.63953	-0.18002
O	1.19805	0.27686	0.42977
B	0.51322	1.09683	-0.53631
C	3.64446	1.28563	-0.97597
C	1.34590	-1.90157	-0.61454
C	3.21179	-1.01229	0.78715
C	0.23240	2.58732	-0.04462
C	5.32827	-1.66511	2.48561
C	4.15769	-1.96448	0.39961
C	3.32522	-0.39612	2.02985
C	4.38038	-0.72715	2.87803
C	5.21497	-2.28411	1.24223

H	4.05700	-2.46783	-0.55589
H	2.58437	0.33139	2.33056
H	4.45962	-0.24912	3.84602
H	5.94450	-3.02184	0.93413
H	6.14807	-1.91850	3.14500
C	-0.08628	-4.23828	-1.22578
C	0.74897	-2.66159	0.39709
C	1.22289	-2.33639	-1.93263
C	0.51092	-3.49864	-2.23759
C	0.03636	-3.81452	0.09818
H	0.87288	-2.34876	1.42736
H	1.69065	-1.79863	-2.74864
H	0.43696	-3.82535	-3.26697
H	-0.40342	-4.39784	0.89765
H	-0.62737	-5.14565	-1.46098
H	0.96064	0.39423	-2.53566
H	3.09709	-0.44624	-2.13925
H	4.65254	0.90440	-0.82725
H	3.31333	1.75994	-0.04979
C	3.52374	2.24749	-2.16100
H	1.48176	3.05009	-2.16829
H	1.87917	2.11257	-3.61656
H	4.13905	1.89962	-2.99188
H	3.83544	3.25994	-1.91202
C	-0.22029	5.22190	0.84289
C	0.81538	3.06355	1.13413
C	-0.58818	3.46853	-0.76680
C	-0.81340	4.77163	-0.33484
C	0.59379	4.36576	1.57749
H	1.45093	2.40069	1.70898
H	-1.05657	3.13186	-1.68827
H	-1.44535	5.43458	-0.91234
H	1.05639	4.71235	2.49302
H	-0.39121	6.23516	1.18330
H	-7.58176	-0.75749	-0.29105
C	-6.62843	-0.39358	0.09062
C	-5.54423	-0.38019	-0.98296
C	-6.09130	-1.27302	1.23326
H	-6.78577	0.62531	0.45441
C	-4.25821	0.08363	-0.33715
H	-5.79316	0.30724	-1.79635
H	-5.41786	-1.37518	-1.41448
C	-4.59175	-1.07188	1.33386
H	-6.29616	-2.32299	1.02085
H	-6.57554	-1.02791	2.17950
C	-2.98015	-0.28243	-0.80464
H	-4.32763	1.07748	0.09520
C	-4.02370	-0.22852	2.28425
H	-3.98061	-1.88572	0.95946
C	-1.90446	0.56693	-0.51087

C	-2.64104	0.01205	2.38141
H	-4.69208	0.39770	2.86816
O	-0.73651	0.39619	-1.05879
H	-2.07191	1.49371	0.03051
C	-1.71575	-0.62455	1.59273
H	-2.31249	0.83525	3.00510
H	-0.67208	-0.33416	1.61813
H	-1.92234	-1.57027	1.10911
C	-2.74110	-1.54785	-1.57795
H	-1.67521	-1.74802	-1.66732
H	-3.21234	-2.40593	-1.08903
H	-3.16607	-1.47629	-2.58222

ja1g-5bts

P	-1.40063	-1.31616	-0.37648
C	-2.39459	1.32286	0.99463
C	-2.83768	0.57285	-0.06702
C	0.20145	-0.49595	-0.19068
C	1.25135	-1.20688	0.41688
C	0.46467	0.80370	-0.65684
C	2.50984	-0.63729	0.56280
C	1.72654	1.36769	-0.51993
C	2.75185	0.65199	0.09460
H	-1.65151	2.09709	0.87007
H	-2.68308	0.93417	-1.07832
H	-2.69403	1.08583	2.00596
H	-3.70231	-0.06700	0.05891
H	1.07198	-2.21338	0.77701
H	-0.32024	1.36923	-1.14364
H	3.30317	-1.20009	1.03851
H	1.91151	2.36767	-0.89223
H	3.73345	1.09503	0.20418

ja1g-6ats

P	1.60394	-0.41610	0.00000
C	0.00000	0.41870	0.00000
C	0.03632	1.82595	0.00000
C	-1.25693	-0.20985	0.00000
C	-1.13191	2.57406	0.00000
C	-2.42582	0.54088	0.00000
C	-2.36921	1.93276	0.00000
C	1.10567	-2.21124	0.00000
C	2.30514	-3.09196	0.00000
H	0.99742	2.32824	0.00000
H	-1.08018	3.65548	0.00000
H	-3.28279	2.51335	0.00000
H	-3.38525	0.03876	0.00000
H	-1.32788	-1.28940	0.00000

H	0.47135	-2.41428	0.87513
H	0.47135	-2.41428	-0.87513
H	3.30644	-2.68556	0.00000
H	2.19080	-4.16652	0.00000

ja1m-r1

Pd	-0.04132	-0.35807	0.29936
C	1.87759	2.02390	-1.33336
C	3.06033	1.16475	0.61689
C	1.89987	1.58888	1.51469
N	0.59504	1.70297	0.80678
C	0.71612	2.50354	-0.44692
C	-0.63286	2.61385	-1.14787
C	-1.66652	3.27465	-0.24121
C	-1.74985	2.55305	1.09919
C	-0.38137	2.34541	1.72509
C	3.17598	2.14840	-0.54338
C	1.78452	0.60343	-1.89757
N	1.84549	-0.44735	-0.85918
C	2.98380	-0.28331	0.10787
C	4.32808	-0.75708	-0.46127
C	3.14392	-2.26336	-2.05577
C	4.25821	-2.17091	-1.02330
C	1.82541	-1.81751	-1.44051
H	1.89646	2.69868	-2.19689
H	3.95284	1.21870	1.24907
H	1.75891	0.87153	2.32794
H	2.14403	2.57303	1.94163
H	0.99660	3.52488	-0.13719
H	-0.50273	3.19768	-2.06541
H	-0.98309	1.61790	-1.44364
H	-1.38558	4.32296	-0.08028
H	-2.64681	3.28393	-0.72630
H	-2.36462	3.12069	1.80476
H	-2.24296	1.58601	0.96304
H	-0.44338	1.71721	2.61576
H	0.03316	3.31895	2.02921
H	4.04010	1.93643	-1.17796
H	3.30471	3.16914	-0.16957
H	2.60667	0.48329	-2.61620
H	0.85505	0.45675	-2.45423
H	2.72426	-0.92664	0.95683
H	5.06175	-0.70803	0.34956
H	4.68825	-0.08097	-1.24490
H	3.39321	-1.66040	-2.93724
H	3.02084	-3.29149	-2.41014
H	4.05910	-2.87896	-0.21039
H	5.22082	-2.45225	-1.46090
H	1.00575	-1.85573	-2.16149

H	-1.42963	-0.40081	1.12076
Cl	1.00504	-1.44508	2.86064
O	-1.05440	-2.11409	-0.34535
C	-2.01984	-1.75668	0.42131
C	-3.22457	-1.10305	-0.21962
C	-3.30552	-1.06203	-1.61614
H	-2.49473	-1.49417	-2.19301
C	-4.40690	-0.49090	-2.24538
H	-4.46155	-0.47708	-3.32986
C	-5.44169	0.05582	-1.48721
H	-6.30106	0.50272	-1.97767
C	-5.37043	0.01946	-0.09600
H	-6.17249	0.44106	0.50207
C	-4.27269	-0.56125	0.53366
H	-4.23125	-0.57591	1.61819
C	-2.20565	-2.52499	1.70953
H	-1.23537	-2.67146	2.18673
H	-2.88116	-2.03825	2.41231
H	-2.63491	-3.49452	1.43525
H	1.55936	-2.49843	-0.62805

ja1m-s2

Pd	-0.13709	0.06928	0.50972
C	2.19340	1.10018	-1.87319
C	3.30892	0.26897	0.12480
C	2.55299	1.29104	0.97428
N	1.29358	1.78956	0.35847
C	1.48604	2.19356	-1.05960
C	0.18030	2.70306	-1.65763
C	-0.32685	3.91369	-0.88199
C	-0.46132	3.57716	0.59815
C	0.79939	2.93874	1.16025
C	3.56715	0.86228	-1.25639
C	1.47010	-0.24347	-2.01818
N	1.33930	-1.00360	-0.74984
C	2.63504	-1.10639	0.01188
C	3.59846	-2.15603	-0.56106
C	1.70130	-3.37280	-1.60996
C	2.94625	-3.51861	-0.74813
C	0.75629	-2.36127	-0.97808
H	2.30089	1.49813	-2.88880
H	4.25592	0.09897	0.64767
H	2.29295	0.86031	1.94527
H	3.22030	2.15090	1.13834
H	2.18528	3.04812	-1.05826
H	0.35549	2.96433	-2.70676
H	-0.57444	1.90776	-1.64244
H	0.37629	4.74535	-1.01764
H	-1.28743	4.25038	-1.28345

H	-0.66794	4.48027	1.18084
H	-1.30396	2.90184	0.75184
H	0.62559	2.57405	2.17517
H	1.60611	3.68762	1.20830
H	4.17013	0.19997	-1.88177
H	4.11925	1.80393	-1.17559
H	2.03443	-0.83429	-2.75154
H	0.46462	-0.11071	-2.42548
H	2.33648	-1.42621	1.01683
H	4.43948	-2.23234	0.13527
H	4.02058	-1.83474	-1.51970
H	1.97517	-3.08333	-2.63139
H	1.16559	-4.32377	-1.69332
H	2.66604	-3.92975	0.22849
H	3.65542	-4.21977	-1.19828
H	-0.15128	-2.22847	-1.57260
H	-1.13827	-1.16796	0.64685
Cl	0.94451	-1.22204	2.99362
O	-1.90305	0.86323	1.43519
C	-2.43487	-0.29120	1.30320
C	-3.37779	-0.51266	0.14430
C	-3.80286	0.59454	-0.59915
H	-3.42727	1.57582	-0.32871
C	-4.69795	0.43874	-1.65255
H	-5.02903	1.30833	-2.21233
C	-5.17488	-0.82860	-1.98452
C	-4.75622	-1.93742	-1.25121
C	-3.86934	-1.78008	-0.19012
H	-3.54941	-2.65457	0.36750
C	-2.57504	-1.14454	2.53888
H	-3.39286	-0.70767	3.12234
H	-2.82584	-2.18301	2.32607
H	-1.64982	-1.10385	3.11668
H	0.46006	-2.72975	0.00634
H	-5.12346	-2.92754	-1.50316
H	-5.87264	-0.95122	-2.80723

ja4q-56cyp5met

C	-1.87984	-0.57892	-0.38139
C	-2.49118	-0.40107	0.97634
C	-1.74786	0.90945	-0.41397
C	-0.54887	1.54707	-0.19296
C	0.63750	0.77838	-0.03958
C	0.57164	-0.70032	-0.15839
C	-0.59335	-1.33663	-0.35163
C	1.94853	1.10830	0.17902
C	2.73425	-0.11437	0.19306
C	1.93257	-1.19535	-0.00989
H	-2.58423	-0.97891	-1.11043

