

Transferrable Selectivity Profiles Enable Prediction In Synergistic Catalyst Space

Yutao Kuang, Junshan Lai and Jolene P. Reid*

Correspondence to: jreid@chem.ubc.ca

Department of Chemistry, University of British Columbia, 2036 Main Mall, Vancouver, British Columbia, V6T 1Z1, Canada

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Full list of authors in the Gaussian reference

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

Computational details

Unless otherwise noted, all reaction components were optimized in the gas-phase with the M06-2X density functional,¹ and the triple- ζ valence quality def2-TZVP basis set of Weigend and Ahlrichs,² as implemented in Gaussian 16 (revision B.01 or C.01).³ All of the optimized geometries were verified by frequency computations as minima (zero imaginary frequencies). Gaussian input files were written using a Python script.⁴ Parameters were acquired from these ground state structures. NBO charges were calculated using NBO6,⁵ at the same level. Sterimol values were calculated using a modified version of Paton's Python script to accommodate non-terminal reference atoms.⁶ For molecules including a metal atom the M06-2X/def2TZP level of theory is not applicable. In these cases the functional is altered to M06 and the calculations and parameter collection performed in the same way. The computational method used for newly calculated molecules are specified where the xyz coordinates are noted. In some cases, parameter tables have been recycled and this is noted where relevant in both the main text discussion and the parameter descriptions below.

Conformational searches were performed with Macromodel version 11.7⁷ and the OPLS3 force field.⁸ Conformations were generated using the mixed Monte Carlo Multiple Minimum (MCMC)/Low-Mode conformational search method and default RMSE atom coordinate cutoff (0.5 Å). Conformers generated within a 10 kJ/mol energy window were chosen for further analysis with DFT.

Multidimensional regression analyses were performed using MATLAB®.⁹

Benchmarking the ability of M06/def2TZVP to reproduce M06-2X/def2TZVP nucleophile geometries

We re-evaluated the geometry of the nucleophile structures by performing a re-optimization at the M06/def2TZVP level of theory. Geometry comparisons quantified by RMSD showed that the structures were unaltered between the two optimization methods. Expectedly, evaluation of the key parameters ($H-X-C_{Nu}$ and $B5_{Nu}$) provided similar results to the M06-2X/def2TZVP optimized system. It should be noted that RMSD was calculated from superimposed structures defined by Atom Specification Language (ASL) as implemented within Maestro.

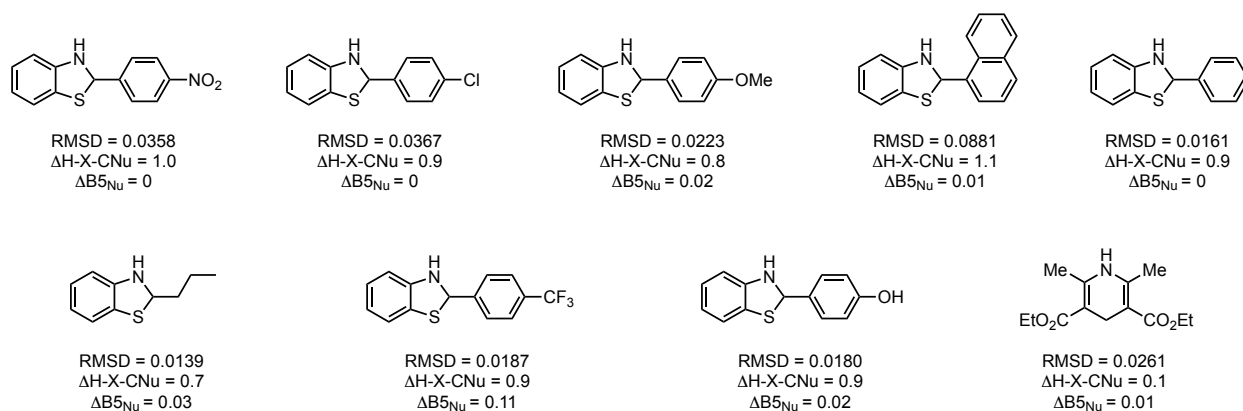
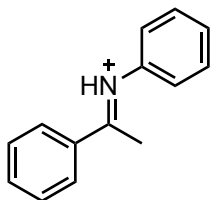


Figure S1. Comparing structural and key parameter changes when the optimization functional is altered from M06-2X to M06.

Cartesian coordinates of the reaction components relevant to chiral Brønsted acid catalysis

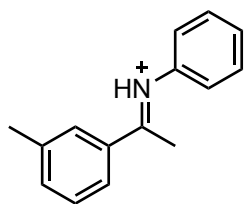
For consistency with the previous statistical model,¹⁰ all iminium components were optimized with Gaussian 09 (rev. D.01). Reaction components required for re-creating the statistical model have been published elsewhere (ref 10).



Hydrogenation *E*-Iminium 1

M06-2X/def2-TZVP Geometry

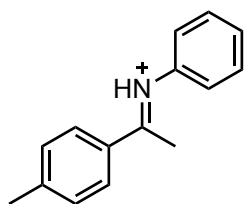
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C	-1.87746	0.17005	-0.02064
C	-2.24826	-1.01384	0.63160
C	-3.57676	-1.38961	0.68878
C	-4.54685	-0.59703	0.08708
C	-0.46779	0.55381	-0.07920
N	0.42119	-0.39343	-0.14018
C	-0.05652	1.98053	-0.05209
C	1.85118	-0.27999	-0.06627
C	2.60869	-0.89506	-1.05207
C	3.99049	-0.81855	-0.97804
C	4.59562	-0.14242	0.07340
C	3.82305	0.45479	1.06046
C	2.44018	0.38485	0.99942
H	-4.94602	1.19445	-1.02571
H	-2.60263	1.88359	-1.12262
H	-1.50809	-1.61174	1.15073
H	-3.85882	-2.29169	1.21431
H	-5.58676	-0.89351	0.12941
H	0.06494	-1.33752	-0.25941
H	-0.72530	2.56646	-0.67893
H	-0.17061	2.36193	0.96604
H	0.97140	2.12017	-0.37389
H	2.12469	-1.41436	-1.87004
H	4.59338	-1.28786	-1.74343
H	4.29663	0.96582	1.88766
H	1.82863	0.82153	1.77878
H	5.67457	-0.08800	0.12845



Hydrogenation *E*-Iminium 2

M06-2X/def2-TZVP Geometry

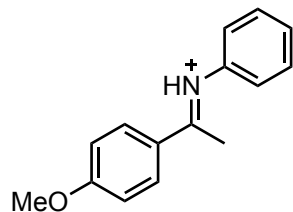
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C	3.06422	-1.82587	-0.57422
C	4.09651	-0.99312	-0.17016
C	0.11152	0.42327	-0.11811
C	-0.21778	1.84008	-0.41863
N	-0.82809	-0.43145	0.16328
C	-2.25057	-0.23998	0.12407
C	-2.98999	-0.61136	1.23760
C	-4.36715	-0.45922	1.20718
C	-4.98708	0.05002	0.07363
C	-4.23426	0.40229	-1.03872
C	-2.85622	0.25348	-1.02231
C	4.99033	1.19663	0.68427
H	2.35376	1.78764	0.57291
H	0.96643	-2.00702	-0.92840
H	3.27889	-2.82917	-0.91606
H	5.11547	-1.36166	-0.18416
H	0.52754	2.49292	0.02908
H	-0.15763	1.99377	-1.49927
H	-1.21056	2.11466	-0.07409
H	-0.52111	-1.35463	0.45663
H	-2.49482	-1.00209	2.11785
H	-4.95488	-0.73854	2.07074
H	-6.06236	0.16464	0.05379
H	-4.71991	0.78225	-1.92704
H	-2.26316	0.49623	-1.89463
H	5.46643	0.78666	1.57596
H	5.75158	1.25829	-0.09392
H	4.65092	2.20497	0.91236



Hydrogenation *E*-Iminium 3

M06-2X/def2-TZVP Geometry

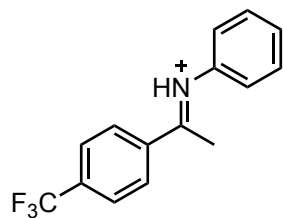
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C	3.25879	-1.32842	-0.12336
C	4.17491	-0.27003	-0.14594
C	0.00296	0.49917	0.27388
C	-0.46484	1.77029	0.89444
N	-0.86295	-0.37036	-0.15959
C	-2.29916	-0.28223	-0.13971
C	-3.01014	-1.29547	0.48554
C	-4.39545	-1.24057	0.48272
C	-5.04997	-0.18840	-0.14378
C	-4.32355	0.81121	-0.77684
C	-2.93779	0.76697	-0.78348
H	1.99539	2.29148	0.25868
H	1.24480	-1.95154	0.07350
H	3.62146	-2.34547	-0.20551
H	-1.48592	1.68333	1.25594
H	0.19938	2.04580	1.70972
H	-0.43619	2.57168	0.15142
H	-0.49080	-1.21407	-0.58298
H	-2.48850	-2.10718	0.97686
H	-4.96208	-2.02054	0.97249
H	-6.13086	-0.15112	-0.14490
H	-4.83451	1.62229	-1.27730
H	-2.36147	1.52481	-1.29837
H	4.38261	1.86017	-0.01742
C	5.63829	-0.54580	-0.29980
H	5.82390	-1.12992	-1.20227
H	6.21596	0.37382	-0.35560
H	6.00303	-1.13202	0.54565



Hydrogenation *E*-Iminium 4

M06-2X/def2-TZVP Geometry

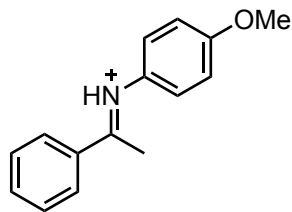
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C	-2.76857	-1.33889	0.52221
C	-3.73429	-0.39794	0.12043
C	0.39930	0.55314	-0.12688
C	0.85063	1.96820	-0.25858
N	1.28677	-0.40784	-0.11365
C	2.71681	-0.29925	-0.04113
C	3.47734	-0.95079	-1.00062
C	4.85976	-0.88262	-0.92048
C	5.46438	-0.17420	0.10922
C	4.68972	0.46300	1.06958
C	3.30675	0.39756	1.00371
H	-1.69685	2.13692	-0.75732
H	-0.73234	-1.76464	0.81878
H	-3.10912	-2.29084	0.90527
H	0.31801	2.43434	-1.08660
H	0.59789	2.52386	0.64581
H	1.91644	2.04239	-0.44426
H	0.93349	-1.35690	-0.15525
H	2.99467	-1.49329	-1.80387
H	5.46342	-1.38227	-1.66564
H	6.54315	-0.12476	0.16808
H	5.16127	1.00166	1.88010
H	2.69182	0.86667	1.76149
H	-4.05001	1.60240	-0.63902
O	-4.99577	-0.78689	0.22217
C	-6.03534	0.11409	-0.14637
H	-6.96301	-0.42195	0.02286
H	-6.00590	1.00829	0.47788
H	-5.95169	0.38458	-1.19995



Hydrogenation *E*-Iminium 5

M06-2X/def2-TZVP Geometry

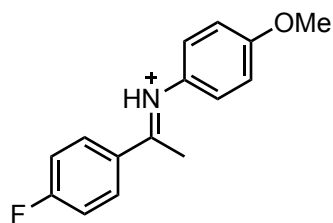
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C	2.59325	1.07436	-0.63863
C	3.06503	-0.04221	0.03764
C	-1.09963	0.72681	-0.06401
N	-1.89343	-0.29871	-0.12789
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C	-3.32807	-0.32498	-0.05788
C	-4.01304	-1.03997	-1.02970
C	-5.39600	-1.09724	-0.96546
C	-6.07298	-0.45527	0.06358
C	-5.37078	0.24087	1.03852
C	-3.98735	0.30647	0.98703
C	4.54981	-0.33222	0.03174
F	4.90004	-1.09869	1.06103
F	4.89231	-0.96933	-1.08902
F	5.25729	0.79371	0.09087
H	2.57594	-1.75165	1.23799
H	0.16401	-1.29214	1.21011
H	0.88273	2.20726	-1.20231
H	3.28722	1.73722	-1.13843
H	-1.45013	-1.20437	-0.25864
H	-1.00443	2.76739	-0.61086
H	-2.66419	2.16680	-0.35447
H	-1.57490	2.47434	1.01491
H	-3.47511	-1.53269	-1.83037
H	-5.94360	-1.64349	-1.72123
H	-5.89805	0.72510	1.84919
H	-3.43004	0.82028	1.75975
H	-7.15248	-0.50550	0.11097



Hydrogenation *E*-Iminium 6

M06-2X/def2-TZVP Geometry

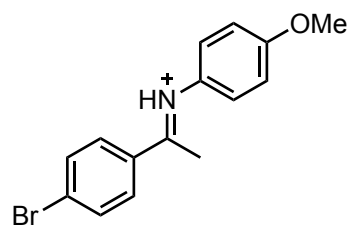
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C	4.40527	-1.39211	0.77674
C	5.38335	-0.70700	0.06623
C	1.34342	0.57989	-0.10936
N	0.42468	-0.33966	-0.06820
C	0.97890	2.01619	-0.21027
C	-0.99482	-0.18498	0.02149
C	-1.79531	-0.93866	-0.82110
C	-3.17408	-0.83359	-0.74576
C	-3.75084	0.02769	0.19049
C	-2.93054	0.76741	1.05295
C	-1.56208	0.65924	0.97385
O	-5.06454	0.20347	0.34514
C	-5.95547	-0.52391	-0.48767
H	5.81123	0.94264	-1.23806
H	3.49234	1.71337	-1.33621
H	2.34535	-1.47958	1.32117
H	4.67113	-2.24690	1.38361
H	6.41208	-1.04002	0.10769
H	0.75555	-1.29981	-0.10594
H	1.06802	2.47774	0.77675
H	1.68594	2.52990	-0.85719
H	-0.03422	2.15590	-0.57778
H	-1.34687	-1.60337	-1.54978
H	-3.78592	-1.42223	-1.41247
H	-3.40028	1.40864	1.78608
H	-0.93504	1.20948	1.66349
H	-5.83649	-1.59862	-0.33542
H	-6.95416	-0.22156	-0.18989
H	-5.79403	-0.27428	-1.53835



Hydrogenation *E*-Iminium 7

M06-2X/def2-TZVP Geometry

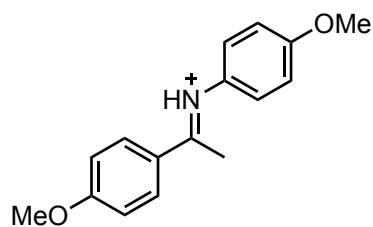
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C	-4.16132	-0.03536	0.20718
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C	-1.98086	0.62579	0.98910
C	-1.40297	-0.16514	-0.00175
N	0.01924	-0.27808	-0.11029
C	0.91224	0.66920	-0.12750
C	2.31989	0.28807	-0.06435
C	0.50051	2.09564	-0.19370
C	3.30395	1.05679	-0.69862
C	4.62883	0.67346	-0.65705
C	4.96838	-0.47118	0.04642
C	4.02606	-1.24340	0.70810
C	2.70299	-0.86060	0.64468
F	6.23761	-0.83291	0.10045
O	-5.47712	0.09827	0.38345
C	-6.35842	-0.62115	-0.46647
H	-1.73576	-1.53001	-1.62353
H	-4.17723	-1.42325	-1.44996
H	-3.82879	1.29126	1.85161
H	-1.35979	1.16587	1.69219
H	0.37379	-1.22727	-0.18177
H	-0.52292	2.20917	-0.54052
H	0.59373	2.54295	0.79928
H	1.17544	2.64470	-0.84622
H	3.04023	1.94036	-1.26194
H	5.40186	1.24064	-1.15672
H	4.34367	-2.11043	1.27058
H	1.97213	-1.43023	1.20652
H	-6.21076	-1.69722	-0.35435
H	-7.36117	-0.35512	-0.14826
H	-6.21479	-0.32954	-1.50893



Hydrogenation *E*-Iminium 8

M06-2X/def2-TZVP Geometry

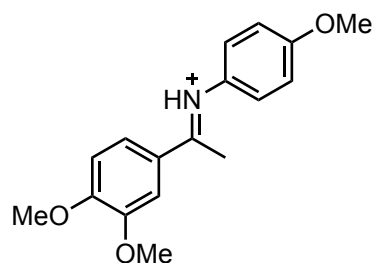
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C	-2.05801	1.36040	-0.71348
C	-3.40153	1.04068	-0.69016
C	-3.82708	-0.08936	-0.00052
C	0.30560	0.84851	-0.12219
C	0.79310	2.25102	-0.17815
N	1.14495	-0.14644	-0.10472
C	2.57048	-0.11807	0.00260
C	3.31023	-0.92855	-0.84323
C	4.69164	-0.95103	-0.75114
C	5.33277	-0.16058	0.20570
C	4.57214	0.63814	1.07061
C	3.20066	0.65641	0.97496
H	-0.88112	-1.19897	1.19259
H	-1.74622	2.23379	-1.26843
H	-4.12040	1.66339	-1.20383
Br	-5.65087	-0.51515	0.04676
H	1.81705	2.31124	-0.53685
H	0.14041	2.84364	-0.81424
H	0.73921	2.69049	0.82116
H	0.73740	-1.07384	-0.18215
H	2.81218	-1.53762	-1.58799
H	5.25583	-1.58120	-1.42180
O	6.65454	-0.10911	0.37894
H	5.08929	1.22142	1.81984
H	2.61827	1.24872	1.66858
C	7.48569	-0.90496	-0.45319
H	7.26250	-1.96549	-0.32176
H	7.36643	-0.62400	-1.50138
H	8.50350	-0.70434	-0.13527
H	-3.26200	-1.76069	1.22381



Hydrogenation *E*-Iminium 9

M06-2X/def2-TZVP Geometry

C	-4.20500	0.79078	-0.41347
C	-2.86856	1.12274	-0.48804
C	-1.86856	0.24219	-0.05664
C	-2.27040	-0.99143	0.49842
C	-3.59252	-1.33041	0.58783
C	-4.58081	-0.44579	0.12212
C	-0.46998	0.60141	-0.15747
N	0.43540	-0.34072	-0.11339
C	-0.04771	2.02183	-0.31742
C	1.85665	-0.20260	-0.00571
C	2.66725	-0.90079	-0.88356
C	4.04637	-0.80968	-0.77772
C	4.61151	-0.01408	0.22013
C	3.78106	0.67411	1.11376
C	2.41337	0.57553	1.00686
O	5.92553	0.14473	0.40661
C	6.82329	-0.53814	-0.45413
H	-4.94606	1.48944	-0.77173
H	-1.54497	-1.67515	0.92317
H	-3.90887	-2.26432	1.03184
H	0.09648	-1.29588	-0.13690
H	1.00967	2.10919	-0.54468
H	-0.62034	2.47691	-1.12405
H	-0.27092	2.58060	0.59331
H	2.22712	-1.51141	-1.66264
H	4.66594	-1.35724	-1.47185
H	4.24191	1.26612	1.89259
H	1.77339	1.08560	1.71616
H	6.69547	-1.61933	-0.36824
H	6.67987	-0.22608	-1.49085
H	7.81980	-0.26144	-0.12518
H	-2.60913	2.08249	-0.91174
O	-5.83325	-0.86162	0.24589
C	-6.89334	-0.01377	-0.18259
H	-7.80831	-0.55912	0.02345
H	-6.81564	0.18668	-1.25241
H	-6.88715	0.92165	0.37929

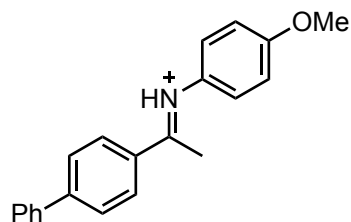


Hydrogenation *E*-Iminium 10

M06-2X/def2-TZVP Geometry

C	-3.71353	0.62915	0.02954
C	-2.38506	0.96995	0.13726
C	-1.38152	-0.02269	0.13722
C	-1.75422	-1.36348	0.06276
C	-3.08745	-1.72157	-0.02491
C	-4.07751	-0.74450	-0.05421
C	0.00710	0.37689	0.22865
N	0.94453	-0.43478	-0.18061
C	0.37777	1.70478	0.79656
C	2.36481	-0.23315	-0.17341
C	3.16996	-1.18414	0.42843
C	4.54829	-1.03462	0.42077
C	5.11881	0.07661	-0.20121
C	4.29503	1.02342	-0.82212
C	2.92771	0.86713	-0.81480
O	6.43276	0.31698	-0.26287
C	7.32265	-0.60992	0.33842
O	-5.37603	-0.98081	-0.14519
O	-4.73599	1.48824	-0.00558
C	-4.45280	2.87215	0.09018
C	-5.82585	-2.32514	-0.25252
H	-2.11032	2.01292	0.18732
H	-1.02220	-2.15837	0.13653
H	-3.35638	-2.76683	-0.05492
H	0.63740	-1.31629	-0.57592
H	1.40176	1.70639	1.16118
H	0.29344	2.47419	0.02446
H	-0.30523	1.96112	1.60264
H	2.72542	-2.04208	0.91797
H	5.16245	-1.78213	0.89995
H	4.76056	1.86566	-1.31530
H	2.29601	1.58568	-1.32126
H	7.23165	-1.59322	-0.12785
H	8.32041	-0.21716	0.17031
H	7.13568	-0.68742	1.41167

H	-3.83097	3.20071	-0.74638
H	-5.41274	3.37697	0.04824
H	-3.95879	3.10356	1.03729
H	-6.90619	-2.26787	-0.33503
H	-5.41130	-2.79814	-1.14473
H	-5.55335	-2.89481	0.63765

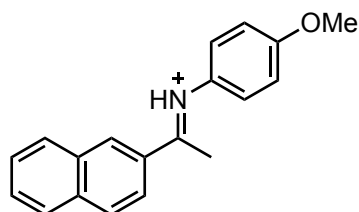


Hydrogenation *E*-Iminium 11

M06-2X/def2-TZVP Geometry

C	2.54588	-1.01240	-0.25400
C	1.18257	-0.84701	-0.34253
C	0.60789	0.42589	-0.20780
C	1.45310	1.52114	0.00653
C	2.81678	1.34634	0.11305
C	3.39357	0.07891	-0.01612
C	-0.82927	0.63866	-0.27700
N	-1.63831	-0.35869	-0.05947
C	-1.37998	1.98415	-0.60499
C	-3.07280	-0.35810	-0.05362
C	-3.74386	-1.28438	-0.84805
C	-5.11892	-1.32084	-0.83289
C	-5.84094	-0.43936	-0.01802
C	-5.15980	0.47247	0.78950
C	-3.77393	0.50395	0.77092
O	-7.17136	-0.54975	-0.07648
C	-7.96252	0.31196	0.72654
H	2.97451	-1.99363	-0.40834
H	1.04011	2.51372	0.12787
H	3.44731	2.19981	0.32344
H	-1.20916	-1.25166	0.15862
H	-2.39006	1.90925	-0.99969
H	-1.41310	2.60166	0.29633
H	-0.73261	2.47781	-1.32548
H	-3.18803	-1.96168	-1.48486
H	-5.66855	-2.02206	-1.44563
H	-5.69442	1.14703	1.44128
H	-3.24372	1.19093	1.41835

H	-8.99497	0.05868	0.50793
H	-7.76094	0.14676	1.78702
H	-7.77956	1.35768	0.47006
H	0.57835	-1.71406	-0.58428
C	7.61224	-0.45702	0.25552
C	6.75500	-1.42915	0.75356
C	5.38384	-1.25859	0.66060
C	4.85229	-0.10604	0.07946
C	5.72293	0.86849	-0.41202
C	7.09371	0.68997	-0.33002
H	8.68345	-0.59391	0.32306
H	7.15612	-2.31992	1.21829
H	4.72182	-2.01044	1.07202
H	5.32639	1.75468	-0.89157
H	7.75949	1.44408	-0.72802

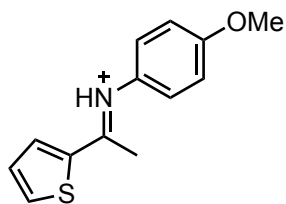


Hydrogenation *E*-Iminium 12

M06-2X/def2-TZVP Geometry

C	-3.11141	-1.82529	-0.08905
C	-1.81189	-1.45045	0.04980
C	-1.47308	-0.07434	0.20288
C	-2.47784	0.87132	0.21933
C	-3.82799	0.50794	0.05527
C	-4.15623	-0.86426	-0.10211
C	-0.09041	0.36755	0.31209
N	0.85950	-0.41393	-0.11560
C	0.24606	1.68778	0.91744
C	2.27360	-0.18179	-0.13709
C	3.11055	-1.16097	0.37073
C	4.48468	-0.98606	0.33865
C	5.01983	0.17765	-0.21648
C	4.16384	1.15064	-0.74793
C	2.80022	0.97069	-0.71509
O	6.32614	0.44606	-0.29460
C	7.24977	-0.50437	0.21336
C	-4.86073	1.47628	0.05044
C	-6.16215	1.09070	-0.10033

C	-6.48725	-0.27457	-0.25278
C	-5.50896	-1.23191	-0.25310
H	-3.36722	-2.87371	-0.17824
H	-1.05428	-2.22287	0.10513
H	-2.24504	1.92309	0.33209
H	0.56753	-1.30169	-0.51042
H	-0.44222	1.90220	1.73092
H	1.26961	1.70079	1.28370
H	0.14416	2.47895	0.17053
H	2.69427	-2.06083	0.80721
H	5.12441	-1.75438	0.74570
H	4.60161	2.03287	-1.19430
H	2.14522	1.71011	-1.15734
H	8.23471	-0.07904	0.04942
H	7.09311	-0.66421	1.28227
H	7.16508	-1.45214	-0.32248
H	-4.60414	2.52175	0.16972
H	-6.95189	1.83000	-0.10310
H	-7.52362	-0.56265	-0.37082
H	-5.76050	-2.27847	-0.37021

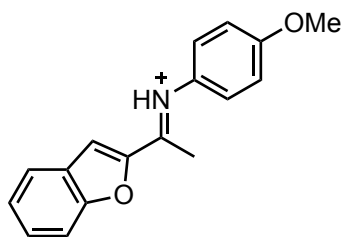


Hydrogenation *E*-Iminium 13

M06-2X/def2-TZVP Geometry

C	-4.95118	-0.63532	-0.39205
S	-3.35641	-1.19218	-0.51864
C	-2.73112	0.29817	0.09279
C	-3.75958	1.18173	0.36299
C	-5.02677	0.64491	0.08746
C	-1.33039	0.54706	0.26833
C	-0.86776	1.90048	0.69035
N	-0.46412	-0.41115	0.06741
C	0.96485	-0.33554	0.08242
C	1.67072	-1.28266	0.82221
C	3.04519	-1.25332	0.82679
C	3.73447	-0.28294	0.08680
C	3.02005	0.65078	-0.66647
C	1.63462	0.61411	-0.67032
H	-3.60812	2.18032	0.74532

H	-0.86953	2.57667	-0.16703
H	-1.55157	2.30352	1.43333
H	0.13633	1.86144	1.10318
H	-0.83409	-1.33614	-0.13130
H	1.14084	-2.02965	1.40047
H	3.61965	-1.97034	1.39671
O	5.06668	-0.33626	0.15610
H	3.52995	1.39278	-1.26212
H	1.08163	1.31557	-1.28190
C	5.82778	0.60915	-0.57955
H	5.60455	1.62614	-0.25077
H	6.86792	0.37939	-0.37279
H	5.63657	0.51161	-1.65006
H	-5.95712	1.17259	0.23132
H	-5.76440	-1.28041	-0.68724

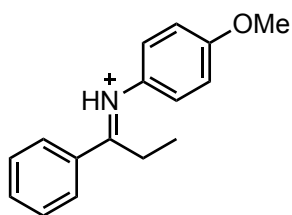


Hydrogenation *E*-Iminium 14

M06-2X/def2-TZVP Geometry

O	-2.10506	-0.66526	0.12930
C	-1.74955	0.62816	-0.13699
C	-2.84560	1.42264	-0.31384
C	-0.35507	0.92072	-0.17897
C	0.10666	2.30822	-0.45209
N	0.47651	-0.06761	0.01316
C	1.90084	-0.04097	0.07125
C	2.59950	-1.04758	-0.57733
C	3.98281	-1.07815	-0.53067
C	4.67139	-0.09443	0.18258
C	3.95516	0.90376	0.85554
C	2.58086	0.92866	0.80681
H	-2.84329	2.47832	-0.53168
H	-0.60736	2.81178	-1.09866
H	0.17473	2.87277	0.47979
H	1.08795	2.30200	-0.92232
H	0.04780	-0.98252	0.12966
H	2.06491	-1.80656	-1.13565
H	4.51150	-1.86404	-1.04847
O	6.00082	-0.03106	0.29080

H	4.50797	1.63770	1.42541
H	2.03703	1.67855	1.36488
C	6.78630	-1.02229	-0.35353
H	6.62804	-1.00046	-1.43361
H	7.81906	-0.77429	-0.13139
H	6.55506	-2.01476	0.03833
C	-3.46471	-0.69684	0.12180
C	-3.97902	0.57817	-0.14724
C	-5.36880	0.76463	-0.19900
C	-6.16967	-0.33067	0.02070
C	-5.61859	-1.59873	0.28882
C	-4.25485	-1.81087	0.34539
H	-5.79172	1.73838	-0.40508
H	-7.24510	-0.22437	-0.01123
H	-6.28622	-2.43339	0.45635
H	-3.82805	-2.78181	0.55144

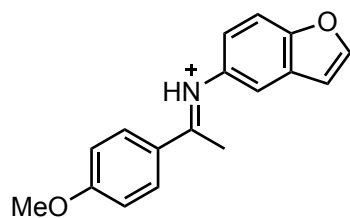


Hydrogenation *E*-Iminium 15

M06-2X/def2-TZVP Geometry

C	-4.95859	-0.02005	-0.78145
C	-3.65524	0.42576	-0.90755
C	-2.64608	-0.12667	-0.11243
C	-2.97586	-1.10417	0.83428
C	-4.28328	-1.53550	0.96457
C	-5.27373	-1.00015	0.15092
C	-1.25897	0.31968	-0.25862
C	-0.94935	1.71828	-0.67061
C	-1.42141	2.74718	0.36516
N	-0.31446	-0.54181	-0.01735
C	1.10188	-0.33915	0.04185
C	1.92345	-1.22227	-0.63780
C	3.29953	-1.07150	-0.58476
C	3.85192	-0.03103	0.16481
C	3.01064	0.84209	0.86693
C	1.64544	0.68635	0.81216
O	5.16098	0.20371	0.28097
C	6.07094	-0.65126	-0.39463