H	-2.64131	1.47702	-0.63382
H	-0.50506	2.62789	-0.15448
H	-0.64233	-2.41716	-0.43090
H	2.34563	2.10421	0.30940
H	3.80442	-0.14576	0.34331
H	2.22782	-2.23268	-0.04527
H	-1.84335	-0.35216	1.83664
H	-3.54191	-0.18164	1.08184

ja4q-tricicl-spiro

C	-0.26901	0.45795	-0.10177
C	0.83785	1.39535	0.22045
C	2.10633	0.95064	0.35709
C	2.47145	-0.40537	0.04834
C	1.55124	-1.25860	-0.52486
C	0.20160	-0.89522	-0.65074
H	0.58704	2.43739	0.36848
H	2.88762	1.64380	0.64447
H	3.50244	-0.71225	0.15756
H	1.87221	-2.21135	-0.92811
H	-0.48336	-1.44360	-1.28022
C	-0.74170	-0.53921	0.91935
C	-2.12053	-0.68603	0.77695
C	-2.57481	0.19577	-0.25259
C	-1.52432	0.90033	-0.76485
H	-0.10852	-0.91122	1.70858
H	-3.59842	0.26447	-0.59383
H	-1.54964	1.61273	-1.57594
H	-2.73794	-1.37363	1.33483

ja5j-ts3E

C	0.63537	2.56040	0.23013
P	-0.81673	-1.52273	0.36806
O	-0.32272	-1.70623	1.82692
O	0.00110	-0.70964	-0.56501
H	0.98676	0.71961	-0.44673
N	1.43737	1.60920	-0.17044
O	-1.00338	-3.01019	-0.22489
O	-2.33782	-0.99110	0.53148
C	-3.30850	-3.61128	-0.13229
C	-2.02823	-3.85288	0.15291
H	-4.02708	-4.38558	0.10519
H	-1.67721	-4.75934	0.62474
C	-3.28218	-1.17254	-0.45604
C	-3.78410	-2.37405	-0.74708
H	-3.61974	-0.24661	-0.89913
H	-4.60006	-2.42191	-1.45705
C	1.19400	3.86654	0.71044

H	2.04048	3.72628	1.37586
H	1.50744	4.43541	-0.17147
H	0.42418	4.42760	1.23095
C	-3.35489	2.64286	-1.29369
C	-3.09725	3.09435	0.00012
C	-1.80748	3.04976	0.50982
C	-0.76517	2.53909	-0.26843
C	-1.02759	2.07125	-1.55787
C	-2.32042	2.12854	-2.06886
H	-4.36043	2.68905	-1.69271
H	-3.90284	3.47558	0.61349
H	-1.60598	3.35948	1.52625
H	-0.22460	1.67438	-2.16351
H	-2.51395	1.77196	-3.07207
N	0.18702	0.59003	2.70923
C	0.29121	1.69729	2.35639
H	-0.10556	-0.78655	2.32083
C	2.82248	1.51536	0.29699
H	3.39488	2.35784	-0.09351
H	2.79195	1.58416	1.39079
C	4.54488	-2.23388	-0.88948
C	3.58931	-2.18825	0.12324
C	3.04079	-0.97121	0.50943
C	3.44016	0.20739	-0.12286
C	4.39314	0.15767	-1.13710
C	4.94827	-1.06055	-1.51889
H	4.97337	-3.18230	-1.18716
H	3.27011	-3.09870	0.61325
H	2.29412	-0.93282	1.29391
H	4.70312	1.07307	-1.62818
H	5.69094	-1.09244	-2.30566

ja5j-TS3Z

C	-2.23862	-0.84008	-0.46789
P	2.30487	-1.10684	0.16567
O	1.99904	-1.59190	1.59819
O	1.16246	-0.77638	-0.72512
H	-0.44857	-0.02046	-0.72022
N	-1.44310	0.19030	-0.54570
O	3.34242	0.10858	0.40802
O	3.23453	-2.22175	-0.55250
C	5.01239	0.01345	-1.26473
C	3.99686	0.65123	-0.68223
H	5.55497	0.52698	-2.04827
H	3.64477	1.63737	-0.95199
C	4.60526	-2.30297	-0.49669
C	5.43673	-1.32780	-0.87102
H	4.94476	-3.28434	-0.19745
H	6.49352	-1.56262	-0.88533

C	-1.79275	-2.13768	-1.07186
H	-2.13073	-2.14831	-2.11262
H	-0.70942	-2.22864	-1.03239
H	-2.26783	-2.96260	-0.54659
C	-6.47421	-0.29100	-0.29515
C	-5.85671	-1.07165	0.67832
C	-4.47675	-1.24256	0.67661
C	-3.70528	-0.62144	-0.30457
C	-4.32629	0.15739	-1.28727
C	-5.70691	0.32190	-1.28098
H	-7.54859	-0.16072	-0.28543
H	-6.44995	-1.54650	1.44876
H	-3.97699	-1.82101	1.43915
H	-3.72694	0.61727	-2.06443
H	-6.17941	0.92488	-2.04530
N	-0.46269	-1.62535	2.04175
C	-1.56202	-1.48565	1.67973
H	0.95332	-1.64347	1.86218
C	-1.73965	1.46135	0.13197
H	-2.49323	2.01248	-0.42878
H	-2.15709	1.20444	1.11036
C	1.85824	3.76656	0.57134
C	1.66645	2.61426	1.33144
C	0.49826	1.87313	1.19012
C	-0.48360	2.27946	0.28503
C	-0.28580	3.42980	-0.47569
C	0.88149	4.17456	-0.33261
H	2.76512	4.34666	0.68750
H	2.42701	2.28470	2.02627
H	0.34400	0.97491	1.77829
H	-1.04731	3.74486	-1.17976
H	1.02602	5.07000	-0.92336

ja8y-bxa

C	0.45136	-2.00551	-1.00347
B	0.95462	-0.53628	-0.67505
O	-0.28295	0.63531	-0.97141
C	-1.29113	1.06812	-0.41393
C	-2.43330	0.17307	0.07894
O	-2.16823	-1.11553	-0.04420
C	-3.21014	-1.99061	0.41843
C	-1.59624	2.52601	-0.39111
N	1.30883	-0.17859	0.83819
C	2.72373	0.31665	0.74137
C	3.71181	-0.83027	0.90397
B	0.44443	0.87240	1.72256
O	2.02438	-0.04895	-1.44538
C	2.74635	0.89505	-0.67378
O	-3.46955	0.64553	0.47252

H	2.88312	1.07858	1.50299
H	3.75916	0.99055	-1.06638
H	2.25457	1.87245	-0.69748
H	1.30086	-1.04722	1.36647
H	-0.75152	0.58376	1.59938
H	0.76971	0.72497	2.88003
H	0.66613	1.98682	1.29879
H	-1.92128	2.81082	0.60802
H	-0.71291	3.08221	-0.68964
H	-2.42787	2.71887	-1.07403
H	-3.39208	-1.81482	1.47667
H	-2.83858	-2.99529	0.24633
H	-4.12300	-1.80846	-0.14442
H	4.73519	-0.45552	0.85055
H	3.58422	-1.32113	1.87160
H	3.57370	-1.56621	0.10930
H	-0.14691	-2.02850	-1.91603
H	1.32957	-2.63456	-1.17408
H	-0.14295	-2.45372	-0.20771

ja8y-bxs

C	-1.70404	2.34673	-0.58170
B	-1.36044	0.79785	-0.51280
N	-1.55408	0.06353	0.87647
B	-0.30788	-0.20596	1.89957
O	0.33440	0.53792	-0.71323
C	1.32896	0.96479	-0.13892
C	2.50638	-0.00322	0.04256
O	3.48494	0.30793	0.67259
O	-1.90881	-0.05068	-1.48540
C	-1.87083	-1.37306	-0.96569
C	-2.25051	-1.21298	0.50977
C	-3.75538	-1.07716	0.69564
C	1.58958	2.36901	0.27630
O	2.30742	-1.15388	-0.57483
C	3.34453	-2.12652	-0.36131
H	-0.86368	-1.78925	-1.06133
H	-2.57789	-1.99850	-1.51115
H	-1.85220	-2.01664	1.12681
H	-3.99855	-0.82433	1.73025
H	-4.14735	-0.30011	0.03532
H	-4.25438	-2.01667	0.45295
H	0.36233	-1.10316	1.42846
H	-0.79496	-0.50654	2.96883
H	0.31327	0.84755	1.98820
H	-2.78186	2.45308	-0.73224
H	-1.44938	2.89113	0.33101
H	-1.21547	2.83909	-1.42514
H	3.04493	-2.99756	-0.93346