H	-5.73097	0.39832	-1.41231
H	-3.42571	1.18330	-1.64436
H	-2.22488	-1.48866	1.51472
H	-4.53263	-2.27790	1.71058
H	-6.29611	-1.33963	0.25251
H	-1.47845	1.89214	-1.61070
H	0.11270	1.82336	-0.87672
H	-1.17843	3.74784	0.01377
H	-2.49802	2.68617	0.51756
H	-0.93397	2.59664	1.32809
H	-0.61774	-1.49816	0.14513
H	1.49366	-2.02461	-1.22554
H	3.92724	-1.76225	-1.12731
H	3.46231	1.62480	1.46087
H	1.00108	1.34299	1.38251
H	5.97819	-1.67744	-0.03324
H	5.90589	-0.61761	-1.47350
H	7.06161	-0.27185	-0.16536

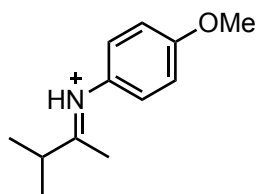


Hydrogenation *E*-Iminium 16

M06-2X/def2-TZVP Geometry

C	-4.21038	1.20025	-0.53116
C	-2.86192	1.39776	-0.66748
C	-1.93863	0.43340	-0.21863
C	-2.44128	-0.71497	0.41200
C	-3.79387	-0.92130	0.56713
C	-4.69664	0.03533	0.08243
C	-0.51488	0.63664	-0.38142
C	0.04487	2.00034	-0.59838
N	0.28574	-0.39578	-0.34757
H	-2.52239	2.30289	-1.15007
H	-1.77052	-1.44440	0.85070
H	-4.14326	-1.80523	1.07890
O	-6.01492	-0.06704	0.17362
H	1.10146	1.97491	-0.84198
H	-0.49548	2.48022	-1.41322

H	-0.11045	2.60932	0.29390
H	-0.15254	-1.31004	-0.33508
H	-4.92550	1.92808	-0.88855
C	-6.58487	-1.22198	0.77937
H	-7.65941	-1.08543	0.72073
H	-6.29697	-2.12263	0.23493
H	-6.27972	-1.29755	1.82421
C	3.76181	-1.24781	-1.29008
C	2.38206	-1.16983	-1.28823
C	1.72139	-0.40934	-0.31642
C	2.38779	0.27514	0.68454
H	4.30030	-1.82371	-2.02913
H	1.80696	-1.68670	-2.04544
H	1.84086	0.82331	1.44122
C	4.42444	-0.54728	-0.29755
C	3.77883	0.21104	0.68953
C	4.83122	0.74533	1.51153
C	5.97659	0.28639	0.97178
O	5.75928	-0.49647	-0.12129
H	4.74270	1.37810	2.37748
H	7.00986	0.42281	1.24205

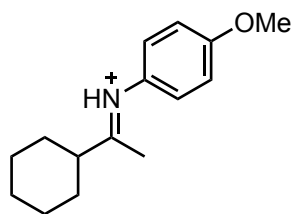


Hydrogenation *E*-Iminium 17

M06-2X/def2-TZVP Geometry

C	3.62828	0.26133	0.25103
C	2.20976	-0.19838	0.40622
N	1.25001	0.51260	-0.08354
C	1.94062	-1.47209	1.12245
C	-0.15785	0.23473	-0.09949
C	-1.02810	1.23965	0.28735
C	-2.39506	1.01859	0.26610
C	-2.88797	-0.21712	-0.15985
C	-1.99656	-1.21623	-0.57291
C	-0.63964	-0.99255	-0.54726
O	-4.18256	-0.53313	-0.21824
C	-5.14232	0.43461	0.18107
C	3.78972	1.63919	-0.37580

C	4.40676	-0.80766	-0.53865
H	4.03117	0.27895	1.27009
H	1.51893	1.39399	-0.51365
H	2.70526	-1.62625	1.88220
H	0.94849	-1.48022	1.56984
H	2.00497	-2.30954	0.42312
H	-0.64475	2.19617	0.62224
H	-3.06232	1.80713	0.57955
H	-2.40241	-2.15506	-0.92398
H	0.04098	-1.75626	-0.89978
H	-6.11103	-0.03823	0.05590
H	-5.00070	0.70999	1.22818
H	-5.08338	1.32253	-0.45156
H	3.26329	2.41800	0.18015
H	4.84417	1.90932	-0.37758
H	3.45978	1.64899	-1.41819
H	4.39370	-1.77713	-0.04329
H	3.99419	-0.91860	-1.54288
H	5.44432	-0.49151	-0.63112

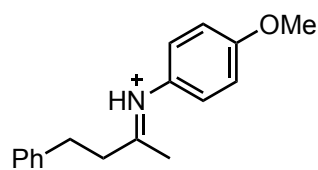


Hydrogenation *E*-Iminium 18

M06-2X/def2-TZVP Geometry

C	-1.13859	0.48793	0.58205
C	-0.75787	1.78899	1.19094
N	-0.24793	-0.31201	0.09712
C	1.17100	-0.13165	-0.00631
C	1.99072	-1.17710	0.38413
C	3.36620	-1.05797	0.27705
C	3.91935	0.11606	-0.23892
C	3.07773	1.15701	-0.65210
C	1.71197	1.03418	-0.54185
O	5.22794	0.33182	-0.38716
C	6.13755	-0.68750	0.00014
H	-2.94822	0.20271	1.55895
H	-0.78829	2.57501	0.43211
H	0.24813	1.75835	1.60587
H	-1.48224	2.05275	1.95959
H	-0.59307	-1.20182	-0.25332

H	1.56139	-2.08708	0.78625
H	3.99300	-1.87815	0.59269
H	3.52712	2.04648	-1.07172
H	1.06866	1.82815	-0.89703
H	7.12841	-0.29513	-0.20506
H	5.97354	-1.59531	-0.58408
H	6.04305	-0.90584	1.06589
C	-4.36317	-1.60899	0.05936
C	-2.86267	-1.31728	0.04037
C	-2.58233	0.10273	0.52851
C	-3.35231	1.13936	-0.32550
C	-4.84730	0.82693	-0.32411
C	-5.12723	-0.59789	-0.78833
H	-4.72241	-1.57196	1.09225
H	-4.53832	-2.62306	-0.30000
H	-2.50737	-1.42892	-0.99230
H	-2.33758	-2.04955	0.66179
H	-3.18122	2.14756	0.05472
H	-2.96427	1.10265	-1.34920
H	-5.23875	0.96503	0.68857
H	-5.36122	1.54648	-0.96227
H	-4.82990	-0.70463	-1.83658
H	-6.19681	-0.80307	-0.74229

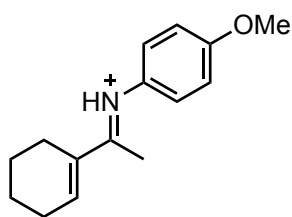


Hydrogenation *E*-Iminium 19

M06-2X/def2-TZVP Geometry

C	-3.01290	-2.12842	-1.07698
C	-3.34883	-0.78927	-0.93365
C	-3.12192	-0.12380	0.27218
C	-2.56116	-0.82922	1.33130
C	-2.23623	-2.17404	1.19545
C	-2.45452	-2.82419	-0.01056
C	-3.41289	1.34926	0.39299
C	-2.47687	2.19835	-0.51009
C	-1.05232	1.97233	-0.12883
C	-0.42038	2.85729	0.87839
N	-0.44456	0.95303	-0.63565
C	0.88715	0.48225	-0.40937
C	1.05640	-0.88456	-0.19812

C	2.32118	-1.38402	0.00232
C	3.43131	-0.52852	-0.02045
C	3.25208	0.83529	-0.25911
C	1.97473	1.33613	-0.45797
O	4.61658	-1.10883	0.18339
C	5.78540	-0.30362	0.16048
H	-3.20512	-2.63462	-2.01403
H	-3.81250	-0.26276	-1.76206
H	-2.38931	-0.32954	2.27814
H	-1.81544	-2.71239	2.03497
H	-2.20643	-3.87195	-0.11748
H	-3.31406	1.66947	1.43142
H	-4.43512	1.57154	0.08363
H	-2.71468	3.25589	-0.39775
H	-2.63585	1.92042	-1.55280
H	-0.05549	3.76382	0.38639
H	0.41019	2.37776	1.39111
H	-1.18294	3.17240	1.59139
H	-1.01387	0.34637	-1.22682
H	0.19194	-1.53980	-0.17840
H	2.48849	-2.43792	0.17712
H	4.09528	1.50762	-0.30761
H	1.84038	2.38718	-0.67854
H	6.61398	-0.97681	0.35552
H	5.91496	0.16358	-0.81793
H	5.74358	0.46175	0.93841

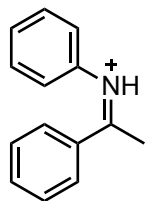


Hydrogenation *E*-Iminium 20

M06-2X/def2-TZVP Geometry

C	4.99672	0.80949	-0.06677
C	3.54824	1.06854	-0.29855
C	2.58430	0.14044	-0.16083
C	2.90665	-1.29256	0.20096
C	4.38937	-1.60919	0.00999
C	5.25553	-0.52116	0.62947
C	1.19396	0.54484	-0.30545
C	0.79750	1.88194	-0.83581

N	0.27319	-0.31197	0.03913
H	2.31979	-1.97340	-0.42422
H	4.60558	-1.68198	-1.05917
H	1.45368	2.16055	-1.65638
H	-0.23133	1.87138	-1.18500
H	0.88782	2.64206	-0.05730
H	0.59932	-1.22566	0.33755
H	5.41592	1.64798	0.49441
C	-3.08522	1.06783	0.79766
C	-1.71608	0.94763	0.74321
C	-1.14749	-0.13957	0.08309
C	-1.94867	-1.11461	-0.48710
H	-3.55488	1.89705	1.30838
H	-1.08801	1.68138	1.23144
H	-1.49989	-1.96360	-0.98835
C	-3.90560	0.09914	0.20499
C	-3.32832	-0.99956	-0.43477
C	-6.10933	-0.64630	-0.25245
O	-5.22072	0.30577	0.31200
H	-7.10926	-0.27876	-0.04626
H	2.62282	-1.48388	1.24263
H	5.49520	0.84053	-1.04410
H	4.60993	-2.58155	0.44832
H	5.02046	-0.42804	1.69315
H	6.31095	-0.77954	0.55751
H	3.28261	2.08155	-0.57830
H	-3.93974	-1.76310	-0.89130
H	-5.97507	-1.62479	0.21291
H	-5.96179	-0.72195	-1.33162

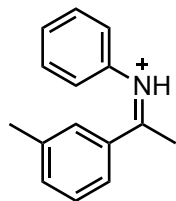


Hydrogenation Z-Iminium 1

M06-2X/def2-TZVP Geometry

C	-1.53104	2.87100	0.02583
C	-0.74921	1.60390	-0.04462
N	0.54692	1.70150	-0.07487
C	-1.45195	0.32519	-0.09475
C	1.54073	0.66814	0.06091

C	2.58279	0.62813	-0.85141
C	3.55516	-0.35172	-0.71032
C	3.47924	-1.26230	0.33421
C	2.43632	-1.19369	1.25010
C	1.45864	-0.22171	1.12123
C	-2.66345	0.18350	0.59050
C	-3.36308	-1.00797	0.51986
C	-2.88508	-2.04580	-0.26909
C	-1.70172	-1.89759	-0.98423
C	-0.97681	-0.72569	-0.88978
H	-0.90634	3.74763	-0.13514
H	-2.34385	2.85207	-0.69824
H	-1.97876	2.95215	1.01976
H	0.92338	2.64238	-0.14169
H	2.62889	1.34091	-1.66579
H	4.37184	-0.39958	-1.41764
H	2.38891	-1.89239	2.07421
H	0.64593	-0.15293	1.83259
H	-3.04906	0.99057	1.19925
H	-4.28661	-1.12287	1.07058
H	-1.34531	-2.69868	-1.61730
H	-0.06081	-0.61607	-1.45454
H	4.24143	-2.02217	0.44252
H	-3.44132	-2.97181	-0.33523

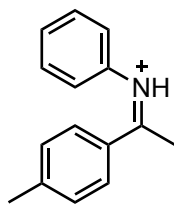


Hydrogenation Z-Iminium 2

M06-2X/def2-TZVP Geometry

C	3.18216	-0.63976	0.15870
C	2.35254	0.45854	0.32166
C	1.06458	0.48270	-0.22939
C	0.61541	-0.59795	-0.99543
C	1.45199	-1.68155	-1.19008
C	2.71159	-1.70596	-0.60965
C	0.25810	1.68808	-0.07679
C	0.92758	3.01982	-0.00935
N	-1.04099	1.67921	-0.01065
C	-1.95214	0.57386	0.13099

C	-3.03999	0.51614	-0.72522
C	-3.94934	-0.52151	-0.58272
C	-3.76602	-1.47390	0.40989
C	-2.67759	-1.38988	1.26997
C	-1.76149	-0.35909	1.13914
C	4.55119	-0.68815	0.77267
H	2.70974	1.29805	0.90502
H	-0.35933	-0.58017	-1.46265
H	1.12227	-2.51132	-1.80054
H	3.35273	-2.56658	-0.76285
H	1.41954	3.11881	0.96154
H	1.69575	3.09567	-0.77678
H	0.21703	3.83797	-0.11143
H	-1.49053	2.58971	-0.01088
H	-3.17029	1.26389	-1.49801
H	-4.80130	-0.58088	-1.24610
H	-4.47977	-2.27880	0.52212
H	-2.54609	-2.12388	2.05332
H	-0.91466	-0.27869	1.80828
H	4.62328	-1.51157	1.48445
H	5.30968	-0.85106	0.00625
H	4.78745	0.23605	1.29642

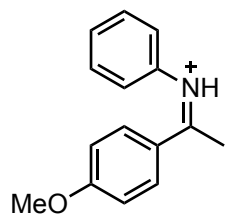


Hydrogenation Z-Iminium 3

M06-2X/def2-TZVP Geometry

C	1.82593	-1.30735	-0.80433
C	0.82020	-0.36808	-0.75990
C	1.01595	0.83961	-0.07041
C	2.24786	1.06927	0.55451
C	3.23353	0.10212	0.53343
C	3.04306	-1.10028	-0.14600
C	0.01632	1.89351	-0.06823
C	0.44710	3.32220	-0.01511
N	-1.26660	1.67098	-0.12124
C	-1.99154	0.43688	0.03011
C	-2.96053	0.12365	-0.90931
C	-3.68908	-1.04695	-0.75355

C	-3.44710	-1.87709	0.33188
C	-2.48198	-1.53763	1.27288
C	-1.74812	-0.37181	1.13028
H	-0.10283	-0.55485	-1.29092
H	2.43303	1.99686	1.07955
H	4.17182	0.28578	1.04062
H	0.80668	3.54423	0.99272
H	-0.37366	4.00224	-0.23476
H	1.26909	3.49734	-0.70612
H	-1.85566	2.49153	-0.22058
H	-3.13602	0.77730	-1.75483
H	-4.44585	-1.30645	-1.48103
H	-4.01908	-2.78716	0.45174
H	-2.30741	-2.17691	2.12748
H	-0.99971	-0.09168	1.86012
H	1.67435	-2.22281	-1.36252
C	4.10716	-2.15288	-0.17675
H	4.25071	-2.52842	-1.18999
H	5.05643	-1.77397	0.19526
H	3.81165	-3.00091	0.44490

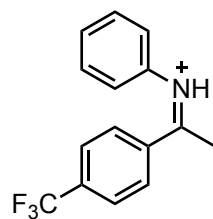


Hydrogenation *Z*-Iminium 4

M06-2X/def2-TZVP Geometry

C	1.55848	-1.08434	-0.79291
C	0.47274	-0.25721	-0.71679
C	0.57250	1.00827	-0.09594
C	1.81770	1.39336	0.42429
C	2.90919	0.55405	0.38469
C	2.78796	-0.69951	-0.22794
C	-0.52081	1.94607	-0.05075
C	-0.24519	3.41399	0.04435
N	-1.78370	1.60481	-0.09400
C	-2.38871	0.30763	0.04566
C	-3.30044	-0.10483	-0.91263
C	-3.91186	-1.34209	-0.76691
C	-3.61096	-2.14194	0.32641

C	-2.70472	-1.70540	1.28575
C	-2.08973	-0.47139	1.15374
H	-0.45253	-0.57303	-1.17645
H	1.93509	2.36056	0.89427
H	3.84496	0.87452	0.81677
H	0.08157	3.65040	1.05972
H	-1.13660	4.00309	-0.16210
H	0.54838	3.70244	-0.64102
H	-2.44615	2.36915	-0.16527
H	-3.52038	0.52557	-1.76523
H	-4.62308	-1.67781	-1.50909
H	-4.09066	-3.10487	0.43778
H	-2.48408	-2.32282	2.14582
H	-1.38738	-0.11573	1.89652
H	1.50196	-2.04323	-1.28918
O	3.77263	-1.57864	-0.33384
C	5.05354	-1.25964	0.20007
H	5.68064	-2.12072	-0.00475
H	4.99005	-1.09663	1.27693
H	5.46498	-0.37751	-0.29256

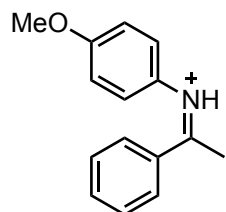


Hydrogenation Z-Iminium 5

M06-2X/def2-TZVP Geometry

C	1.36566	3.53781	-0.10858
C	1.39163	2.04897	-0.08986
N	2.54827	1.46345	-0.13693
C	0.12849	1.30743	-0.04874
C	2.87743	0.07093	0.03139
C	3.72034	-0.51604	-0.89899
C	4.06589	-1.84942	-0.73696
C	3.57788	-2.56702	0.34617
C	2.74882	-1.95474	1.27856
C	2.39369	-0.62434	1.12899
C	-0.94039	1.82133	0.68630
C	-2.15727	1.15840	0.69980

C	-2.31313	0.00922	-0.05583
C	-1.26595	-0.49186	-0.82257
C	-0.04272	0.14429	-0.81047
C	-3.63013	-0.73333	-0.08041
F	-4.54258	-0.15156	0.69136
F	-4.11153	-0.78982	-1.32233
F	-3.46636	-1.98715	0.34479
H	0.65853	3.88784	-0.85988
H	1.01326	3.89793	0.86111
H	2.34987	3.96441	-0.29221
H	3.35214	2.07164	-0.26640
H	4.09053	0.05393	-1.74262
H	4.71845	-2.32363	-1.45727
H	2.38602	-2.51119	2.13216
H	1.75791	-0.13288	1.85403
H	-0.82770	2.72552	1.26935
H	-2.98117	1.53964	1.28688
H	-1.41372	-1.37951	-1.42448
H	0.76796	-0.24527	-1.41122
H	3.85273	-3.60566	0.47174

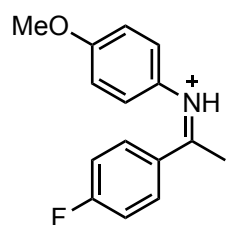


Hydrogenation Z-Iminium 6

M06-2X/def2-TZVP Geometry

C	2.84308	2.59725	0.04742
C	1.81072	1.52382	-0.02809
N	0.56555	1.89520	-0.05317
C	2.23228	0.12641	-0.09252
C	-0.63270	1.11681	0.07064
C	-1.69394	1.40538	-0.76797
C	-2.88046	0.69655	-0.65557
C	-2.99691	-0.29959	0.31450
C	-1.91809	-0.56744	1.17032
C	-0.74421	0.13713	1.05487
O	-4.09112	-1.03795	0.51244
C	-5.23116	-0.80206	-0.30005
C	3.38913	-0.26805	0.58687
C	3.83472	-1.57505	0.49613
C	3.15723	-2.48303	-0.30588

C	2.02720	-2.08784	-1.01378
C	1.55376	-0.79488	-0.90009
H	3.62263	2.42062	-0.69208
H	2.41393	3.58787	-0.09146
H	3.31381	2.56781	1.03328
H	0.40683	2.89637	-0.11496
H	-1.59948	2.17699	-1.52295
H	-3.70014	0.92897	-1.31853
H	-2.04228	-1.32714	1.92980
H	0.07987	-0.06351	1.72704
H	-5.98851	-1.50027	0.04164
H	-5.59191	0.22076	-0.17357
H	-5.00427	-0.99191	-1.35118
H	3.93167	0.43560	1.20413
H	4.71633	-1.88101	1.04263
H	3.51572	-3.50072	-0.38845
H	1.51522	-2.79135	-1.65609
H	0.67673	-0.49428	-1.45741

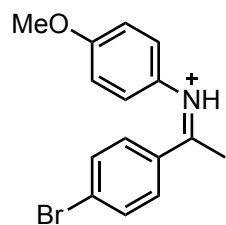


Hydrogenation Z-Iminium 7

M06-2X/def2-TZVP Geometry

C	1.18878	0.41079	-0.94750
C	2.30226	-0.41245	-0.92812
C	3.25555	-0.26767	0.08362
C	3.08215	0.71593	1.06562
C	1.97425	1.53276	1.04162
C	1.02259	1.36565	0.04028
N	-0.11726	2.23757	0.02023
C	-1.38027	1.94971	-0.10357
C	-1.90826	0.59469	-0.01412
C	-2.31525	3.09053	-0.33292
C	-3.07290	0.27119	-0.72247
C	-3.63185	-0.98689	-0.62439
C	-3.03912	-1.90566	0.22581
C	-1.90816	-1.60780	0.97298
C	-1.33668	-0.36134	0.83982

F	-3.57545	-3.10788	0.33890
O	4.36051	-1.00934	0.18936
C	4.61184	-2.00632	-0.78962
H	0.45309	0.30511	-1.73476
H	2.42631	-1.14867	-1.70805
H	3.83772	0.81912	1.83220
H	1.84065	2.28996	1.80484
H	0.10889	3.22720	0.04944
H	-3.19081	2.99863	0.30716
H	-1.83188	4.05104	-0.16384
H	-2.65790	3.06663	-1.37058
H	-3.53841	0.99765	-1.37495
H	-4.51678	-1.26372	-1.18013
H	-1.50115	-2.35145	1.64390
H	-0.46049	-0.12074	1.42559
H	4.71276	-1.55899	-1.78059
H	5.54856	-2.47391	-0.50374
H	3.81563	-2.75379	-0.79533

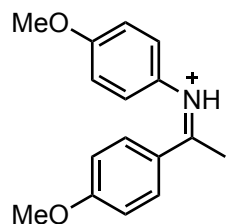


Hydrogenation Z-Iminium 8

M06-2X/def2-TZVP Geometry

C	-1.59846	-0.55662	-0.78857
C	-0.59514	0.38874	-0.76354
C	-0.76664	1.58512	-0.05287
C	-1.97247	1.81150	0.62062
C	-2.96533	0.85125	0.62886
C	-2.77456	-0.33014	-0.07797
C	0.23922	2.63960	-0.08297
C	-0.19239	4.06793	-0.05005
N	1.51792	2.40873	-0.15192
C	2.24164	1.18131	0.01167
C	3.26196	0.89003	-0.87517
C	3.99856	-0.27582	-0.72641
C	3.70854	-1.14347	0.32733
C	2.68389	-0.82354	1.23096

C	1.95687	0.33225	1.07922
H	0.31230	0.20602	-1.32246
H	-2.13540	2.73258	1.16411
H	-3.88586	1.01724	1.17006
Br	-4.12279	-1.63188	-0.08690
H	-1.02525	4.22843	-0.73201
H	-0.53753	4.31085	0.95817
H	0.62410	4.74456	-0.29537
H	2.10561	3.22691	-0.27976
H	3.48244	1.56278	-1.69531
H	4.78980	-0.49393	-1.42750
O	4.35352	-2.28794	0.56328
H	2.49514	-1.49976	2.05333
H	1.17593	0.58202	1.78565
C	5.41715	-2.66297	-0.29926
H	5.78857	-3.60910	0.08052
H	5.05851	-2.79353	-1.32220
H	6.21552	-1.91875	-0.27479
H	-1.47678	-1.46915	-1.35471

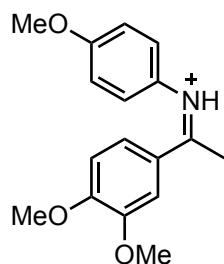


Hydrogenation Z-Iminium 9

M06-2X/def2-TZVP Geometry

C	-1.38292	3.59164	0.04469
C	-0.70405	2.26103	-0.04880
N	0.60303	2.28959	-0.09000
C	-1.49284	1.05297	-0.09509
C	1.55098	1.22311	0.05059
C	2.58600	1.12309	-0.85999
C	3.53293	0.11707	-0.72810
C	3.43626	-0.78548	0.33036
C	2.39016	-0.66178	1.25578
C	1.45663	0.33856	1.12230
O	4.29275	-1.78834	0.54994
C	5.38687	-1.95379	-0.33802
C	-2.79648	1.07556	0.42054

C	-3.61403	-0.03328	0.37343
C	-3.14834	-1.20136	-0.24071
C	-1.85861	-1.22834	-0.79985
C	-1.04408	-0.13287	-0.71728
H	-2.22268	3.64446	-0.64468
H	-1.76883	3.72741	1.05777
H	-0.69265	4.40835	-0.15855
H	1.01826	3.21186	-0.16233
H	2.65564	1.82081	-1.68584
H	4.33396	0.04971	-1.44861
H	2.34813	-1.35976	2.08065
H	0.65556	0.43841	1.84359
H	5.03636	-2.15173	-1.35333
H	6.02928	-1.07080	-0.33101
H	5.94204	-2.81116	0.02905
H	-4.60393	0.01554	0.80120
H	-1.53575	-2.13336	-1.29587
H	-0.06380	-0.17982	-1.16925
H	-3.17957	1.97108	0.89125
C	-5.16877	-2.37309	0.17842
H	-5.15477	-2.20547	1.25664
H	-5.80931	-1.63706	-0.31015
H	-5.53209	-3.37341	-0.03277
O	-3.84967	-2.32046	-0.35336

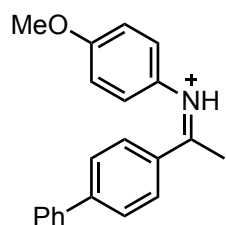


Hydrogenation Z-Iminium 10

M06-2X/def2-TZVP Geometry

C	-1.21107	3.93904	-0.03053
C	-0.55271	2.59792	0.06366
N	0.75130	2.61124	0.19029
C	-1.34728	1.39602	0.01479
C	1.68730	1.53076	0.06738
C	2.61135	1.31487	1.08408
C	3.51645	0.28151	0.97176
C	3.50970	-0.54219	-0.15992

C	2.58740	-0.30657	-1.18213
C	1.68201	0.73587	-1.06482
O	4.42119	-1.52168	-0.17618
C	4.48474	-2.37205	-1.30967
C	-0.92110	0.18063	0.60162
C	-1.71504	-0.93709	0.55380
C	-2.97543	-0.87816	-0.11158
C	-3.39862	0.32045	-0.67582
C	-2.60088	1.44814	-0.59569
O	-3.66122	-2.00805	-0.12419
O	-1.40918	-2.12432	1.08890
C	-4.93457	-2.03363	-0.75711
C	-0.16227	-2.25133	1.74775
H	-2.10863	3.97302	0.58214
H	-0.53463	4.73662	0.27166
H	-1.49995	4.12484	-1.06773
H	1.17214	3.52501	0.31689
H	2.61246	1.94558	1.96473
H	4.24721	0.09027	1.74562
H	2.57589	-0.91604	-2.07341
H	0.96556	0.92095	-1.85521
H	5.28238	-3.07986	-1.10771
H	3.54369	-2.90977	-1.44578
H	4.72087	-1.80144	-2.21031
H	0.02020	0.13285	1.12449
H	-4.35427	0.37985	-1.17425
H	-2.95962	2.36520	-1.04197
H	-5.30105	-3.04808	-0.64058
H	-5.61884	-1.33546	-0.27193
H	-4.84043	-1.79319	-1.81761
H	-0.09872	-3.28541	2.07140
H	0.66327	-2.02472	1.06625
H	-0.11282	-1.59167	2.61774

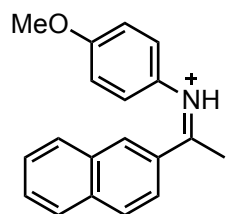


Hydrogenation Z-Iminium 11

M06-2X/def2-TZVP Geometry

C	-0.93201	4.20451	-0.19417
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C	-1.09776	2.71930	-0.17248
N	-2.32217	2.27168	-0.22307
C	0.07536	1.86709	-0.11102
C	-2.82708	0.94640	-0.00957
C	-3.73990	0.42959	-0.91015
C	-4.26548	-0.83979	-0.71549
C	-3.87270	-1.58365	0.39715
C	-2.95982	-1.03842	1.31192
C	-2.44287	0.21969	1.11477
O	-4.31404	-2.81282	0.67987
C	-5.25152	-3.41879	-0.19630
C	1.25039	2.36696	0.46850
C	2.39846	1.60485	0.49853
C	2.43370	0.33359	-0.08456
C	1.26746	-0.14605	-0.69579
C	0.10606	0.59302	-0.70007
H	-0.13245	4.48976	-0.87466
H	-1.85406	4.70926	-0.47697
H	-0.65702	4.54652	0.80666
H	-3.03901	2.97334	-0.37575
H	-4.03726	1.00667	-1.77762
H	-4.97431	-1.23353	-1.42842
H	-2.68715	-1.62614	2.17775
H	-1.74367	0.64091	1.82574
H	-4.82909	-3.53424	-1.19673
H	-5.46265	-4.39663	0.22485
H	-6.17207	-2.83342	-0.24425
H	3.29525	2.01193	0.94589
H	1.27064	-1.12718	-1.15140
H	-0.77248	0.18862	-1.18266
H	1.26655	3.35463	0.90994
C	6.00120	-1.99858	-0.03481
C	5.68912	-1.18234	1.04412
C	4.53318	-0.41977	1.02632
C	3.66662	-0.47296	-0.06725
C	3.98757	-1.30108	-1.14461
C	5.14993	-2.05360	-1.13026
H	6.90670	-2.59066	-0.02239
H	6.34497	-1.14438	1.90367
H	4.28517	0.19490	1.88277
H	3.34376	-1.33017	-2.01473
H	5.39623	-2.67915	-1.97787