H	4.29799	-1.73562	-0.71032
H	3.40915	-2.35841	0.69968
H	2.25536	2.80149	-0.47933
H	0.67123	2.94156	0.32554
H	2.12159	2.37711	1.22407
H	-2.19580	0.63575	1.42001

ja20-rs7

C	-2.84988	-1.52463	0.06844
C	-3.19213	-0.21619	-0.64691
C	-1.85787	0.53572	-0.58110
N	-0.87678	-0.53286	-0.79173
C	-1.45182	-1.85677	-0.45791
C	0.35555	-0.38805	-1.24568
C	0.94253	0.97423	-1.47171
C	1.66921	1.43966	-0.17960
C	2.55674	0.32170	0.36426
C	1.81564	-0.99387	0.62804
O	0.76748	-0.95574	1.38272
C	-1.75735	1.24866	0.78840
O	-0.91571	0.80340	1.67943
C	2.74555	-2.16680	0.90999
C	2.47697	2.70121	-0.47571
C	1.27502	-1.44673	-1.18129
O	-2.52156	2.17340	0.96615
H	0.20226	1.71691	-1.76660
H	1.67919	0.89696	-2.27490
H	2.97606	0.63971	1.32479
H	3.39675	0.14436	-0.31639
H	0.91884	1.67413	0.57459
H	0.91627	-2.46188	-1.08202
H	2.17254	-1.33831	-1.77665
H	-1.78240	1.29883	-1.35168
H	2.16041	-3.08142	0.99875
H	3.23162	-1.98250	1.87199
H	3.51298	-2.28793	0.14461
H	-1.48927	-2.45791	-1.37073
H	-0.82745	-2.34454	0.28446
H	-3.55934	-2.32631	-0.12998
H	-3.45856	-0.40524	-1.68928
H	-2.80621	-1.35764	1.14593
H	-3.98193	0.36098	-0.17255
H	-0.18697	0.04203	1.43484
H	2.96501	3.06601	0.42944
H	1.83588	3.49845	-0.85727
H	3.25113	2.49805	-1.22096

ja20-sr7

C	2.93322	-1.45775	0.24936
C	1.99783	-0.32522	0.69475
N	0.66779	-0.89261	0.39943
C	0.75697	-2.03055	-0.53351
C	2.21473	-1.98917	-0.99184
C	2.44511	0.99182	0.00435
O	1.67707	1.59823	-0.84606
C	-0.45204	-0.50159	0.98141
C	-0.60147	0.80874	1.45488
C	-1.70708	-1.31590	0.84808
C	-2.61095	-0.78424	-0.29322
C	-3.97363	-1.46857	-0.23435
C	-2.72412	0.73435	-0.19686
C	-1.34696	1.38565	-0.26932
O	-0.61050	0.91905	-1.23091
C	-1.31468	2.88895	-0.04943
O	3.55420	1.37189	0.32535
H	-1.82260	3.18463	0.86942
H	-1.81872	3.35803	-0.89931
H	-0.28224	3.23682	-0.03527
H	-1.39646	0.99423	2.16560
H	-3.29756	1.10561	-1.05300
H	-3.25596	1.03472	0.71161
H	-1.49335	-2.37420	0.69616
H	0.54195	-2.96411	-0.00702
H	-2.25814	-1.22001	1.78785
H	0.27502	1.43421	1.56976
H	0.04316	-1.89226	-1.34337
H	-2.13064	-1.00645	-1.24716
H	2.06397	-0.13172	1.76494
H	3.93364	-1.07681	0.06456
H	2.56784	-2.96576	-1.31924
H	2.32372	-1.28133	-1.81599
H	2.97911	-2.23071	1.02027
H	0.65274	1.23336	-1.04302
H	-3.87536	-2.55389	-0.30860
H	-4.48150	-1.23828	0.70618
H	-4.61093	-1.13023	-1.05318

ja37f-ts4a

C	3.47818	-0.54583	-0.85065
C	2.12725	-0.55878	-0.51881
C	1.59603	-1.72356	0.04122
C	2.41851	-2.81130	0.31470
C	3.77332	-2.78706	0.01597
C	4.28902	-1.64215	-0.57793
C	1.22642	0.63817	-0.83307
C	0.14633	0.07928	-1.81671
N	-0.95707	1.00665	-2.10278

C	-0.91094	1.45170	-3.50073
C	-0.25397	0.27056	-4.21476
C	0.76271	-0.25366	-3.19224
C	-2.06681	0.86407	-1.36472
C	-3.33794	1.42777	-1.60005
C	-4.42694	1.12052	-0.78753
C	-4.35459	0.45059	0.42983
C	1.78074	-4.01055	0.95064
F	1.19702	-3.68233	2.11876
C	5.75637	-1.55527	-0.87493
F	6.44019	-1.06525	0.17392
C	0.58862	1.25375	0.42171
C	0.58993	0.66231	1.68257
C	0.02628	1.32119	2.77337
C	-0.54255	2.57818	2.64378
C	-0.55563	3.16460	1.38310
C	-0.00443	2.51505	0.28649
C	-1.28043	4.46056	1.17642
F	-1.37869	5.16414	2.31428
C	-0.03901	0.61293	4.09263
F	-1.13873	-0.16782	4.16559
O	1.93285	1.65410	-1.51513
Si	3.04244	2.84361	-1.03365
C	2.28470	4.52801	-1.36808
C	4.53254	2.68262	-2.17279
C	3.54615	2.66816	0.76892
F	-0.66886	5.23841	0.26554
F	-2.53000	4.24547	0.72784
F	-0.10270	1.47381	5.11911
F	1.02037	-0.18553	4.28632
F	0.81440	-4.52450	0.16950
F	2.66741	-4.98544	1.19750
F	6.00295	-0.74157	-1.91761
F	6.27749	-2.75810	-1.16055
N	-3.65154	-1.47038	-0.64017
C	-2.80430	-1.85382	0.42533
O	-1.59438	-1.73519	0.48092
N	-2.95799	-1.17511	-1.69264
C	-3.76490	-1.01263	-2.85724
O	-5.08204	-1.29950	-2.78642
C	-5.56188	-2.58457	-2.33103
C	-6.62951	-2.37802	-1.28047
O	-3.28581	-0.58965	-3.88232
O	-3.54155	-2.37759	1.40280
C	-2.80837	-2.86517	2.55031
C	-2.21879	-4.23398	2.27010
H	-0.30395	-0.80228	-1.36355
H	-1.91068	1.65254	-3.87337
H	-0.30140	2.35685	-3.56524
H	-1.02445	-0.47222	-4.40895

H	0.21220	0.56312	-5.15547
H	0.93189	-1.32507	-3.28833
H	1.71715	0.25862	-3.30091
H	-1.87565	0.39835	-0.41089
H	-3.52545	1.92046	-2.54421
H	-5.40334	1.21341	-1.25290
H	1.52565	4.81245	-0.64086
H	3.06861	5.28942	-1.34894
H	1.83023	4.54771	-2.36194
H	5.18956	1.84072	-1.94948
H	4.20239	2.58584	-3.20978
H	5.13334	3.59305	-2.10165
H	2.74076	2.95453	1.44728
H	3.85533	1.65040	1.01554
H	4.39684	3.32850	0.95837
H	-0.02468	2.99045	-0.68390
H	-0.97137	3.08518	3.49648
H	1.04302	-0.30331	1.84846
H	0.54084	-1.80004	0.27618
H	4.40515	-3.63787	0.22700
H	3.90026	0.31074	-1.35001
H	-2.03668	-2.14376	2.81059
H	-3.55275	-2.90310	3.34189
H	-5.96851	-3.07595	-3.21604
H	-1.47985	-4.17961	1.47287
H	-1.72422	-4.60996	3.16738
H	-3.00534	-4.93371	1.98633
H	-6.18161	-1.94831	-0.38649
H	-7.40328	-1.70945	-1.66005
H	-7.09204	-3.33367	-1.02617
H	-4.73647	-3.17701	-1.94458
C	-3.36075	0.81777	1.50931
H	-2.70243	0.01695	1.84891
H	-2.74260	1.64969	1.17916
H	-3.92149	1.14815	2.38790
H	-5.28132	0.02185	0.79118

ja37f-ts4b

C	3.60123	-0.28250	-0.81296
C	2.25191	-0.41523	-0.50537
C	1.80537	-1.63503	0.01173
C	2.70859	-2.65948	0.27074
C	4.06277	-2.51664	-0.00207
C	4.49332	-1.31941	-0.55748
C	1.26300	0.71250	-0.80067
C	0.27485	0.10313	-1.85121
N	-0.87022	0.96106	-2.17669
C	-0.84234	1.37117	-3.58480
C	-0.08291	0.22456	-4.25019

C	0.97081	-0.15436	-3.20279
C	-1.97460	0.80169	-1.43480
C	-3.24388	1.35886	-1.64461
C	-4.29541	1.11607	-0.75411
C	-4.18766	0.38707	0.41239
C	-5.37943	0.02082	1.24167
C	2.16601	-3.91598	0.88379
F	1.18606	-4.44419	0.12908
C	5.93195	-1.13794	-0.94005
F	6.34286	0.12401	-0.70992
C	0.53106	1.20967	0.45670
C	0.60070	0.59832	1.70669
C	-0.07327	1.14088	2.79833
C	-0.83639	2.29238	2.67535
C	-0.90638	2.90469	1.42943
C	-0.22391	2.38250	0.33881
C	-1.78363	4.10741	1.24628
F	-1.88933	4.81790	2.38099
C	-0.00624	0.45052	4.12808
F	-1.04431	-0.39489	4.29732
O	1.90057	1.81453	-1.41145
Si	2.83993	3.09273	-0.80845
C	1.92058	4.69813	-1.12617
C	4.41599	3.12462	-1.83648
C	3.25484	2.88862	1.01369
F	-1.30857	4.92828	0.29225
F	-3.02612	3.75470	0.88038
F	-0.05579	1.32911	5.14157
F	1.11493	-0.27191	4.26172
F	3.11122	-4.85329	1.04162
F	1.62817	-3.66940	2.09321
F	6.13113	-1.37992	-2.24615
F	6.73770	-1.96096	-0.25254
N	-3.53039	-1.55884	-0.69778
C	-2.65086	-1.90145	0.36460
O	-1.45447	-1.68695	0.42694
N	-2.85228	-1.23601	-1.74722
C	-3.66513	-1.07015	-2.91318
O	-4.98639	-1.32731	-2.81780
C	-5.44591	-2.65076	-2.45926
C	-6.54931	-2.52379	-1.43487
O	-3.17417	-0.68697	-3.94685
O	-3.34566	-2.50797	1.32504
C	-2.58574	-2.91213	2.48862
C	-1.84603	-4.20996	2.22873
H	-0.13294	-0.81817	-1.43706
H	-1.85163	1.47549	-3.97144
H	-0.30634	2.31993	-3.67394
H	-0.78447	-0.59291	-4.40871
H	0.35737	0.51253	-5.20461

H	1.29166	-1.19182	-3.28443
H	1.84636	0.48779	-3.29217
H	-1.76522	0.35035	-0.47845
H	-3.45166	1.88796	-2.56473
H	-5.29256	1.37902	-1.09252
H	-3.23027	0.35668	0.92309
H	-6.30075	0.12718	0.66851
H	-5.44601	0.65930	2.12792
H	-5.29842	-1.01193	1.58505
H	2.60021	5.54255	-0.98588
H	1.56139	4.73041	-2.15779
H	1.06686	4.84338	-0.46466
H	5.15126	2.37770	-1.53188
H	4.18814	2.96875	-2.89340
H	4.88914	4.10526	-1.74100
H	4.04105	3.60362	1.27140
H	2.39655	3.08317	1.65849
H	3.63181	1.88797	1.23640
H	-0.27739	2.88583	-0.61548
H	-1.34809	2.71392	3.52943
H	1.19581	-0.28823	1.86311
H	0.75523	-1.79484	0.23102
H	4.75943	-3.31481	0.20894
H	3.95918	0.62686	-1.26955
H	-1.90634	-2.10729	2.75791
H	-3.33777	-3.02949	3.26517
H	-5.80665	-3.10649	-3.38249
H	-1.09966	-4.08198	1.44709
H	-1.33441	-4.52668	3.13923
H	-2.54642	-4.99162	1.93319
H	-6.13865	-2.11923	-0.51204
H	-7.33119	-1.86009	-1.80631
H	-6.98987	-3.50253	-1.23562
H	-4.61783	-3.23990	-2.07184

jo1f-ts1

C	2.59680	-1.20814	0.25923
C	1.40432	-2.10859	-0.13680
N	0.24982	-1.19931	-0.09701
C	0.73979	0.01328	-0.15956
N	2.12324	0.07529	-0.24182
N	0.20190	1.22139	-0.08219
C	1.26897	2.21864	-0.12426
C	2.50761	1.38551	0.27042
N	-2.26565	-1.67440	-0.27367
C	-2.97825	-1.03896	0.57508
H	-0.84977	1.42664	-0.09706
C	-2.59538	1.54741	-0.07816
N	-3.74493	1.32746	-0.06878

H	-1.06007	-1.52464	-0.22975
H	3.53307	-1.51059	-0.20612
H	2.72472	-1.17778	1.34953
H	1.27113	-2.94248	0.55139
H	1.54882	-2.50975	-1.14459
H	1.07173	3.03165	0.57161
H	1.38155	2.63143	-1.13004
H	3.42500	1.75032	-0.18717
H	2.63043	1.35684	1.36108
H	-2.74742	-2.06004	-1.07660
H	-4.05572	-0.99013	0.51984
H	-2.48731	-0.58924	1.42639

jo1f-ts2

C	2.28481	-1.54077	0.34309
C	0.95728	-2.22576	-0.04647
N	0.00906	-1.10558	-0.06502
C	0.70538	0.00302	-0.17358
N	2.06748	-0.20930	-0.21355
N	0.40541	1.28582	-0.17789
C	1.64318	2.06589	-0.20856
C	2.69392	1.02795	0.24424
N	-2.57820	-1.42000	-0.42807
C	-3.39901	-0.81704	0.37286
H	-0.56823	1.68237	-0.14531
C	-3.04750	1.37501	0.25948
N	-2.18381	2.13240	0.03864
H	-1.09999	-1.24008	-0.21500
H	3.15570	-2.02641	-0.09172
H	2.39922	-1.49101	1.43314
H	0.64895	-2.98175	0.67256
H	1.03137	-2.68519	-1.03525
H	1.57747	2.91896	0.46272
H	1.85050	2.42089	-1.22011
H	3.66620	1.18524	-0.21724
H	2.80289	1.02572	1.33581
H	-2.95505	-1.50813	-1.36565
H	-4.44852	-0.67722	0.14287
H	-3.12840	-0.73661	1.41813

jo5k-enda

C	2.64598	-1.09152	0.61799
C	0.20783	-1.10498	1.21092
O	0.46421	-0.41016	2.22137
N	1.26463	-1.38038	0.31152
C	4.30877	0.78601	0.77227
O	2.38293	-2.54658	-1.24801
C	1.18018	-2.57104	-0.50256

H	5.71003	2.41350	0.85808
C	3.36390	-2.11550	-0.30842
H	1.17360	-3.48290	0.12521
C	-0.06831	-2.51891	-1.34492
H	3.71170	-2.97681	0.27515
H	4.94515	0.11157	1.33889
C	-1.27402	-2.47939	-0.38560
H	2.87129	-1.30217	1.66983
H	1.98654	3.20126	-1.14316
H	4.23411	3.97762	-0.38732
C	-1.06266	-1.54888	0.78541
H	4.19665	-1.68157	-0.85787
H	1.26333	0.89454	-0.69180
C	2.23948	1.22458	-0.36565
C	4.73815	2.08367	0.50770
C	3.05814	0.34207	0.33366
C	2.65781	2.52903	-0.62217
C	3.91012	2.96173	-0.19213
H	-0.00967	-1.61565	-1.95749
H	-1.47577	-3.50800	-0.04985
H	-2.16743	-2.18159	-0.95362
H	-0.12204	-3.38546	-2.00922
H	-1.84426	-1.49074	1.53083
C	-1.44933	0.72113	-0.19700
H	-0.82799	0.98818	0.64263
H	-0.98976	0.21840	-1.02973
Cl	-1.38041	2.65267	-1.14329
C	-2.89104	0.52641	0.02760
C	-3.72034	0.06107	-0.99809
C	-3.46299	0.84602	1.26555
C	-5.08541	-0.11146	-0.78308
H	-3.28905	-0.14347	-1.97160
C	-4.82489	0.67814	1.47883
H	-2.81850	1.20658	2.05917
C	-5.64436	0.19350	0.45616
H	-5.71419	-0.47653	-1.58740
H	-5.25123	0.92181	2.44531
H	-6.70726	0.06252	0.62352

jo5k-exb

C	1.57510	0.54195	-0.73042
C	0.13330	-1.06689	0.55020
O	0.45425	-1.97690	-0.25250
N	0.62923	0.21621	0.30297
C	3.76051	-0.26894	-1.68232
O	1.32100	2.29266	0.82812
C	0.25602	1.38181	1.07488
H	5.66988	-0.91324	-2.43164
C	1.64493	2.07829	-0.54109

H	-0.67644	1.82166	0.69215
H	-0.93299	-2.20359	1.96924
C	0.10801	1.02941	2.53518
H	0.89819	2.56824	-1.17726
H	3.37839	-0.00863	-2.66474
C	-0.96282	-0.06867	2.64478
H	1.19274	0.29204	-1.72631
H	5.07421	-1.27423	1.80250
H	6.53093	-1.54587	-0.18849
C	-0.74217	-1.18600	1.65453
H	2.63422	2.48972	-0.73096
H	2.77657	-0.36755	1.54787
C	3.42610	-0.46959	0.68759
C	5.04922	-0.78171	-1.55243
C	2.93992	-0.10232	-0.56611
C	4.71305	-0.98376	0.82257
C	5.53193	-1.13893	-0.29503
H	1.07348	0.66563	2.89730
H	-1.94631	0.41462	2.50662
H	-0.96233	-0.45929	3.66791
H	-0.17110	1.92016	3.10444
C	-2.77673	-1.50205	0.25120
H	-2.10448	-2.24704	-0.14180
H	-3.17149	-1.64196	1.24228
Cl	-4.54822	-2.26550	-0.71516
C	-2.69021	-0.13269	-0.27396
C	-3.43305	0.90338	0.30753
C	-1.91450	0.14626	-1.40778
C	-3.38375	2.19317	-0.21331
H	-4.07075	0.68083	1.15569
C	-1.86586	1.43499	-1.92593
H	-1.33959	-0.65600	-1.85613
C	-2.59632	2.46673	-1.33127
H	-3.96383	2.98369	0.24927
H	-1.25491	1.63786	-2.79908
H	-2.55710	3.47012	-1.73968

jo8a-7

C	1.80401	-2.46483	0.83936
C	-0.27387	-1.78997	0.18324
C	-0.90024	-2.40838	1.40752
C	-0.10245	-3.63629	1.86081
C	1.35000	-3.20420	2.06774
C	2.25991	-1.16810	0.91079
N	2.77807	-0.45422	-0.09120
C	3.05191	-1.01099	-1.41162
C	2.95368	1.00176	-0.05033
C	3.94492	0.05400	-2.04730
C	3.36307	1.35547	-1.49165

C	1.70424	1.79964	0.36710
O	1.73143	3.01287	0.13103
O	0.75274	1.15393	0.92287
H	2.00112	-3.05174	-0.05023
H	0.02283	-0.75726	0.15444
H	-0.13504	-2.38833	-0.70259
H	-1.92518	-2.69970	1.18537
H	-0.93195	-1.65981	2.20325
H	-0.14974	-4.40015	1.07817
H	-0.53611	-4.06919	2.76510
H	1.40854	-2.53915	2.93486
H	1.98825	-4.06717	2.27724
H	2.12601	-0.61608	1.83273
H	3.54131	-1.98109	-1.31387
H	2.11984	-1.14520	-1.97298
H	3.75151	1.25974	0.65306
H	4.97319	-0.08337	-1.70643
H	3.93217	0.01169	-3.13551
H	4.05298	2.19526	-1.51618
H	2.47291	1.64261	-2.05321
H	-0.38178	2.06860	0.99310
I	-2.48842	-0.81142	-1.12342
N	-1.21778	2.80313	0.97028
C	-0.76431	3.98842	1.72738
C	-1.42845	3.13083	-0.45986
C	-2.41992	2.18646	1.56930
H	-0.62130	3.70282	2.76835
H	0.18318	4.30600	1.29925
H	-1.51988	4.77221	1.65858
H	-2.21033	3.88732	-0.54213
H	-1.72616	2.22072	-0.97911
H	-0.48387	3.50136	-0.85130
H	-2.19076	1.90058	2.59463
H	-2.68873	1.30611	0.98660
H	-3.23730	2.90917	1.56041

jo8a-8

C	1.24716	-2.26758	1.09122
C	1.95316	-2.12399	-0.07898
N	2.62965	-1.05094	-0.50157
C	3.28992	-1.02014	-1.81476
C	3.06559	0.05820	0.35941
C	4.05943	0.30263	-1.79985
C	4.35907	0.51509	-0.31246
C	1.99473	1.17118	0.41117
O	2.19293	2.22902	-0.20053
O	0.96100	0.88479	1.10526
C	-0.71951	-1.60366	0.18740
C	-1.40153	-2.89345	0.57194