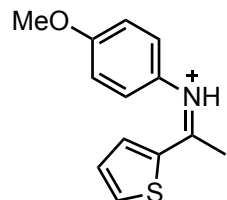


Hydrogenation Z-Iminium 12

M06-2X/def2-TZVP Geometry

C	-0.90074	3.64024	-0.01671
C	-0.26161	2.29285	-0.10774
N	1.04101	2.26298	-0.08699
C	-1.09146	1.10488	-0.23432
C	1.94355	1.16160	0.06274
C	3.10150	1.15786	-0.69417
C	4.02644	0.13583	-0.54631
C	3.78461	-0.88134	0.37743
C	2.61428	-0.85614	1.14976
C	1.70059	0.15962	1.00013
O	4.60867	-1.90788	0.60430
C	5.83313	-1.96930	-0.11077
C	-0.67404	-0.02168	-1.00307
C	-1.50922	-1.08350	-1.15824
C	-2.78896	-1.11416	-0.54347
C	-3.20994	0.00577	0.22145
C	-2.34729	1.11173	0.33862
C	-3.66098	-2.21465	-0.67887
C	-4.89050	-2.19880	-0.07809
C	-5.30866	-1.08632	0.68462
C	-4.48727	-0.00585	0.83240
H	-0.17278	4.44126	-0.13294
H	-1.68358	3.74115	-0.76579
H	-1.36396	3.75082	0.96671
H	1.49872	3.16846	-0.11345
H	3.28566	1.94723	-1.41333
H	4.92375	0.14473	-1.14638
H	2.46068	-1.64313	1.87520
H	0.80623	0.18246	1.60911
H	6.44970	-1.09390	0.10368
H	6.33707	-2.86485	0.23848
H	5.65247	-2.04596	-1.18497
H	0.28892	-0.01713	-1.49391
H	-1.20521	-1.92657	-1.76619
H	-2.68945	1.96417	0.91285
H	-3.34493	-3.06869	-1.26477

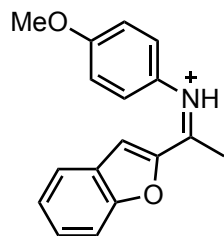
H	-5.55481	-3.04619	-0.18632
H	-6.28514	-1.09600	1.14998
H	-4.80034	0.85247	1.41429



Hydrogenation Z-Iminium 13

M06-2X/def2-TZVP Geometry

C	2.16034	2.52564	0.05749
S	1.00105	1.30092	0.05666
C	2.22619	0.07790	-0.04628
C	3.48746	0.66363	-0.07545
C	3.45013	2.05742	-0.01578
C	2.02442	-1.33309	-0.10091
C	3.21700	-2.23442	-0.20399
N	0.85493	-1.91665	-0.06852
C	-0.43150	-1.28168	0.04070
C	-1.12912	-0.95093	-1.10681
C	-2.36381	-0.32742	-1.00791
C	-2.89614	-0.04694	0.25234
C	-2.18355	-0.40105	1.40603
C	-0.95881	-1.01979	1.30233
H	4.40480	0.09665	-0.13762
H	3.86757	-2.08850	0.65786
H	2.91948	-3.27974	-0.24352
H	3.78555	-1.99760	-1.10265
H	0.85671	-2.92926	-0.11855
H	-0.70706	-1.16698	-2.08032
H	-2.90037	-0.07149	-1.90902
O	-4.07433	0.54857	0.45751
H	-2.62267	-0.18255	2.36964
H	-0.40392	-1.29216	2.19134
C	-4.86099	0.91146	-0.66661
H	-5.12384	0.03091	-1.25610
H	-5.76211	1.36390	-0.26565
H	-4.33412	1.63541	-1.29161
H	4.32109	2.69434	-0.02541
H	1.84235	3.55606	0.11366

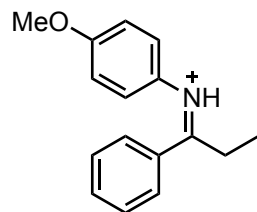


Hydrogenation Z-Iminium 14

M06-2X/def2-TZVP Geometry

O	2.65184	1.10503	-0.06759
C	1.28029	1.03757	-0.03904
C	0.85944	-0.27143	0.00800
C	0.64115	2.30967	-0.07926
C	1.49712	3.52769	-0.16274
N	-0.65586	2.46478	-0.04973
C	-1.63918	1.42116	0.05469
C	-2.20739	0.90093	-1.09269
C	-3.13557	-0.12704	-0.99885
C	-3.49074	-0.62378	0.25655
C	-2.91016	-0.08084	1.41092
C	-1.99110	0.93968	1.31191
H	-0.15848	-0.62154	0.03866
H	2.16485	3.56100	0.69861
H	2.12803	3.46943	-1.04977
H	0.89787	4.43436	-0.19650
H	-0.99676	3.41856	-0.09430
H	-1.92242	1.28667	-2.06340
H	-3.57608	-0.52492	-1.90061
O	-4.37354	-1.60756	0.45727
H	-3.20980	-0.47545	2.37206
H	-1.53957	1.36036	2.20158
C	-5.02546	-2.17812	-0.66663
H	-4.30327	-2.64657	-1.33858
H	-5.69656	-2.93304	-0.27009
H	-5.60070	-1.42277	-1.20568
C	3.10371	-0.16528	-0.03729
C	2.03156	-1.06696	0.00906
C	2.28846	-2.44947	0.04693
C	3.59890	-2.85405	0.03627
C	4.65584	-1.91841	-0.01091
C	4.43452	-0.55851	-0.04841

H	1.47766	-3.16411	0.08426
H	3.83727	-3.90821	0.06495
H	5.67403	-2.28439	-0.01745
H	5.24018	0.16042	-0.08413

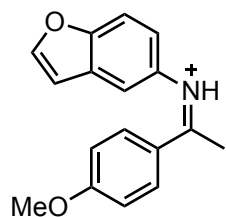


Hydrogenation Z-Iminium 15

M06-2X/def2-TZVP Geometry

C	-3.28774	-2.34614	-0.55091
C	-3.05619	-0.98509	-0.66173
C	-2.03913	-0.38846	0.08657
C	-1.28263	-1.16243	0.97363
C	-1.54395	-2.51317	1.10306
C	-2.53689	-3.10819	0.33329
C	-1.82579	1.05997	0.01501
C	-3.01573	1.96835	-0.01743
C	-2.73575	3.46211	0.00073
N	-0.64251	1.59026	0.02405
C	0.64352	0.96481	-0.09513
C	1.66482	1.39515	0.73163
C	2.92635	0.82750	0.62967
C	3.15780	-0.16876	-0.31937
C	2.11783	-0.57763	-1.16660
C	0.86899	-0.01459	-1.05979
O	4.33102	-0.78054	-0.50230
C	5.43069	-0.40355	0.31211
H	-4.06048	-2.80947	-1.14909
H	-3.64998	-0.40035	-1.35155
H	-0.50813	-0.70385	1.57455
H	-0.97147	-3.10522	1.80408
H	-2.72890	-4.16892	0.42803
H	-3.65344	1.67249	0.81997
H	-3.58506	1.69917	-0.91266
H	-2.21542	3.76817	0.91084
H	-2.15895	3.78192	-0.86931
H	-3.67716	4.00661	-0.02297
H	-0.61252	2.60430	0.08167
H	1.48279	2.16578	1.47150

H	3.71305	1.16797	1.28572
H	2.32766	-1.33402	-1.91044
H	0.07238	-0.32591	-1.72259
H	5.21706	-0.59685	1.36546
H	6.26466	-1.01922	-0.00911
H	5.67617	0.65057	0.16728

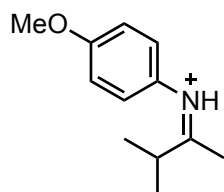


Hydrogenation Z-Iminium 16

M06-2X/def2-TZVP Geometry

C	-3.72584	0.04392	0.29398
C	-2.88551	1.13493	0.34028
C	-1.56076	1.06482	-0.11608
C	-1.11397	-0.15203	-0.67819
C	-1.94998	-1.23071	-0.76116
C	-3.26207	-1.15509	-0.26068
C	-0.74387	2.25261	-0.06946
C	-1.38889	3.60296	-0.04026
N	0.56417	2.24518	-0.05383
H	-3.26669	2.05409	0.76455
H	-0.11708	-0.23558	-1.08582
H	-1.62804	-2.15876	-1.21284
O	-3.98570	-2.26000	-0.36702
H	-0.66885	4.39469	-0.23788
H	-1.80900	3.77644	0.95323
H	-2.19919	3.65930	-0.76340
H	1.01100	3.15237	-0.12662
H	-4.73163	0.12825	0.67651
C	-5.32890	-2.26147	0.10434
H	-5.92666	-1.52850	-0.43942
H	-5.35983	-2.05476	1.17517
H	-5.70765	-3.25960	-0.08810
C	2.17454	-0.68700	1.55111
C	1.30600	0.35722	1.30232
C	1.47163	1.14986	0.16046
C	2.49634	0.96124	-0.74735
H	2.07758	-1.31380	2.42617
H	0.49499	0.56868	1.98623
H	2.59434	1.59864	-1.61710

C	3.19201	-0.88357	0.63216
C	3.38240	-0.08753	-0.50534
C	4.54295	-0.62700	-1.16101
C	4.94012	-1.66108	-0.39479
O	4.14115	-1.83798	0.69430
H	5.01043	-0.28889	-2.06948
H	5.75640	-2.35740	-0.48476

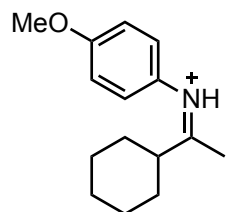


Hydrogenation Z-Iminium 17

M06-2X/def2-TZVP Geometry

C	-3.61466	1.38098	-0.46305
C	-2.37421	0.60464	-0.19513
N	-1.24292	1.13238	-0.53286
C	-2.46573	-0.72775	0.47414
C	0.09201	0.61911	-0.38133
C	1.04117	1.44414	0.19678
C	2.34657	1.00423	0.34205
C	2.69938	-0.26994	-0.10754
C	1.73411	-1.08424	-0.71429
C	0.43922	-0.64231	-0.85683
O	3.92381	-0.79146	-0.01369
C	4.95339	-0.01681	0.58343
C	-3.02806	-1.76649	-0.51199
C	-3.34832	-0.63940	1.72527
H	-4.37727	0.73275	-0.89475
H	-4.00828	1.74775	0.48810
H	-3.44183	2.22672	-1.12569
H	-1.28870	2.05796	-0.95179
H	-1.46214	-1.02963	0.77176
H	0.76585	2.43104	0.54916
H	3.07475	1.65563	0.80131
H	2.03709	-2.05674	-1.07714
H	-0.29335	-1.26440	-1.35318
H	5.12662	0.90027	0.01666
H	4.70490	0.22414	1.61907
H	5.84448	-0.63553	0.55727
H	-2.46575	-1.80764	-1.44454
H	-2.98319	-2.74866	-0.04322
H	-4.07147	-1.55759	-0.74922

H	-2.99363	0.12195	2.42048
H	-4.38721	-0.42934	1.46963
H	-3.32016	-1.60058	2.23659

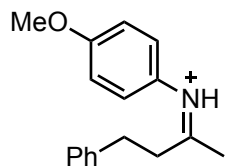


Hydrogenation *Z*-Iminium 18

M06-2X/def2-TZVP Geometry

C	-1.46865	1.58326	-0.13941
C	-2.51151	2.64118	-0.21276
N	-0.23079	1.94310	-0.25722
C	0.94923	1.11734	-0.23024
C	1.92062	1.37552	0.71967
C	3.07711	0.61137	0.75049
C	3.25703	-0.40984	-0.18440
C	2.27271	-0.64628	-1.15257
C	1.12719	0.11554	-1.17958
O	4.33060	-1.20218	-0.23905
C	5.37278	-1.00533	0.70487
H	-0.95858	-0.40525	0.32807
H	-2.11868	3.58955	-0.57393
H	-2.93248	2.78479	0.78536
H	-3.32795	2.31657	-0.85786
H	-0.05714	2.93682	-0.38342
H	1.77807	2.16367	1.44889
H	3.82488	0.81753	1.50144
H	2.44218	-1.42798	-1.88025
H	0.38063	-0.05160	-1.94477
H	5.80600	-0.00841	0.60109
H	6.12473	-1.75469	0.47922
H	5.00567	-1.15020	1.72301
C	-2.82358	-1.91167	-0.93266
C	-2.49401	-0.44098	-1.17947
C	-1.85816	0.16715	0.09224
C	-2.84048	0.04200	1.27329
C	-3.16621	-1.42988	1.51604
C	-3.75301	-2.07889	0.26586
H	-1.89365	-2.46204	-0.75755
H	-3.27669	-2.33264	-1.83078

H	-3.41253	0.10237	-1.41998
H	-1.82406	-0.33625	-2.03466
H	-2.41191	0.49424	2.17066
H	-3.76373	0.58017	1.03952
H	-2.25433	-1.95762	1.81185
H	-3.86255	-1.51073	2.35117
H	-4.72036	-1.61853	0.04043
H	-3.94305	-3.13688	0.44706

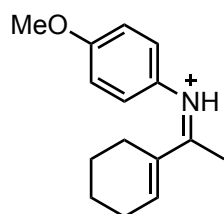


Hydrogenation *Z*-Iminium 19

M06-2X/def2-TZVP Geometry

C	0.97048	-2.82466	0.57971
C	1.27395	-1.67875	1.30031
C	2.20720	-0.76485	0.81921
C	2.83108	-1.01923	-0.40011
C	2.52748	-2.16361	-1.12680
C	1.59488	-3.06847	-0.63674
C	2.52066	0.48499	1.59858
C	1.53933	1.64828	1.29081
C	1.61800	2.03934	-0.14086
C	2.81208	2.77614	-0.62972
N	0.68031	1.74981	-0.97640
C	-0.57484	1.09229	-0.68702
C	-1.61899	1.82490	-0.15412
C	-2.83066	1.20199	0.10608
C	-2.98321	-0.15583	-0.18152
C	-1.91511	-0.87710	-0.72796
C	-0.71219	-0.25750	-0.98352
O	-4.10640	-0.84956	0.03212
C	-5.23080	-0.17555	0.57438
H	0.25373	-3.53362	0.97348
H	0.78997	-1.49939	2.25406
H	3.58839	-0.33636	-0.77277
H	3.03242	-2.35822	-2.06404
H	1.36800	-3.96824	-1.19330
H	3.54674	0.80397	1.41129
H	2.44064	0.29308	2.66855
H	1.82209	2.51646	1.89064
H	0.52583	1.34961	1.55150

H	2.79743	3.77811	-0.19223
H	2.83894	2.86181	-1.71426
H	3.72198	2.29070	-0.27784
H	0.83381	2.00915	-1.94797
H	-1.49487	2.87972	0.05853
H	-3.64202	1.77924	0.52323
H	-2.05633	-1.92858	-0.93813
H	0.12161	-0.81714	-1.39069
H	-5.00078	0.23198	1.56133
H	-5.56216	0.62441	-0.09117
H	-6.01251	-0.92322	0.66334