C	-0.74797	-3.50087	1.81712
C	0.75015	-3.61287	1.54432
H	1.27365	-1.45866	1.81144
H	1.94011	-2.94459	-0.79357
H	3.96638	-1.87576	-1.90486
H	2.55362	-1.07132	-2.61757
H	3.20869	-0.32450	1.37216
H	4.95335	0.25963	-2.42055
H	3.42109	1.11433	-2.14517
H	5.18685	-0.12171	0.00889
H	4.58115	1.55262	-0.07731
H	0.06132	2.02466	0.93874
H	-0.31972	-1.44163	-0.79620
H	-0.63119	-0.77775	0.87235
H	-1.34965	-3.59326	-0.26510
H	-2.45444	-2.70096	0.76724
H	-1.19875	-4.46540	2.06012
H	-0.91414	-2.83568	2.67008
H	1.28742	-3.95343	2.43412
H	0.92262	-4.35585	0.75864
I	-2.86690	-0.22951	-0.88097
N	-0.54985	2.95583	0.86197
C	-1.81871	2.75267	1.59189
C	0.27221	4.01880	1.47590
C	-0.78297	3.22703	-0.57602
H	-2.37297	1.94743	1.11154
H	-2.39988	3.67586	1.56794
H	-1.58854	2.48648	2.62233
H	1.22032	4.04779	0.94501
H	0.44259	3.76640	2.52132
H	-0.25405	4.97159	1.40359
H	0.18926	3.26803	-1.06030
H	-1.31573	4.17409	-0.67731
H	-1.37795	2.41269	-0.98672

jo8v-ts2a

O	-0.15357	1.64051	0.45781
C	-0.92367	2.40905	-0.16998
H	-1.02781	2.31549	-1.25015
H	-1.15501	3.37266	0.28008
C	-2.98926	1.92078	0.32621
H	-3.50335	2.69352	-0.22833
H	-2.83760	2.04664	1.38987
C	-2.89053	0.67889	-0.21370
H	-3.16007	0.48259	-1.24957
O	-2.37816	-0.32524	0.46947
Si	-2.36589	-1.96241	-0.04113
H	-2.88087	-1.97361	-1.43314
H	-0.98947	-2.47794	0.07379

H	-3.29282	-2.67754	0.86715
Ti	1.05115	0.05720	0.04446
Cl	0.57944	-0.61511	2.10583
Cl	2.12323	-1.81787	-0.49506
Cl	2.75561	1.42341	-0.06358
Cl	-0.16894	-0.05754	-1.89574

jo8v-ts2b

O	0.55574	0.59313	0.79997
C	1.07330	1.75417	0.98779
H	1.70809	1.87080	1.86591
H	0.48450	2.63531	0.72695
C	2.32538	2.17801	-0.47334
H	2.70713	3.15734	-0.21586
H	1.61222	2.10242	-1.28468
C	3.09523	1.08147	-0.17267
H	3.92895	1.15076	0.52778
O	2.76020	-0.10030	-0.59341
Si	3.23189	-1.57832	0.16681
H	2.41645	-1.80275	1.37566
H	3.11973	-2.62455	-0.86299
H	4.65069	-1.33101	0.54899
Ti	-1.15911	-0.08671	0.03994
Cl	-1.19390	1.83563	-1.15008
Cl	-3.04025	-0.79841	-0.92125
Cl	-1.99066	-0.02139	2.08788
Cl	-0.00252	-1.90870	-0.58119

jo15c-3ars

C	3.16897	-1.36193	0.30088
C	1.94326	-0.64133	-0.25505
C	1.95223	0.83691	0.09412
C	1.40842	1.26075	1.27051
O	0.77812	-1.24834	0.21735
Ti	-0.94828	-0.65147	-0.03817
O	-1.89634	-1.12371	1.44922
O	-1.45363	-1.55586	-1.54709
O	-1.94535	1.00422	-0.62624
C	-2.77935	1.79216	0.18679
O	-0.27882	1.16304	0.00126
H	-2.01558	-1.17349	-2.22579
H	-2.50524	-1.85313	1.57896
H	-2.71136	1.51402	1.24357
H	-2.52895	2.85022	0.06333
H	-3.80800	1.62692	-0.15766
H	1.41233	2.31101	1.53872
H	1.04996	0.55635	2.01200
C	2.58722	1.77075	-0.88027

H	1.97130	-0.72228	-1.35422
H	3.14309	-2.40925	-0.00758
H	4.09647	-0.91481	-0.06852
H	3.16935	-1.32199	1.39282
H	2.57546	2.80250	-0.52646
H	3.62820	1.48070	-1.06412
H	2.06868	1.72694	-1.84302

jo15c-3ass

C	-3.25210	-1.11902	-0.53348
C	-1.95157	-0.36268	-0.75143
O	-0.86379	-1.13102	-0.30932
Ti	0.85714	-0.66383	0.12251
O	0.39148	1.23560	0.04476
C	-1.87247	0.97264	-0.03276
C	-2.29767	1.04504	1.39597
C	-1.33055	2.04395	-0.68482
O	1.85810	-1.34378	-1.26104
O	1.09972	-1.49357	1.73505
O	2.11975	0.83967	0.46659
C	2.94641	1.46350	-0.48172
H	1.84369	-1.33822	2.32169
H	1.61444	-2.08647	-1.81736
H	2.71852	1.14410	-1.50361
H	2.85967	2.55104	-0.39671
H	3.97623	1.16756	-0.24597
H	-1.23792	3.00883	-0.19982
H	-1.10852	2.00165	-1.74521
H	-1.90799	0.19703	1.96624
H	-1.95643	1.96757	1.86652
H	-3.39074	1.00520	1.46616
H	-1.83654	-0.17652	-1.82961
H	-4.10932	-0.53040	-0.87435
H	-3.22533	-2.05099	-1.10183
H	-3.39120	-1.37191	0.51983

jo78-end

C	1.25164	-1.13424	-0.12481
C	0.28372	-0.69030	-1.15181
C	0.28372	0.69029	-1.15181
C	1.25164	1.13424	-0.12481
O	1.71173	0.00000	0.53351
O	1.62089	2.23137	0.17077
O	1.62089	-2.23137	0.17077
C	-1.60149	-1.15513	0.00038
C	-1.21344	-0.70325	1.25680
C	-1.21344	0.70325	1.25680
C	-1.60149	1.15513	0.00038

C	-2.25721	-0.00000	-0.70748
H	-0.84377	-1.32788	2.05749
H	-0.84377	1.32789	2.05748
H	-1.76472	2.19311	-0.25362
H	-0.00302	1.35274	-1.95284
H	-0.00302	-1.35274	-1.95284
H	-1.76472	-2.19311	-0.25361
H	-2.18663	-0.00000	-1.79285
H	-3.32040	-0.00000	-0.43147

jo78-ex

C	2.45303	-0.70355	-0.36464
C	2.45337	0.70369	-0.36414
C	1.43069	1.15671	0.46078
C	-0.25508	0.69000	-1.01603
C	-0.25477	-0.68986	-1.01581
C	1.42982	-1.15668	0.45973
C	1.01406	-0.00017	1.32255
C	-1.36859	-1.13298	-0.14537
C	-1.36877	1.13304	-0.14562
O	-1.96142	-0.00006	0.40403
O	-1.75332	-2.23361	0.11527
O	-1.75386	2.23356	0.11493
H	3.07094	-1.32794	-0.99465
H	3.07158	1.32824	-0.99370
H	1.23346	2.19091	0.70740
H	0.13145	1.35339	-1.77025
H	0.13128	-1.35319	-1.77037
H	1.23257	-2.19096	0.70601
H	-0.00573	0.00007	1.69674
H	1.68068	-0.00086	2.19631

jo82-Esin

C	0.38925	0.09992	0.05807
C	1.55797	-0.21554	-0.66659
C	2.75618	-0.30967	0.12196
O	2.85404	0.09595	1.27593
O	3.80692	-0.85437	-0.53623
C	5.02259	-0.87894	0.21078
C	-0.93353	-0.08066	-0.63310
C	-1.42880	-1.52510	-0.59952
O	-2.83700	-1.36695	-0.60326
O	-1.95723	0.62202	0.07333
C	-3.12400	-0.21499	0.16882
C	-4.30743	0.49243	-0.45458
C	-3.34044	-0.57403	1.62967
H	0.36931	-0.16854	1.11169
H	1.53064	-0.55453	-1.69197

H	4.90537	-1.47574	1.11417
H	5.31900	0.13017	0.49426
H	5.76366	-1.32407	-0.44771
H	-0.87890	0.29153	-1.66084
H	-1.08121	-2.03409	0.30601
H	-1.13866	-2.10258	-1.47319
H	-5.18259	-0.15710	-0.42975
H	-4.07197	0.73712	-1.48965
H	-4.52644	1.40853	0.09425
H	-4.22114	-1.20890	1.72952
H	-3.48290	0.33234	2.21904
H	-2.47174	-1.10763	2.01736
N	0.43401	1.89660	0.32937
O	1.20257	2.41696	-0.67512
H	-0.50618	2.27992	0.29250
H	0.88489	2.05762	1.22757
H	1.64557	1.55029	-1.00903

Jo82-Zsin

C	-0.33076	0.65781	-0.79727
C	-1.67839	0.33283	-1.05836
C	0.60977	-0.24427	-0.04162
C	1.20724	-1.34056	-0.91548
O	2.46520	-1.56421	-0.30138
O	1.76854	0.51619	0.32721
C	2.93156	-0.31188	0.17436
C	3.58798	-0.53398	1.52092
C	3.85182	0.34344	-0.84201
C	-2.44924	-0.34576	-0.05051
O	-2.12376	-0.48334	1.12541
O	-3.64579	-0.78843	-0.50797
C	-4.47757	-1.38235	0.48783
H	0.18622	1.13885	-1.62610
H	-2.10808	0.50043	-2.03369
H	0.13045	-0.66235	0.84159
H	1.32114	-1.00117	-1.95173
H	0.63749	-2.26579	-0.89613
H	4.43186	-1.21597	1.41398
H	2.86098	-0.97124	2.20458
H	3.94290	0.41408	1.92588
H	4.74966	-0.26035	-0.97522
H	4.13693	1.33973	-0.50214
H	3.33852	0.43365	-1.80029
H	-4.69217	-0.67012	1.28340
H	-3.99297	-2.25564	0.92171
H	-5.39135	-1.66857	-0.02573
N	-0.35681	2.07068	0.37945
O	-1.54358	2.71865	0.17353
H	-0.32550	1.69049	1.32388