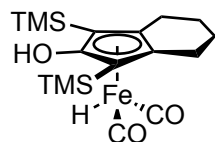


Hydrogenation *Z*-Iminium 20

M06-2X/def2-TZVP Geometry

C	3.89012	-1.42830	0.56887
C	3.28882	-0.06705	0.52829
C	2.10383	0.22628	-0.04086
C	1.30475	-0.83355	-0.77779
C	2.20997	-1.99124	-1.19191
C	2.97052	-2.51399	0.02035
C	1.68444	1.62091	-0.03728
C	2.68631	2.72937	0.05200
N	0.43741	1.98476	-0.15404
H	0.82767	-0.38392	-1.65127
H	2.91698	-1.65664	-1.95631
H	3.06675	2.78798	1.07423
H	3.52800	2.54530	-0.61102
H	2.23732	3.69186	-0.18658
H	0.27231	2.97945	-0.26993
H	4.20900	-1.64320	1.59235
C	-2.07074	-0.29177	1.32907
C	-0.91503	0.43420	1.15922
C	-0.74699	1.19387	0.00484
C	-1.73987	1.25340	-0.95646
H	-2.23505	-0.88704	2.21668
H	-0.14176	0.42076	1.91762
H	-1.60319	1.85678	-1.84560
C	-3.07636	-0.25804	0.35340

C	-2.90636	0.52326	-0.79185
C	-5.22775	-0.98886	-0.32572
O	-4.16040	-0.99483	0.61007
H	-5.98957	-1.64158	0.08782
H	0.49850	-1.21967	-0.15223
H	4.82019	-1.37736	-0.01167
H	1.60288	-2.77882	-1.63688
H	2.25557	-2.81411	0.79086
H	3.55380	-3.39810	-0.23293
H	3.87042	0.71985	0.99636
H	-3.67135	0.57076	-1.55199
H	-5.63269	0.01802	-0.44469
H	-4.89834	-1.37589	-1.29207



Knölker's Complex

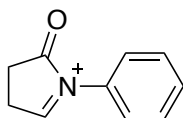
M06/def2-TZVP Geometry

C	-0.74862	1.19362	-0.57827
C	0.65756	1.11321	-0.67906
C	1.51357	2.33301	-0.79817
C	0.76073	3.57315	-0.34037
C	-0.60885	3.64350	-0.99382
C	-1.49492	2.49353	-0.53661
C	-1.29359	-0.13996	-0.57957
C	-0.16775	-0.98628	-0.75483
C	1.04212	-0.26627	-0.77473
H	2.45018	2.22313	-0.24334
H	0.63756	3.54846	0.75130
H	-1.09466	4.59723	-0.77392
H	-1.85051	2.69553	0.48351
O	-0.17513	-2.33950	-0.80691
Si	2.70334	-1.09870	-0.94558
Si	-3.09973	-0.57360	-0.44882
Fe	-0.12129	0.43220	1.38896
C	-0.29990	-1.47698	2.14686
O	-0.56499	-2.45477	2.64451
H	-1.08341	-2.66017	-0.82236
H	1.80962	2.45993	-1.84912
H	1.34362	4.46858	-0.56961
H	-0.48253	3.59732	-2.08272
H	-2.39185	2.43369	-1.16243

C	-4.02606	-0.05344	-1.98799
H	-5.08175	-0.32665	-1.90895
H	-3.97370	1.02576	-2.14696
H	-3.61699	-0.54019	-2.87607
C	-3.85870	0.24514	1.04781
H	-3.77582	1.33319	1.00124
H	-4.92010	-0.00776	1.11930
H	-3.36906	-0.07695	1.97056
C	-3.31320	-2.43311	-0.26034
H	-3.02340	-2.99403	-1.15517
H	-2.78005	-2.83960	0.60367
H	-4.37450	-2.64423	-0.10383
C	2.75493	-2.03847	-2.56000
H	1.94413	-2.76815	-2.60497
H	2.64966	-1.36342	-3.41211
C	4.10757	0.14003	-0.92498
H	4.02035	0.87904	-1.72411
H	4.18264	0.67377	0.02559
H	5.04925	-0.39632	-1.07203
C	2.96407	-2.29972	0.46802
H	3.06039	-1.77886	1.42466
H	2.12841	-2.99897	0.54446
H	3.87772	-2.88050	0.31547
H	3.70242	-2.57308	-2.66711
C	1.79730	0.86618	2.14177
O	2.71326	1.33800	2.60066
H	-0.83730	1.29557	2.62323

Cartesian coordinates of reaction components relevant to chiral phosphate catalysis

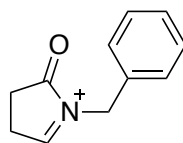
Additional reaction components required for re-creating the statistical model have been published elsewhere.¹¹



Iminium 1

M06/def2-TZVP Geometry

C	1.45125	-1.28476	0.44582
N	0.76445	-0.24882	0.12385
C	1.69908	0.88501	-0.29408
C	3.07950	0.33267	-0.12413
C	2.90748	-1.10958	0.32060
C	-0.65855	-0.14720	0.07066
C	-1.27674	0.99556	0.55459
C	-2.65635	1.06289	0.51792
C	-3.39529	0.01333	-0.00342
C	-2.76109	-1.11680	-0.49563
C	-1.38400	-1.20321	-0.46368
O	1.28539	1.91548	-0.65907
H	0.95982	-2.19267	0.78448
H	3.61720	0.44399	-1.06686
H	3.60816	0.94870	0.60632
H	3.39079	-1.34847	1.27270
H	3.30161	-1.84081	-0.39328
H	-0.69541	1.81023	0.96505
H	-3.15660	1.94348	0.90012
H	-4.47573	0.07963	-0.03499
H	-3.34004	-1.92782	-0.91860
H	-0.87587	-2.06575	-0.88124

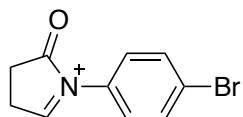


Iminium 2

M06/def2-TZVP Geometry

C	1.06221	1.10187	-0.00009
N	1.20495	-0.16846	-0.00005

C	2.65721	-0.54540	-0.00012
C	3.40541	0.75278	0.00007
C	2.33934	1.83826	-0.00007
C	0.15878	-1.21854	-0.00003
O	2.98693	-1.67094	0.00015
H	0.07001	1.54869	-0.00011
H	4.05863	0.78194	0.87398
H	4.05894	0.78199	-0.87359
H	2.37551	2.50197	-0.86963
H	2.37540	2.50208	0.86942
H	0.36285	-1.83678	-0.87808
H	0.36288	-1.83678	0.87802
C	-3.73032	0.52186	0.00003
C	-3.10415	0.23071	1.20111
C	-1.84776	-0.34908	1.20187
C	-1.21348	-0.64134	-0.00001
C	-1.84781	-0.34910	-1.20186
C	-3.10420	0.23069	-1.20107
H	-4.71729	0.96814	0.00004
H	-3.60108	0.44449	2.13933
H	-1.36299	-0.59483	2.14226
H	-1.36307	-0.59486	-2.14227
H	-3.60116	0.44446	-2.13928

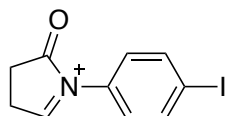


Iminium 3

M06/def2-TZVP Geometry

C	-2.98771	-1.27772	0.43053
N	-2.27896	-0.24972	0.12584
C	-3.19243	0.90420	-0.28968
C	-4.58269	0.37400	-0.13502
C	-4.43920	-1.07684	0.29099
C	-0.85793	-0.17078	0.08154
C	-0.21922	0.96800	0.55189
C	1.15881	1.01854	0.52785
C	1.88285	-0.05415	0.02619
C	1.23664	-1.18510	-0.45605
C	-0.13942	-1.24380	-0.43014
O	-2.75858	1.93035	-0.64319
H	-2.51684	-2.19737	0.76612
H	-5.10405	0.98925	0.60146
H	-5.11316	0.50854	-1.07881

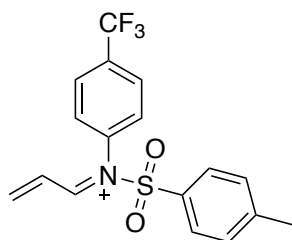
H	-4.83724	-1.79029	-0.43867
H	-4.93834	-1.32107	1.23349
H	-0.78461	1.80063	0.94815
H	1.67652	1.89326	0.90002
Br	3.75202	0.02853	-0.01579
H	1.81210	-2.00670	-0.86276
H	-0.65182	-2.10747	-0.84005



Iminium 4

M06/def2-TZVP Geometry

C	3.56705	-1.27641	0.42629
N	2.85558	-0.24881	0.12459
C	3.76609	0.90739	-0.28827
C	5.15779	0.38114	-0.13278
C	5.01812	-1.07192	0.28681
C	1.43495	-0.17324	0.08061
C	0.79302	0.96447	0.54889
C	-0.58556	1.00904	0.52746
C	-1.31542	-0.06495	0.03040
C	-0.65854	-1.19364	-0.44992
C	0.71796	-1.24950	-0.42651
O	3.33095	1.93309	-0.64194
H	3.09831	-2.19773	0.75986
H	5.69043	0.52189	-1.07437
H	5.67486	0.99476	0.60812
H	5.51884	-1.31889	1.22770
H	5.41751	-1.78056	-0.44679
H	1.35618	1.80008	0.94229
H	-1.09669	1.88731	0.90164
I	-3.39013	0.02098	-0.01098
H	-1.22399	-2.02312	-0.85612
H	1.23205	-2.11295	-0.83519

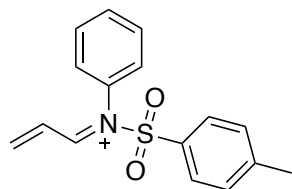


Iminium 5

M06/def2-TZVP Geometry

C	-1.09673	-3.46509	-1.38565
C	-1.76513	-4.42904	-2.02475
C	-1.82308	-2.52170	-0.60129
N	-1.30838	-1.54577	0.06912
S	-2.42736	-0.49027	1.08981
C	0.08370	-1.19823	0.06308
C	-2.03775	1.06155	0.44498
O	-3.70829	-0.94472	0.68350
O	-1.91225	-0.66133	2.39648
C	-1.07344	1.83604	1.08127
C	-0.73386	3.05102	0.52689
C	-1.33562	3.50205	-0.64712
C	-2.29838	2.69970	-1.26202
C	-2.65745	1.48248	-0.72763
C	-0.98512	4.83224	-1.21562
C	0.86110	-1.46200	1.17523
C	2.18649	-1.05947	1.17137
C	2.70603	-0.40260	0.07074
C	1.91446	-0.14741	-1.04130
C	0.59372	-0.54213	-1.04887
C	4.13923	0.06425	0.03947
F	4.79068	-0.25142	1.14651
F	4.78378	-0.47592	-0.98973
F	4.19100	1.38637	-0.10745
H	-0.01635	-3.38931	-1.43524
H	-1.25530	-5.17554	-2.62109
H	-2.84650	-4.50189	-1.96908
H	-2.90742	-2.61603	-0.53212
H	-0.61025	1.48855	1.99675
H	0.01128	3.67040	1.01334
H	-2.77732	3.04820	-2.17020
H	-3.41800	0.86935	-1.19690
H	-1.11333	4.85460	-2.29794
H	-1.63971	5.60230	-0.79711
H	0.03968	5.11553	-0.97531
H	0.43401	-1.96588	2.03326

H	2.81394	-1.25916	2.03028
H	2.33634	0.36609	-1.89752
H	-0.04854	-0.33534	-1.89843

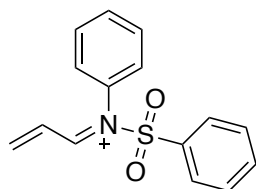


Iminium 6

M06/def2-TZVP Geometry

C	3.28793	-0.62485	-1.46482
C	4.09943	-1.43686	-2.14722
C	2.27991	-1.19294	-0.63092
N	1.42979	-0.52833	0.07768
S	0.25304	-1.46157	1.13879
C	1.30814	0.90303	0.06901
C	-1.24317	-0.91099	0.47573
O	0.53587	-2.80694	0.78651
O	0.48785	-0.92289	2.42577
C	-1.88891	0.17229	1.06013
C	-3.06077	0.62478	0.49202
C	-3.59218	0.01984	-0.64531
C	-2.91582	-1.06234	-1.21120
C	-1.74576	-1.53562	-0.66154
C	-4.87730	0.49381	-1.22867
C	0.69676	1.50572	-1.02015
C	0.53558	2.87859	-1.01908
C	0.97612	3.62653	0.06159
C	1.58305	3.00827	1.14265
C	1.75214	1.63467	1.15708
H	3.38087	0.45398	-1.51694
H	4.88636	-1.05130	-2.78347
H	4.00157	-2.51611	-2.08938
H	2.20713	-2.27836	-0.55529
H	-1.47712	0.64062	1.94600
H	-3.58146	1.46378	0.93963
H	-3.32740	-1.54269	-2.09192
H	-1.23245	-2.38807	-1.09083
H	-4.89215	0.38034	-2.31310
H	-5.70905	-0.09627	-0.83312
H	-5.07307	1.53683	-0.98064

H	0.34369	0.89745	-1.84686
H	0.06216	3.36484	-1.86284
H	1.93016	3.59728	1.98231
H	2.21636	1.13439	1.99786
H	0.84654	4.70181	0.06021

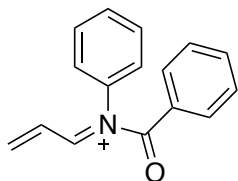


Iminium 7

M06/def2-TZVP Geometry

C	-3.14849	-0.89922	-1.05430
C	-3.98800	-1.79703	-1.57733
C	-1.97908	-1.35645	-0.37930
N	-1.08672	-0.60155	0.17046
S	0.29912	-1.40196	1.06745
C	-1.08488	0.83419	0.10724
C	1.63818	-0.72275	0.20008
O	0.19563	-0.86372	2.37149
O	0.10421	-2.77456	0.76598
C	2.24974	0.42049	0.69917
C	3.28821	0.97655	-0.02278
C	3.69196	0.39728	-1.21583
C	3.07232	-0.74696	-1.69883
C	2.03446	-1.31947	-0.99138
C	-1.40753	1.57105	1.23385
C	-1.35142	2.95199	1.15745
C	-0.97366	3.57229	-0.02234
C	-0.65298	2.81893	-1.14091
C	-0.70397	1.43891	-1.08137
H	-3.33764	0.16642	-1.11628
H	-4.89541	-1.49782	-2.08711
H	-3.79307	-2.86251	-1.51015
H	-1.80540	-2.42945	-0.29141
H	1.91940	0.85257	1.63584
H	3.78764	1.86187	0.34970
H	3.40822	-1.19903	-2.62346
H	1.54989	-2.22379	-1.34006
H	-1.69220	1.07014	2.15083
H	-1.60678	3.54507	2.02663
H	-0.35893	3.30656	-2.06190
H	-0.44040	0.82803	-1.93885
H	-0.93048	4.65335	-0.07160