H	0.42128	2.70152	0.22087
H	-2.02906	2.01517	-0.38267

jo82-coll5a

C	-2.62137	-0.03294	0.04440
H	-1.48897	-0.09155	-0.50855
H	-2.87311	1.02293	0.06728
H	-3.25508	-0.61287	-0.61981
H	-2.51879	-0.47507	1.03123
O	-0.37490	-0.11036	-1.07337
C	0.63549	0.00754	-0.09451
O	1.82168	0.10548	-0.75247
C	0.70806	-1.25106	0.78667
H	0.86382	-2.12156	0.15143
H	-0.23738	-1.36515	1.31767
H	1.52213	-1.16490	1.50467
C	0.46855	1.28883	0.73988
H	0.41827	2.14584	0.06993
H	1.30879	1.40126	1.42320
H	-0.45833	1.22591	1.31096

jo82-perp5a

C	2.61047	-0.11110	-0.00928
H	1.48970	-0.50481	-0.39237
H	3.22145	-1.00851	-0.03639
H	2.93046	0.65039	-0.71431
H	2.44062	0.26086	0.99643
O	0.30645	-0.88650	-0.63722
C	-0.55043	-0.02622	0.05690
O	-0.33232	0.01011	1.40754
C	-1.96251	-0.56902	-0.22270
H	-2.03268	-1.59211	0.14289
H	-2.14581	-0.55872	-1.29627
H	-2.69255	0.05657	0.28918
C	-0.41113	1.43616	-0.41536
H	-0.51180	1.44273	-1.50039
H	0.57005	1.82691	-0.14575
H	-1.18089	2.05890	0.03703

jo90-5conc2

P	-2.36415	-0.11586	0.02841
Pd	-0.16636	-0.79615	0.04943
Br	2.21788	-1.28863	0.03400
C	1.71389	0.64200	-1.04018
H	2.75837	0.74352	-1.33884
H	1.10172	0.43916	-1.92057
S	1.27198	2.26260	-0.37802

O	-0.20294	2.38984	-0.15113
C	2.04945	2.10989	1.24979
H	1.54857	1.30411	1.79045
H	3.11369	1.89753	1.13265
H	1.90417	3.06614	1.75347
C	-3.65755	-1.42517	0.13847
H	-4.66498	-0.99670	0.13095
H	-3.55477	-2.11219	-0.70448
H	-3.52005	-1.99809	1.05830
C	-2.91633	0.82685	-1.45092
H	-2.78778	0.21391	-2.34593
H	-3.96671	1.12323	-1.36676
H	-2.29072	1.71693	-1.54170
C	-2.86208	1.01534	1.38979
H	-3.91294	1.30893	1.30133
H	-2.70643	0.52126	2.35134
H	-2.22570	1.90115	1.34569

jo90-5sn2

Pd	-1.04849	-0.98287	-0.14580
P	-2.56320	0.69676	0.09559
O	0.62323	-2.37222	-0.38372
S	1.80789	-1.37966	-0.34075
C	0.99915	0.19803	-0.09132
H	0.76102	0.53743	0.90860
H	0.71133	0.73579	-0.98305
C	2.50881	-1.62102	1.30866
H	3.29163	-0.88263	1.47609
H	1.70610	-1.54301	2.04410
H	2.91718	-2.63231	1.30925
Br	3.06143	1.48888	-0.09363
C	-3.17260	1.47258	-1.45736
H	-3.90242	2.26116	-1.24977
H	-2.33119	1.90030	-2.00668
H	-3.63501	0.71109	-2.08867
C	-4.13545	0.25095	0.94020
H	-4.80912	1.11073	1.00712
H	-4.63203	-0.55016	0.38862
H	-3.91823	-0.11497	1.94575
C	-2.01208	2.16377	1.05774
H	-1.12030	2.59641	0.59757
H	-2.79436	2.92747	1.10074
H	-1.75526	1.85919	2.07471

ol1s-ts1rs

C	0.82250	1.73032	-0.10126
C	2.09691	1.37657	0.56347
C	2.15168	1.20012	1.95676

C	3.36570	0.97070	2.59787
C	4.55300	0.95442	1.87336
C	4.51886	1.18258	0.50040
C	3.30625	1.38540	-0.14595
H	0.92206	2.28319	-1.03246
H	1.24544	1.33293	2.53633
H	3.38348	0.83723	3.67286
H	5.49788	0.77773	2.37203
H	5.43712	1.17552	-0.07342
H	3.28572	1.53381	-1.21770
C	-0.13761	3.17781	1.14478
O	-0.64472	2.62679	2.14569
C	-1.01144	3.80020	0.08859
C	-2.37959	3.53573	0.07624
C	-3.19472	4.11143	-0.89314
C	-2.64948	4.96377	-1.85007
C	-1.28347	5.24070	-1.83444
C	-0.47039	4.65971	-0.86822
H	0.85224	3.65858	1.22403
H	-2.78569	2.88248	0.83834
H	-4.25710	3.90058	-0.89979
H	-3.28580	5.41588	-2.60075
H	-0.85713	5.91168	-2.57010
H	0.59387	4.87356	-0.84648
C	-0.19291	-0.83506	-1.51857
C	-0.74957	-1.88856	0.59087
C	0.14219	-2.02280	-0.62698
H	-0.48219	-2.60857	1.37287
O	-2.06239	-2.12172	0.11009
O	1.48255	-1.95026	-0.19007
H	-1.16092	-0.98894	-1.99483
H	-0.04917	-2.97018	-1.14625
C	0.88482	-0.58454	-2.55829
H	0.77184	-1.33211	-3.35496
H	0.79811	0.40793	-2.99975
O	2.17949	-0.66842	-1.99697
C	2.36695	-1.86543	-1.28573
H	2.14375	-2.70732	-1.96281
C	3.79015	-1.92927	-0.80280
C	4.09415	-2.31404	0.49809
C	5.42349	-2.38130	0.90644
C	6.44705	-2.07077	0.01816
C	6.14025	-1.68869	-1.28639
C	4.81472	-1.61779	-1.69629
H	3.29408	-2.53430	1.18999
H	5.65662	-2.66866	1.92393
H	7.47986	-2.12431	0.33891
H	6.93318	-1.44339	-1.98172
H	4.56745	-1.30442	-2.70257
C	-1.77967	-0.10415	2.02534

H	-1.68683	-0.68406	2.95331
H	-1.78398	0.95717	2.25221
O	-3.00310	-0.42807	1.37909
C	-3.05979	-1.78394	1.06072
H	-2.86257	-2.37169	1.97197
C	-4.40599	-2.12412	0.47848
C	-4.55720	-3.28314	-0.28133
C	-5.80610	-3.62525	-0.78732
C	-6.90815	-2.81243	-0.53521
C	-6.75587	-1.65638	0.22365
C	-5.50742	-1.31088	0.73250
H	-3.69502	-3.90537	-0.48160
H	-5.91869	-4.52454	-1.37962
H	-7.88047	-3.07883	-0.92996
H	-7.60903	-1.01915	0.41884
H	-5.37799	-0.41049	1.31630
S	-0.49740	0.61624	-0.36222
C	-0.59902	-0.46364	1.12899
H	0.35193	-0.36202	1.64904

o11s-ts1sr

C	1.11253	1.32646	0.12183
C	1.65062	2.51360	-0.56679
C	1.02330	3.76704	-0.45243
C	1.57638	4.89269	-1.04881
C	2.77730	4.80462	-1.75102
C	3.42031	3.57387	-1.84771
C	2.86299	2.43801	-1.26903
H	1.70006	0.42298	0.01138
H	0.11901	3.84925	0.14110
H	1.07653	5.84846	-0.94875
H	3.20931	5.68550	-2.20862
H	4.35759	3.49317	-2.38515
H	3.35051	1.47575	-1.37184
C	1.00747	1.95242	2.20908
O	-0.15221	2.31612	2.48903
C	1.59370	0.70932	2.83085
C	2.87965	0.27414	2.50353
C	3.40701	-0.86840	3.09189
C	2.65295	-1.58716	4.02043
C	1.37936	-1.14505	4.36762
C	0.85538	0.00437	3.78037
H	1.76907	2.69686	1.93112
H	3.45759	0.83240	1.77403
H	4.40365	-1.19936	2.82694
H	3.06365	-2.47728	4.48087
H	0.80194	-1.68707	5.10690
H	-0.11785	0.38905	4.05906
C	-0.71712	0.01440	-1.80424

C	-1.57847	-1.44996	-0.06568
C	-0.73340	-1.43331	-1.32394
H	-1.53213	-2.41905	0.44369
O	-2.89457	-1.16669	-0.50737
O	0.56798	-1.84190	-0.95432
H	-1.68284	0.27580	-2.23520
H	-1.15057	-2.09722	-2.09083
C	0.40719	0.24643	-2.80667
H	0.10022	-0.19706	-3.76340
H	0.61032	1.30531	-2.95498
O	1.62478	-0.33513	-2.37550
C	1.49168	-1.68460	-2.00830
H	1.12162	-2.25382	-2.87639
C	2.84658	-2.16809	-1.56375
C	3.07399	-2.62670	-0.27002
C	4.35127	-3.04231	0.10002
C	5.39672	-2.99970	-0.81543
C	5.16817	-2.53337	-2.10869
C	3.89648	-2.11694	-2.48078
H	2.26342	-2.65133	0.44434
H	4.52422	-3.39718	1.10821
H	6.38740	-3.32495	-0.52413
H	5.98003	-2.49238	-2.82348
H	3.71387	-1.73893	-3.47950
C	-2.10135	0.07147	1.87357
H	-2.19969	-0.73696	2.61079
H	-1.80579	0.99133	2.36921
O	-3.34876	0.29037	1.23149
C	-3.77517	-0.85394	0.56027
H	-3.76362	-1.70421	1.26138
C	-5.15240	-0.64061	-0.00924
C	-5.61811	-1.48541	-1.01594
C	-6.90320	-1.32373	-1.52067
C	-7.72761	-0.31870	-1.02132
C	-7.26133	0.52368	-0.01725
C	-5.97546	0.36446	0.49143
H	-4.96875	-2.25792	-1.40645
H	-7.26039	-1.97979	-2.30438
H	-8.72827	-0.19224	-1.41487
H	-7.89709	1.30940	0.37058
H	-5.60196	1.01947	1.26577
S	-0.56229	1.04187	-0.25405
C	-1.04639	-0.34820	0.85523
H	-0.12843	-0.66492	1.35027