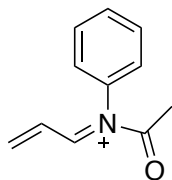
H 4.50860 0.83822 -1.77482



Iminium 8

M06/def2-TZVP Geometry

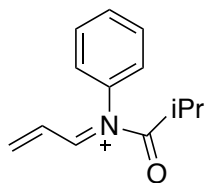
C	3.30342	-1.21212	-0.28546
C	4.21032	-2.15543	-0.56467
C	1.93295	-1.60867	-0.15822
N	0.92195	-0.82910	0.07011
C	-0.39496	-1.52449	0.36105
C	1.03254	0.60335	0.19137
C	-1.62474	-0.81740	-0.00966
O	-0.31001	-2.59228	0.87305
C	-2.77634	-1.16884	0.69857
C	-3.98692	-0.58988	0.36562
C	-4.05479	0.31451	-0.68756
C	-2.91420	0.64399	-1.41033
C	-1.69405	0.08857	-1.06899
C	0.57395	1.20147	1.35452
C	0.66931	2.57920	1.47802
C	1.20759	3.33681	0.44646
C	1.65511	2.72211	-0.71636
C	1.56774	1.34573	-0.85191
H	3.58137	-0.17934	-0.12847
H	5.26298	-1.91747	-0.64412
H	3.92348	-3.18891	-0.72183
H	1.69035	-2.66589	-0.21776
H	-2.70510	-1.89051	1.50165
H	-4.87889	-0.84810	0.91961
H	-2.97786	1.33367	-2.24063
H	-0.81347	0.34304	-1.64208
H	0.15469	0.60045	2.15202
H	0.32182	3.05921	2.38249
H	2.06534	3.31434	-1.52292
H	1.88940	0.85500	-1.76284
H	1.27497	4.41162	0.54666
H	-5.00425	0.76134	-0.95182



Iminium 9

M06/def2-TZVP Geometry

C	-1.45053	-2.05597	0.00005
C	-2.47072	-2.92323	0.00006
C	-1.73773	-0.66701	0.00002
N	-0.86053	0.29154	0.00000
C	-1.40142	1.71011	-0.00003
C	0.55998	0.02767	0.00000
O	-2.57397	1.84085	-0.00001
C	1.21962	-0.09538	1.21003
C	2.58124	-0.34457	1.20246
C	3.25857	-0.46684	0.00001
C	2.58123	-0.34463	-1.20244
C	1.21962	-0.09544	-1.21002
H	-0.41865	-2.38828	0.00005
H	-2.30728	-3.99407	0.00008
H	-3.50211	-2.58525	0.00005
H	-2.77521	-0.33058	0.00001
H	0.67333	0.00298	2.14210
H	3.11290	-0.44503	2.14038
H	3.11288	-0.44514	-2.14037
H	0.67332	0.00287	-2.14209
H	4.32395	-0.66082	0.00001
C	-0.35962	2.75840	-0.00009
H	-0.84749	3.72940	-0.00012
H	0.28423	2.66388	0.87686
H	0.28419	2.66381	-0.87706

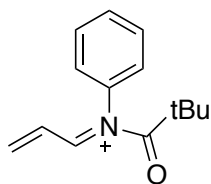


Iminium 10

M06/def2-TZVP Geometry

C	-1.56243	2.46456	0.00399
C	-1.79150	3.78030	0.09037

C	-0.21888	2.00805	-0.04512
N	0.17037	0.77069	-0.11327
C	1.68088	0.54771	-0.21805
C	-0.76864	-0.32449	-0.10369
O	2.34017	1.50460	-0.42525
C	-1.40053	-0.66602	1.07980
C	-2.30347	-1.71486	1.07677
C	-2.56417	-2.40293	-0.09677
C	-1.92762	-2.04567	-1.27481
C	-1.02198	-0.99991	-1.28534
H	-2.37336	1.74675	-0.04011
H	-2.79693	4.18234	0.11697
H	-0.97671	4.49564	0.13798
H	0.59165	2.73733	-0.04670
H	-1.18448	-0.11649	1.99017
H	-2.80359	-1.99430	1.99560
H	-2.13838	-2.58078	-2.19221
H	-0.51722	-0.70714	-2.19972
H	-3.27051	-3.22378	-0.09414
C	2.14423	-0.84612	0.03975
C	3.49832	-1.07482	-0.60395
C	2.21463	-1.02194	1.56107
H	1.40854	-1.54986	-0.35833
H	3.82431	-2.09687	-0.41063
H	3.46809	-0.92353	-1.68332
H	4.24325	-0.39461	-0.18862
H	2.56003	-2.03116	1.78550
H	2.92964	-0.31564	1.98867
H	1.24875	-0.88270	2.04967

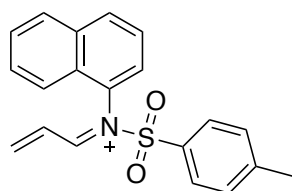


Iminium 11

M06/def2-TZVP Geometry

C	-1.48730	2.65095	0.07790
C	-1.57145	3.97958	0.19343
C	-0.21065	2.05424	-0.12450
N	0.03861	0.78753	-0.22607
C	1.48720	0.41468	-0.57774
C	-0.97088	-0.23336	-0.14341

O	1.95995	1.04270	-1.45724
C	-1.21307	-0.99533	-1.27395
C	-2.14862	-2.01121	-1.20507
C	-2.82182	-2.25659	-0.01871
C	-2.57451	-1.47983	1.10203
C	-1.64456	-0.45718	1.04597
H	-2.36754	2.01975	0.11317
H	-2.52282	4.47990	0.32486
H	-0.68860	4.60984	0.15944
H	0.65174	2.71146	-0.23020
H	-0.67229	-0.79366	-2.19264
H	-2.35190	-2.61331	-2.08168
H	-3.10401	-1.67285	2.02657
H	-1.42965	0.15008	1.91892
H	-3.54764	-3.05866	0.03247
C	2.16432	-0.60967	0.30487
C	3.64524	-0.58251	-0.05925
C	1.98403	-0.18812	1.76363
C	1.62866	-2.02826	0.08863
H	4.17863	-1.28217	0.58578
H	3.80706	-0.87956	-1.09598
H	4.07706	0.40979	0.07906
H	2.57459	-0.85622	2.39302
H	2.34457	0.82985	1.93617
H	0.94747	-0.25829	2.09755
H	2.28024	-2.71389	0.63409
H	0.61459	-2.16858	0.46250
H	1.65910	-2.31204	-0.96563

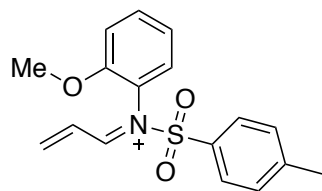


Iminium 12

M06/def2-TZVP Geometry

C	0.78467	-1.72217	0.35769
C	1.49381	-0.97169	1.29198
C	2.79120	-0.61687	1.00055
C	3.39479	-1.00304	-0.19713
C	2.66517	-1.77084	-1.10198
C	1.36024	-2.13001	-0.83954
C	4.79986	-0.60189	-0.48316

S	-0.87303	-2.09548	0.66073
O	-1.36206	-3.11005	-0.20379
O	-1.18686	-2.02322	2.03865
N	-1.67891	-0.58257	-0.01612
C	-2.56522	-0.72303	-0.94286
C	-1.28531	0.67618	0.55467
C	-1.78669	1.02144	1.77903
C	-1.35436	2.20385	2.39579
C	-0.42555	2.99223	1.77999
C	0.10374	2.65477	0.51716
C	-0.33471	1.47007	-0.13389
C	-3.31603	0.33808	-1.53012
C	-4.20887	0.05405	-2.48137
C	1.06754	3.46453	-0.11889
C	1.57427	3.12479	-1.33886
C	1.13304	1.95662	-1.98283
C	0.20042	1.14821	-1.39787
H	1.02916	-0.67897	2.22611
H	3.35992	-0.03254	1.71581
H	3.13380	-2.09312	-2.02484
H	0.79409	-2.73041	-1.54167
H	4.90906	0.48423	-0.43429
H	5.47971	-1.01989	0.26313
H	5.12795	-0.93687	-1.46618
H	-2.73677	-1.74542	-1.28175
H	-2.49936	0.37049	2.27081
H	-1.75721	2.47760	3.36232
H	-0.07808	3.90225	2.25689
H	-3.14729	1.35170	-1.18382
H	-4.80499	0.82636	-2.95127
H	-4.37268	-0.96430	-2.81879
H	1.39489	4.36792	0.38391
H	2.31190	3.75639	-1.81822
H	1.53532	1.69674	-2.95474
H	-0.11933	0.24805	-1.91124

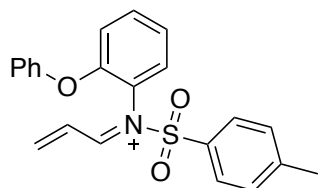


Iminium 13

M06/def2-TZVP Geometry

C	-1.19010	-1.15846	-0.49413
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C	-1.77944	-0.15916	-1.26051
C	-2.97170	0.38423	-0.83092
C	-3.58538	-0.05745	0.34012
C	-2.96788	-1.06171	1.08628
C	-1.77223	-1.61421	0.68345
C	-4.89618	0.50501	0.76879
S	0.32988	-1.81698	-0.98936
O	0.61179	-3.05068	-0.34616
O	0.58078	-1.57506	-2.36096
N	1.47733	-0.65894	-0.15128
C	2.28973	-1.13132	0.73336
C	1.34690	0.72736	-0.48424
C	1.78126	1.18991	-1.71383
C	1.56923	2.51141	-2.05745
C	0.91435	3.34678	-1.16872
C	0.47718	2.88858	0.06317
C	0.69065	1.56590	0.42628
C	3.26610	-0.37409	1.44371
C	4.05375	-0.99344	2.32562
O	0.31862	1.01074	1.58905
C	-0.49095	1.76750	2.46898
H	-1.31145	0.17494	-2.17890
H	-3.44725	1.16069	-1.41971
H	-3.44371	-1.41732	1.99353
H	-1.29884	-2.40100	1.25825
H	-5.71425	-0.09394	0.35840
H	-5.00427	0.49326	1.85380
H	-5.03399	1.52561	0.41123
H	2.21364	-2.20305	0.91772
H	2.27069	0.50411	-2.39444
H	1.91120	2.88401	-3.01379
H	0.74048	4.38281	-1.43334
H	-0.02826	3.56485	0.73939
H	3.35628	0.68674	1.23906
H	4.81783	-0.46166	2.87877
H	3.95870	-2.05663	2.52091
H	-0.72711	1.11513	3.30621
H	0.03807	2.64939	2.83975
H	-1.41838	2.07525	1.97660

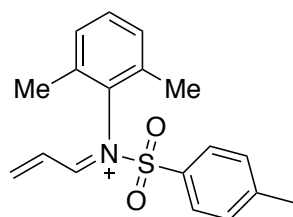


Iminium 14

M06/def2-TZVP Geometry

C	-0.74417	1.96916	-0.42906
C	0.12979	1.96307	-1.51258
C	1.39099	2.48499	-1.34445
C	1.79572	3.01042	-0.11572
C	0.90121	2.99723	0.95067
C	-0.37003	2.47717	0.80818
C	3.17341	3.55455	0.03750
S	-2.34303	1.34242	-0.63611
O	-3.18937	1.71656	0.43495
O	-2.74894	1.36077	-1.99635
N	-2.05521	-0.43873	-0.33437
C	-2.30865	-1.26871	-1.29080
C	-1.49635	-0.80494	0.93139
C	-2.25811	-0.71057	2.08499
C	-1.68846	-1.02819	3.30161
C	-0.36458	-1.43684	3.34852
C	0.40022	-1.53043	2.19985
C	-0.15743	-1.20589	0.97218
O	0.48300	-1.28402	-0.21278
C	1.86439	-1.41881	-0.25853
C	2.38068	-2.52842	-0.89496
C	3.75480	-2.65158	-1.02179
C	4.59222	-1.67598	-0.50986
C	4.05563	-0.56883	0.12837
C	2.68435	-0.42949	0.25318
C	-2.19488	-2.68713	-1.20699
C	-2.50346	-3.42710	-2.27424
H	-0.18898	1.57141	-2.47110
H	2.08440	2.49420	-2.17842
H	1.20483	3.41016	1.90594
H	-1.07221	2.47940	1.63317
H	3.34692	3.95391	1.03586
H	3.91421	2.77326	-0.15520
H	3.36148	4.34949	-0.68747
H	-2.65943	-0.82090	-2.22056
H	-3.28819	-0.38419	2.01386
H	-2.27643	-0.96357	4.20750

H	0.08454	-1.69646	4.29956
H	1.43081	-1.85833	2.24795
H	1.70618	-3.27991	-1.28818
H	4.17076	-3.51799	-1.52108
H	5.66588	-1.77774	-0.60649
H	4.71102	0.19271	0.53450
H	2.24663	0.43199	0.74724
H	-1.87624	-3.13341	-0.27173
H	-2.44853	-4.50835	-2.25263
H	-2.82379	-2.97177	-3.20565

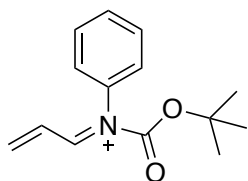


Iminium 15

M06/def2-TZVP Geometry

C	1.58831	-0.69136	-0.57439
C	1.99575	0.53890	-1.07822
C	3.19043	1.06772	-0.63842
C	3.98420	0.38830	0.28517
C	3.54612	-0.84426	0.77146
C	2.35467	-1.39231	0.35097
C	5.29485	0.94760	0.71646
S	0.11174	-1.38402	-1.14540
O	-0.29158	-0.78263	-2.36127
O	0.06561	-2.78315	-0.90628
N	-1.12480	-0.74666	0.05885
C	-1.73040	-1.60690	0.80670
C	-1.41836	0.66860	0.06856
C	-0.74579	1.48595	0.97931
C	-1.03141	2.84490	0.93632
C	-1.95075	3.35313	0.04084
C	-2.63347	2.50737	-0.81380
C	-2.39197	1.14180	-0.81799
C	-2.75825	-1.29695	1.74672
C	-3.31396	-2.28496	2.45279
C	0.23348	0.97399	1.98695
C	-3.18200	0.23811	-1.70778
H	1.38776	1.05865	-1.80875
H	3.52621	2.02327	-1.02535

H	4.16139	-1.38246	1.48378
H	2.02736	-2.35961	0.71303
H	5.54406	0.64887	1.73493
H	6.09265	0.57536	0.06725
H	5.30927	2.03571	0.65432
H	-1.41998	-2.64515	0.68625
H	-0.52768	3.50472	1.63397
H	-2.15716	4.41641	0.02495
H	-3.38266	2.90529	-1.48855
H	-3.06922	-0.26390	1.85929
H	-4.10126	-2.09704	3.17225
H	-2.99860	-3.31612	2.33019
H	0.05479	-0.06232	2.27758
H	1.25783	1.03232	1.60964
H	0.19017	1.58133	2.89113
H	-4.01144	0.78279	-2.15592
H	-2.57281	-0.17055	-2.51485
H	-3.60579	-0.60824	-1.16019

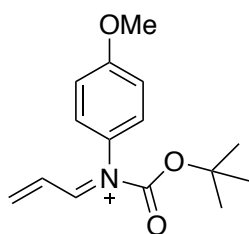


Iminium 16

M06/def2-TZVP Geometry

N	-0.66908	-0.84648	-0.04241
C	-1.42364	-1.90268	-0.05049
C	-1.20560	0.49514	-0.02714
C	-1.78169	0.96795	1.13794
C	-2.29698	2.25245	1.15253
C	-2.22932	3.03944	0.01527
C	-1.64678	2.54914	-1.14309
C	-1.12548	1.26868	-1.17053
C	0.81261	-1.08873	-0.01215
O	1.40060	0.05054	0.04940
O	1.21308	-2.20524	-0.04381
C	2.90565	0.16400	0.06921
C	3.10487	1.65739	0.11983
C	3.44762	-0.43103	-1.20618
C	3.42048	-0.51532	1.31301
C	-2.84210	-1.91248	-0.11607
C	-3.47860	-3.08901	-0.09530
H	-0.87880	-2.84600	-0.01657