ol7q-bi

C	0.10008	0.55378	1.72224
C	0.22235	-0.62858	1.03514
H	0.94596	0.88442	2.31059

H	-0.86090	0.98536	1.95168
C	1.52801	-1.38470	1.00811
C	2.08360	-1.46409	-0.41381
H	2.24275	-0.93585	1.69814
B	-1.94324	-0.48224	-0.26991
C	-3.16236	-0.65595	0.75569
H	-3.46461	-1.70487	0.80498
H	-2.91594	-0.33749	1.77238
H	-4.02966	-0.07815	0.42702
C	-2.16278	-0.97207	-1.77844
H	-2.32026	-2.05315	-1.80725
H	-3.03789	-0.49840	-2.22910
H	-1.29577	-0.75058	-2.40970
C	-0.41539	1.46240	-0.32530
O	-1.61907	1.07374	-0.29180
H	0.33275	0.86078	-0.84019
C	-0.13202	2.91202	-0.10461
H	0.89923	3.06229	0.20822
H	-0.28518	3.42990	-1.05681
H	-0.82187	3.32493	0.62841
O	-0.67331	-1.15451	0.24540
H	1.36367	-1.97740	-1.04833
O	2.27405	-0.18774	-1.00309
C	3.28556	0.57756	-0.38252
H	3.48430	1.43041	-1.02970
H	2.97586	0.94468	0.60163
H	4.20662	-0.00576	-0.26943
H	1.33177	-2.40457	1.35064
H	3.02964	-2.01951	-0.41684

ol7q-bo

C	0.58097	-1.34277	1.16139
C	-0.18438	-0.52203	0.37908
H	0.17168	-2.30526	1.43604
H	1.43100	-0.98338	1.71862
H	-1.77166	-1.96341	0.21568
B	1.53827	1.28363	0.00281
C	1.83559	1.94585	1.43131
H	1.22307	2.84284	1.55264
H	1.61826	1.28658	2.27525
H	2.88187	2.25163	1.50623
C	1.75356	2.19715	-1.29252
H	1.03535	3.02075	-1.29571
H	2.75517	2.63237	-1.31276
H	1.60892	1.63611	-2.22126
C	2.16776	-1.05852	-0.56777
O	2.56567	0.03992	-0.10673
H	1.38510	-1.06139	-1.32737
C	3.02547	-2.26928	-0.41869

H	2.42831	-3.17680	-0.47082
H	3.74241	-2.27627	-1.24599
H	3.57631	-2.22146	0.51798
O	0.16636	0.65674	-0.08349
C	-1.51027	-0.97827	-0.16903
C	-2.61356	0.01077	0.18441
H	-1.44881	-1.03234	-1.25996
H	-2.36592	0.99986	-0.21625
O	-3.81298	-0.47612	-0.37667
H	-2.70796	0.09999	1.27568
C	-4.89504	0.38907	-0.11843
H	-5.77884	-0.04560	-0.58156
H	-5.07017	0.49694	0.95891
H	-4.71846	1.38455	-0.54281

Frequencies at which the RMSD differences were higher than 0.2 Å, 0.3 Å and 0.4 Å.

	HF	BLYP	HCTH	B3LYP	B3P86	B3PW91	PBE1PBE	O3LYP	BHANDHLYP	BMK	MPWB1K	M05(-2X)	M05(-2X)-UF
HF		8	7	6	6	6	7	6	6	6	7	7	7
BLYP	8		2	3	5	5	5	3	4	4	6	6	7
HCTH	7	2		2	2	2	2	2	2	2	4	4	4
B3LYP	6	3	2		0	0	1	1	0	0	1	3	3
B3P86	6	5	2	0		0	1	1	0	0	1	2	2
B3PW91	6	5	2	0	0		1	1	0	1	2	3	3
PBE1PBE	7	5	2	1	1	1		2	1	1	0	2	2
O3LYP	6	3	2	1	1	1	2		1	4	6	4	5
BHANDHLYP	6	4	2	0	0	0	1	1		0	1	3	3
BMK	6	4	2	0	0	1	1	4	0		1	3	2
MPWB1K	7	6	4	1	1	2	0	6	1	1		2	2
M05(-2X)	7	6	4	3	2	3	2	4	3	3	2		0
M05(-2X)-UF	7	7	4	3	2	3	2	5	3	2	2	0	

	HF	BLYP	HCTH	B3LYP	B3P86	B3PW91	PBE1PBE	O3LYP	BHANDHLYP	BMK	MPWB1K	M05(-2X)	M05(-2X)-UF
HF		8	7	6	7	7	7	6	6	6	11	7	7
BLYP	8		4	5	5	5	5	5	5	6	8	8	8
HCTH	7	4		2	2	2	2	3	6	9	8	7	
B3LYP	6	5	2		0	0	1	1	0	1	7	4	4
B3P86	7	5	2	0		0	1	1	0	0	4	4	4
B3PW91	7	5	2	0	0		2	1	0	2	4	4	4
PBE1PBE	7	5	2	1	1	2		2	1	1	1	4	4
O3LYP	6	5	2	1	1	1	2		2	6	10	9	9
BHANDHLYP	6	5	3	0	0	0	1	2		0	2	4	4
BMK	6	6	6	1	0	2	1	6	0		3	4	4
MPWB1K	11	8	9	7	4	4	1	10	2	3		5	5
M05(-2X)	7	8	8	4	4	4	4	9	4	4	5		0
M05(-2X)-UF	7	8	7	4	4	4	4	9	4	4	5	0	

	HF	BLYP	HCTH	B3LYP	B3P86	B3PW91	PBE1PBE	O3LYP	BHANDHLYP	BMK	MPWB1K	M05(-2X)	M05(-2X)-UF
HF		12	11	8	11	11	11	12	6	11	15	12	12
BLYP	12		5	5	5	5	6	5	8	8	13	11	11
HCTH	11	5		3	7	4	8	2	6	11	13	10	10
B3LYP	8	5	3		0	1	1	3	1	4	11	9	9
B3P86	11	5	7	0		1	1	7	3	3	7	7	5
B3PW91	11	5	4	1	1		2	4	3	6	10	9	9
PBE1PBE	11	6	8	1	1	2		10	2	2	5	5	4
O3LYP	12	5	2	3	7	4	10		9	11	14	12	11
BHANDHLYP	6	8	6	1	3	3	2	9		4	11	5	5
BMK	11	8	11	4	3	6	2	11	4		7	8	6
MPWB1K	15	13	13	11	7	10	5	14	11	7		10	11
M05(-2X)	12	11	10	9	7	9	5	12	5	8	10		0
M05(-2X)-UF	12	11	10	9	5	9	4	11	5	6	11	0	

Frequencies at which the maximum deviations distances of bonds forming (or breaking) in the TS were higher than 0.1 Å, 0.2 Å and 0.4 Å.

	HF	BLYP	HCTH	B3LYP	B3P86	B3PW91	PBE1PBE	O3LYP	BHANDHLYP	BMK	MPWB1K	M05(-2X)	M05(-2X)-UF
HF		18	15	17	18	18	20	16	14	18	18	17	17
BLYP	18		4	5	12	11	13	5	12	15	13	10	11
HCTH	15	4		8	11	10	11	2	14	14	10	10	10
B3LYP	17	5	8		6	3	9	6	5	6	8	8	9
B3P86	18	12	11	6		0	0	10	9	7	8	7	7
B3PW91	18	11	10	3	0		0	8	9	5	5	4	4
PBE1PBE	20	13	11	9	0	0		11	9	6	5	6	5
O3LYP	16	5	2	6	10	8	11		13	11	10	10	10
BHANDHLYP	14	12	14	5	9	9	9	13		5	4	9	10
BMK	18	15	14	6	7	5	6	11	5		2	8	8
MPWB1K	18	13	10	8	8	5	5	10	4	2		3	2
M05(-2X)	17	10	10	8	7	4	6	10	9	8	3		0
M05(-2X)-UF	17	11	10	9	7	4	5	10	10	8	2	0	

	HF	BLYP	HCTH	B3LYP	B3P86	B3PW91	PBE1PBE	O3LYP	BHANDHLYP	BMK	MPWB1K	M05(-2X)	M05(-2X)-UF
HF		13	11	10	11	11	8	6	10	9	13	13	
BLYP	13		3	2	5	2	5	2	5	4	6	6	6
HCTH	11	3		2	6	3	9	0	6	7	7	7	1
B3LYP	10	2	2		3	1	3	2	0	0	2	1	1
B3P86	11	5	6	3		0	0	4	3	2	1	0	0
B3PW91	11	2	3	1	0		0	1	3	1	1	0	0
PBE1PBE	11	5	9	3	0	0		4	3	2	1	0	0
O3LYP	8	2	0	2	4	1	4		4	3	5	3	3
BHANDHLYP	6	5	6	0	3	3	3	4		0	1	3	4
BMK	10	4	7	0	2	1	2	3	0		0	1	1
MPWB1K	9	6	7	2	1	1	1	5	1	0		0	0
M05(-2X)	13	6	7	1	0	0	0	3	3	1	0		0
M05(-2X)-UF	13	6	6	1	0	0	0	3	4	1	0	0	

	HF	BLYP	HCTH	B3LYP	B3P86	B3PW91	PBE1PBE	O3LYP	BHANDHLYP	BMK	MPWB1K	M05(-2X)	M05(-2X)-UF
HF		4	2	3	5	3	5	2	1	3	3	4	4
BLYP	4		1	2	2	2	2	2	2	2	2	2	2
HCTH	2	1		0	0	0	0	0	1	0	1	1	1
B3LYP	3	2	0		0	0	0	0	0	0	0	0	0
B3P86	5	2	0	0		0	0	0	2	0	0	0	0
B3PW91	3	2	0	0	0		0	0	1	0	0	0	0
PBE1PBE	5	2	0	0	0	0		0	2	0	0	0	0
O3LYP	2	2	0	0	0	0	0		1	0	0	1	1
BHANDHLYP	1	2	1	0	2	1	2	1		0	0	0	0
BMK	3	2	0	0	0	0	0	0	0		0	0	0
MPWB1K	3	2	1	0	0	0	0	0	0	0		0	0
M05(-2X)	4	2	1	0	0	0	0	1	0	0	0		0
M05(-2X)-UF	4	2	1	0	0	0	0	1	0	0	0	0	

Times that maximum dihedral angle deviations were higher than 30°, 60° and 90°

	HF	BLYP	HCTH	B3LYP	B3P86	B3PW91	PBE1PBE	O3LYP	BHANDHLYP	BMK	MPWB1K	M05(-2X)	M05(-2X)-UF
HF	6	7	6	6	6	7	6	6	6	6	7	7	
BLYP	6	1	2	3	2	3	2	4	5	6	5	5	
HCTH	7	1	2	2	2	2	2	3	5	5	4	5	
B3LYP	6	2	2		0	1	1	1	3	5	4	5	
B3P86	6	3	2	0		0	1	1	1	4	4	4	
B3PW91	6	2	2	0	0		1	0	1	4	4	4	
PBE1PBE	7	3	2	1	1	1		2	2	2	4	4	
O3LYP	6	2	2	1	1	0	2		2	4	6	4	5
BHANDHLYP	6	4	3	1	1	1	2	2		3	5	4	3
BMK	6	5	5	3	1	4	2	4	3		2	5	5
MPWB1K	6	6	5	5	4	4	2	6	5	2		6	6
M05(-2X)	7	5	4	4	4	4	4	4	4	5	6		0
M05(-2X)-UF	7	5	5	5	4	4	4	5	3	5	6	0	

	HF	BLYP	HCTH	B3LYP	B3P86	B3PW91	PBE1PBE	O3LYP	BHANDHLYP	BMK	MPWB1K	M05(-2X)	M05(-2X)-UF
HF	4	5	3	3	3	3	4	2	2	4	5	4	4
BLYP	4		0	2	2	2	2	2	2	2	2	2	2
HCTH	5	0		2	2	2	2	2	2	2	2	2	2
B3LYP	3	2	2		0	0	0	0	0	0	1	1	1
B3P86	3	2	2	0		0	0	0	0	0	0	1	1
B3PW91	3	2	2	0	0		0	0	0	0	0	1	1
PBE1PBE	4	2	2	0	0	0		0	1	1	0	0	0
O3LYP	4	2	2	0	0	0	0		0	0	0	1	1
BHANDHLYP	2	2	2	0	0	0	1	0		1	1	1	1
BMK	4	2	2	0	0	0	1	0	1		1	1	1
MPWB1K	5	2	2	1	0	0	0	0	1	1		0	0
M05(-2X)	4	2	2	1	1	1	0	1	1	1	0		0
M05(-2X)-UF	4	2	2	1	1	1	0	1	1	1	0	0	

[illegible]

Comparison with experimental data

For 7 of the reactions studied, we have been able to find experimental data that can be related to the difference between transition states. In the following tables, we compare this difference with the Gibbs free energy offered by method 1 and method 2.

It is important to mention that this comparison cannot be considered as an absolute benchmark of different functionals. First, the set of reactions is rather limited. Secondly, we have only considered two possible transition states, and a more reliable study would require the inclusion of other transition state structures which could have a non negligible contribution to the formation of the products. Finally, our calculations have been done in the gas phase and no solvation model was used.

jo78

Experimental difference: >2.5 kcal/mol

	method 1		method 2	
	Gibbs free energy difference	error	Gibbs free energy difference	error
HF	2.07	-0.43	1.74	-0.76
BLYP	0.30	-2.20	1.44	-1.06
HCTH	-0.05	-2.55	0.84	-1.66
B3LYP	0.92	-1.58	1.70	-0.80
B3LYP-UF	0.97	-1.53	1.78	-0.72
B3P86	1.18	-1.32	1.94	-0.56
B3PW91	1.12	-1.38	1.87	-0.63
PBE1PBE	1.34	-1.16	1.98	-0.52
O3LYP	0.80	-1.70	1.61	-0.89
BHANDHLYP	1.51	-0.99	1.81	-0.69
BMK	1.60	-0.90	1.98	-0.52
MPWB1K	1.73	-0.77	1.87	-0.63
M05-2X	2.12	-0.38	2.16	-0.34
M05-2X-UF	1.92	-0.58	1.92	-0.58

jo15

Experimental difference: 0.75 kcal/mol

	method 1		method 2	
	Gibbs free energy difference	error	Gibbs free energy difference	error
HF	0.51	0.24	1.31	-0.56
BLYP	1.28	-0.53	1.31	-0.56
HCTH	1.62	-0.87	1.12	-0.37
B3LYP	1.59	-0.84	1.38	-0.63
B3LYP-UF	1.39	-0.64	1.24	-0.49
B3P86	1.63	-0.88	1.43	-0.68
B3PW91	1.79	-1.04	1.39	-0.64
PBE1PBE	1.71	-0.96	1.39	-0.64
O3LYP	1.88	-1.13	1.20	-0.45
BHANDHLYP	1.59	-0.84	1.66	-0.91
BMK	0.87	-0.12	1.07	-0.32
MPWB1K	2.36	-1.61	2.20	-1.45
M05-2X	2.07	-1.32	1.67	-0.92
M05-2X-UF	1.07	-0.32	1.05	-0.30

ja20

Experimental difference: 0.53 kcal/mol

	method 1		method 2	
	Gibbs free energy difference	error	Gibbs free energy difference	error
HF	0.72	0.19	1.26	0.73
BLYP	0.84	0.31	1.30	0.77
HCTH	0.40	-0.13	1.40	0.87
B3LYP	0.68	0.15	1.21	0.68
B3LYP-UF	0.67	0.14	1.17	0.64
B3P86	0.83	0.30	0.98	0.45
B3PW91	0.71	0.18	1.12	0.59
PBE1PBE	0.82	0.29	0.95	0.42
O3LYP	0.33	-0.20	1.47	0.94
BHANDHLYP	0.75	0.22	0.81	0.28
BMK	2.63	2.10	1.91	1.38
MPWB1K	0.57	0.04	0.24	-0.29
M05-2X	1.11	0.58	1.12	0.59
M05-2X-UF	1.07	0.54	1.07	0.54

jo8a

Experimental difference: 0.99 kcal/mol

	method 1		method 2	
	Gibbs free energy difference	error	Gibbs free energy difference	error
HF	2.81	1.82	1.44	0.45
BLYP	1.22	0.23	1.40	0.41
HCTH	1.66	0.67	2.16	1.17
B3LYP	1.61	0.62	1.60	0.61
B3LYP-UF	1.53	0.54	1.48	0.49
B3P86	1.55	0.56	1.48	0.49
B3PW91	1.55	0.56	1.34	0.35
PBE1PBE	1.59	0.60	1.46	0.47
O3LYP	1.54	0.55	1.46	0.47
BHANDHLYP	2.10	1.11	1.62	0.63
BMK	1.42	0.43	1.68	0.69
MPWB1K	1.41	0.42	1.19	0.20
M05-2X	2.73	1.74	2.75	1.76
M05-2X-UF	1.46	0.47	1.43	0.44

ja37

Experimental difference: >2.5 kcal/mol

	method 1		method 2	
	Gibbs free energy difference	error	Gibbs free energy difference	error
HF	11.64	0.0	10.34	0.0
BLYP	8.02	0.0	8.72	0.0
HCTH	8.95	0.0	9.42	0.0
B3LYP	8.63	0.0	7.73	0.0
B3LYP-UF	8.73	0.0	7.84	0.0
B3P86	8.42	0.0	6.74	0.0
B3PW91	8.61	0.0	6.84	0.0
PBE1PBE	8.38	0.0	6.80	0.0
O3LYP	8.95	0.0	8.14	0.0
BHANDHLYP	9.14	0.0	7.31	0.0
BMK	8.83	0.0	7.88	0.0
MPWB1K	7.20	0.0	6.01	0.0
M05-2X	6.15	0.0	6.06	0.0
M05-2X-UF	6.92	0.0	6.91	0.0

an02

Experimental difference: 1.75 kcal/mol

	method 1		method 2	
	Gibbs free energy difference	error	Gibbs free energy difference	error
HF	2.40	0.65	0.78	-0.97
BLYP	1.27	-0.48	0.92	-0.83
HCTH	1.92	0.17	1.64	-0.11
B3LYP	0.94	-0.81	1.13	-0.62
B3LYP-UF	1.68	-0.07	1.51	-0.24
B3P86	0.89	-0.86	1.23	-0.52
B3PW91	0.72	-1.03	0.90	-0.85
PBE1PBE	1.07	-0.68	1.09	-0.66
O3LYP	1.48	-0.27	0.99	-0.76
BHANDHLYP	1.32	-0.43	1.26	-0.49
BMK	-0.15	-1.90	0.48	-1.27
MPWB1K	2.24	0.49	2.87	1.12
M05-2X	2.22	0.47	1.96	0.21
M05-2X-UF	1.66	-0.09	1.66	-0.09

jo5k

Experimental difference: 1.46 kcal/mol

	method 1		method 2	
	Gibbs free energy difference	error	Gibbs free energy difference	error
HF	-0.48	1.94	1.30	0.16
BLYP	-0.05	1.51	1.08	0.38
HCTH	-0.46	1.92	0.24	1.22
B3LYP	-0.40	1.86	1.42	0.04
B3LYP-UF	-0.23	1.69	1.67	-0.21
B3P86	-0.26	1.72	1.53	-0.07
B3PW91	-0.30	1.76	1.93	-0.47
PBE1PBE	-0.08	1.54	1.70	-0.24
O3LYP	-1.08	2.54	0.16	1.30
BHANDHLYP	-0.08	1.54	1.71	-0.25
BMK	-0.42	1.88	0.23	1.23
MPWB1K	2.88	-1.42	2.37	-0.91
M05-2X	1.80	-0.34	1.78	-0.32
M05-2X-UF	2.16	-0.70	2.16	-0.70

Mean unsigned errors

(excluding ja37)

	method 1	method 2
	error	error
HF	0.88	0.55
BLYP	0.88	0.86
HCTH	1.05	1.05
B3LYP	0.98	0.69
B3LYP-UF	0.77	0.60
B3P86	0.94	0.59
B3PW91	0.99	0.71
PBE1PBE	0.87	0.60
O3LYP	1.06	0.94
BHANDHLYP	0.86	0.59
BMK	1.22	0.96
MPWB1K	0.79	0.79
M05-2X	0.80	0.70
M05-2X-UF	0.45	0.44