H	-1.81791	0.34013	2.02164
H	-2.74927	2.63850	2.05741
H	-2.63293	4.04425	0.03096
H	-1.59813	3.16646	-2.03133
H	-0.65999	0.87268	-2.06593
H	2.65484	2.08213	1.01840
H	4.17346	1.87669	0.13428
H	2.66726	2.13992	-0.75599
H	3.30438	-1.50972	-1.25307
H	2.98824	0.03660	-2.07956
H	4.52008	-0.23231	-1.24932
H	3.27129	-1.59401	1.28588
H	4.49286	-0.32601	1.38921
H	2.94586	-0.10363	2.20574
H	-3.37892	-0.97379	-0.19001
H	-4.55814	-3.15278	-0.15484
H	-2.93627	-4.02567	-0.01566

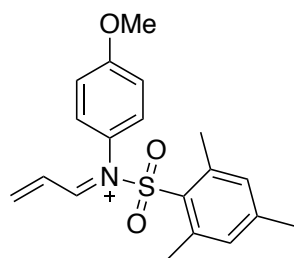


Iminium 17

M06/def2-TZVP Geometry

N	0.55075	1.29772	0.04088
C	0.56668	2.59740	0.00470
C	-0.66075	0.52726	0.11485
C	-0.89662	-0.28964	1.21485
C	-2.05677	-1.01767	1.27723
C	-2.99294	-0.95346	0.23818
C	-2.74235	-0.14020	-0.86529
C	-1.57362	0.59671	-0.92060
C	1.89194	0.62767	-0.04616
O	1.70318	-0.64010	-0.12561
O	2.87310	1.29557	-0.03394
C	2.85271	-1.61294	-0.12896
C	3.62349	-1.44215	1.15649
C	3.68495	-1.37489	-1.36352
C	2.13664	-2.93889	-0.17885
O	-4.08049	-1.70342	0.39347
C	-5.07143	-1.69680	-0.61395

C	-0.55617	3.45315	0.15889
C	-0.37995	4.77539	0.06009
H	1.55581	3.03215	-0.13271
H	-0.17119	-0.34548	2.01884
H	-2.27508	-1.65423	2.12556
H	-3.44328	-0.08453	-1.68675
H	-1.36569	1.21699	-1.78612
H	2.96298	-1.54558	2.02059
H	4.37469	-2.23175	1.21673
H	4.13902	-0.48381	1.20585
H	3.06916	-1.43005	-2.26321
H	4.20002	-0.41566	-1.33429
H	4.43932	-2.16138	-1.42762
H	1.53802	-3.02569	-1.08685
H	2.87071	-3.74587	-0.17206
H	1.48256	-3.06072	0.68682
H	-5.85534	-2.37000	-0.27704
H	-5.49165	-0.69600	-0.75006
H	-4.67160	-2.05892	-1.56562
H	-1.52764	3.02178	0.37047
H	-1.19976	5.46992	0.19501
H	0.59233	5.20267	-0.16273

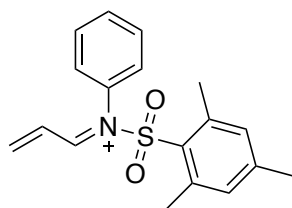


Iminium 18

M06/def2-TZVP Geometry

C	1.75385	-0.27451	0.53112
C	1.30466	-1.53289	0.99350
C	1.77693	-2.65108	0.32521
C	2.63692	-2.57611	-0.75830
C	3.03020	-1.31954	-1.19852
C	2.61629	-0.15281	-0.58486
S	1.19747	1.18160	1.30310
O	0.45748	0.94013	2.48526
O	2.12245	2.25533	1.21389
N	-0.12586	1.69803	0.12751
C	-0.07147	2.87845	-0.38798
C	-1.18735	0.76045	-0.09726
C	-2.26063	0.72155	0.77318

C	-3.26307	-0.21262	0.58488
C	-3.17968	-1.11572	-0.47449
C	-2.08508	-1.06512	-1.34394
C	-1.09273	-0.13418	-1.15762
C	3.14551	-3.80797	-1.42061
C	0.35883	-1.77327	2.12759
C	3.10506	1.13604	-1.16895
C	-1.04730	3.44258	-1.26404
C	-0.87348	4.68559	-1.71848
O	-4.08617	-2.05463	-0.73927
C	-5.22067	-2.16922	0.09504
H	1.45192	-3.62726	0.66966
H	3.69251	-1.24546	-2.05504
H	0.79898	3.47499	-0.11143
H	-2.30536	1.41394	1.60611
H	-4.10138	-0.23229	1.26765
H	-2.04514	-1.77290	-2.16246
H	-0.23793	-0.09631	-1.82566
H	4.10654	-4.09690	-0.98550
H	2.46403	-4.64821	-1.28806
H	3.31093	-3.65155	-2.48705
H	0.19617	-2.84411	2.23677
H	0.73675	-1.38712	3.07320
H	-0.61022	-1.29893	1.95810
H	2.28797	1.80462	-1.45238
H	3.73792	1.68760	-0.47496
H	3.68147	0.93018	-2.06924
H	-1.91149	2.84671	-1.53530
H	-1.58960	5.15481	-2.38152
H	-0.00697	5.27554	-1.43774
H	-5.82020	-1.25435	0.07811
H	-5.81196	-2.99000	-0.30260
H	-4.93423	-2.39937	1.12549

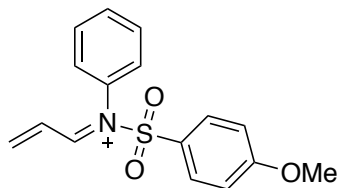


Iminium 19

M06/def2-TZVP Geometry

C	1.20988	-0.64187	0.56235
C	1.89539	0.53474	0.94386

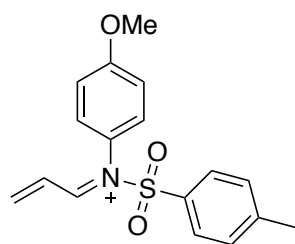
C	3.06163	0.82970	0.25615
C	3.55416	0.03945	-0.76971
C	2.83539	-1.09257	-1.13035
C	1.66862	-1.46726	-0.49277
S	-0.27017	-1.07892	1.36171
O	-0.50696	-2.47824	1.38534
O	-0.57192	-0.25662	2.47290
N	-1.51078	-0.49796	0.12092
C	-2.38245	-1.33485	-0.32820
C	-1.48882	0.90071	-0.20330
C	-0.71212	1.33365	-1.26545
C	-0.66395	2.68809	-1.54396
C	-1.38104	3.58325	-0.76610
C	-2.15435	3.13263	0.29190
C	-2.21069	1.78165	0.58487
C	4.83217	0.37866	-1.45234
C	1.47951	1.49429	2.01362
C	0.98582	-2.70415	-0.98740
C	-3.44228	-1.02110	-1.23144
C	-4.28549	-1.98618	-1.60551
H	3.60911	1.72271	0.53897
H	3.20336	-1.71361	-1.94070
H	-2.28041	-2.35951	0.03212
H	-0.15161	0.61698	-1.85711
H	-0.06520	3.04423	-2.37292
H	-1.33878	4.64244	-0.98816
H	-2.71470	3.83528	0.89583
H	-2.79225	1.40824	1.41980
H	5.66308	-0.14493	-0.97081
H	4.82303	0.07108	-2.49846
H	5.04739	1.44581	-1.39896
H	2.20092	2.30779	2.06532
H	0.49591	1.92580	1.81824
H	1.42526	1.02343	2.99440
H	0.95681	-3.48723	-0.23082
H	-0.04756	-2.51875	-1.29179
H	1.51561	-3.08713	-1.85784
H	-3.54085	-0.00249	-1.58973
H	-5.10561	-1.79350	-2.28593
H	-4.18250	-3.00223	-1.23841



Iminium 20

M06/def2-TZVP Geometry

C	0.82883	-1.12484	0.48194
C	1.28569	-1.74159	-0.68685
C	2.50780	-1.39129	-1.19056
C	3.29254	-0.42741	-0.53859
C	2.82525	0.18423	0.62867
C	1.59233	-0.16269	1.13399
S	-0.72832	-1.51531	1.08538
O	-1.17095	-2.79616	0.66268
O	-0.93198	-1.00816	2.39122
N	-1.77046	-0.39698	0.05082
C	-2.70080	-0.91722	-0.67594
C	-1.45393	1.00282	0.08535
C	-0.76566	1.55019	-0.98701
C	-0.41566	2.88678	-0.94354
C	-0.74701	3.65360	0.16262
C	-1.43237	3.09065	1.22684
C	-1.79031	1.75383	1.19853
O	4.46132	-0.16754	-1.10217
C	-3.61980	-0.19291	-1.49269
C	-4.53397	-0.86540	-2.19604
C	5.33799	0.76749	-0.49853
H	0.68593	-2.50213	-1.17298
H	2.90560	-1.85625	-2.08382
H	3.42315	0.92145	1.14629
H	1.21992	0.30139	2.03947
H	-2.77722	-2.00415	-0.63235
H	-0.50183	0.92603	-1.83481
H	0.11859	3.32961	-1.77486
H	-0.47071	4.70037	0.19407
H	-1.69398	3.69486	2.08648
H	-2.31789	1.29505	2.02556
H	-3.56368	0.88954	-1.51362
H	-5.25937	-0.35732	-2.81915
H	-4.58556	-1.94903	-2.16897
H	4.88595	1.76209	-0.45792
H	5.62045	0.44833	0.50800
H	6.22435	0.80148	-1.12614

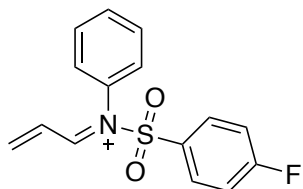


Iminium 21

M06/def2-TZVP Geometry

C	1.87780	-0.40226	0.54237
C	2.73936	-0.46840	-0.54758
C	2.96811	-1.69289	-1.13468
C	2.35330	-2.84936	-0.65292
C	1.49362	-2.74849	0.43921
C	1.24606	-1.53424	1.04311
C	2.64040	-4.17156	-1.27451
S	1.53161	1.13889	1.24432
O	0.86628	1.01055	2.48702
O	2.56245	2.08463	1.00226
N	0.20234	1.69943	0.11005
C	0.39685	2.77888	-0.57215
C	-0.94653	0.85250	-0.01386
C	-1.09144	0.08625	-1.16753
C	-2.15641	-0.77129	-1.28083
C	-3.08825	-0.87956	-0.24267
C	-2.92964	-0.11120	0.91034
C	-1.85409	0.75022	1.02426
O	-4.08411	-1.73814	-0.44743
C	-5.07007	-1.90171	0.55214
C	-0.54439	3.37653	-1.46162
C	-0.20727	4.49335	-2.11139
H	3.23174	0.42567	-0.91207
H	3.64411	-1.76437	-1.97947
H	1.01405	-3.64267	0.82121
H	0.57951	-1.45555	1.89338
H	1.81376	-4.86892	-1.13876
H	2.85070	-4.07763	-2.34021
H	3.52324	-4.62086	-0.81062
H	1.36278	3.26206	-0.42305
H	-0.35399	0.16053	-1.96077
H	-2.29684	-1.38077	-2.16477
H	-3.64092	-0.17524	1.72227
H	-1.72161	1.34175	1.92177

H	-5.77331	-2.63744	0.17072
H	-4.63298	-2.27190	1.48405
H	-5.60006	-0.96426	0.74364
H	-1.51945	2.91737	-1.57828
H	-0.89563	4.99036	-2.78349
H	0.77120	4.94663	-1.98988

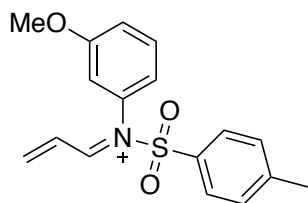


Iminium 22

M06/def2-TZVP Geometry

C	-1.28491	-0.88074	0.45130
C	-1.78626	-1.51693	-0.68107
C	-2.94139	-1.04050	-1.25801
C	-3.56477	0.05962	-0.68851
C	-3.07524	0.69488	0.44102
C	-1.91770	0.22141	1.01843
F	-4.66492	0.51318	-1.24013
S	0.19477	-1.44957	1.13960
O	0.41230	-0.90556	2.42698
O	0.45604	-2.80215	0.80015
N	1.39937	-0.54395	0.09410
C	2.25537	-1.22615	-0.59207
C	1.29900	0.88961	0.07351
C	0.71793	1.49327	-1.03175
C	0.57677	2.86836	-1.04332
C	1.00762	3.61741	0.04065
C	1.58506	2.99821	1.13731
C	1.73351	1.62233	1.16474
C	3.28736	-0.67804	-1.40856
C	4.10045	-1.50696	-2.06920
H	-1.28387	-2.38627	-1.08827
H	-3.37911	-1.50806	-2.13055
H	-3.61042	1.54184	0.85052
H	-1.50680	0.68990	1.90451
H	2.16624	-2.30986	-0.51066
H	0.37378	0.88472	-1.86209
H	0.12710	3.35550	-1.89946
H	0.89396	4.69440	0.02927
H	1.92531	3.58825	1.97904
H	2.17448	1.12145	2.01765
H	3.39695	0.39891	-1.46639

H	4.90524	-1.13728	-2.69248
H	3.98592	-2.58429	-2.00597

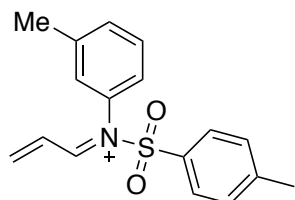


Iminium 23

M06/def2-TZVP Geometry

C	-0.69101	-1.77409	0.27542
C	-1.56550	-1.16062	1.16423
C	-2.86737	-0.94614	0.76418
C	-3.30514	-1.32801	-0.50217
C	-2.40045	-1.93880	-1.37217
C	-1.09604	-2.16695	-0.99635
S	0.95959	-1.99010	0.73283
O	1.14921	-1.80344	2.12233
O	1.59788	-3.01374	-0.01507
N	1.68927	-0.46822	0.00346
C	2.66134	-0.59360	-0.83563
C	1.12116	0.79054	0.40402
C	1.40800	1.29972	1.65980
C	0.80347	2.49059	2.01835
C	-0.06206	3.14896	1.16043
C	-0.33849	2.61789	-0.09734
C	0.26436	1.41964	-0.47642
C	-4.72130	-1.12314	-0.91356
O	-1.15800	3.16625	-0.99884
C	-1.78817	4.39174	-0.68706
C	3.37665	0.48167	-1.44149
C	4.36414	0.20349	-2.29611
H	-1.22416	-0.86411	2.14869
H	-3.56514	-0.47554	1.44762
H	-2.73644	-2.24587	-2.35639
H	-0.39914	-2.65626	-1.66661
H	2.94795	-1.61861	-1.07308
H	2.07491	0.77436	2.33047
H	1.01062	2.91997	2.99080
H	-0.51802	4.07719	1.47748
H	0.03732	0.99246	-1.44741
H	-4.79887	-0.88352	-1.97467
H	-5.29663	-2.03875	-0.74927
H	-5.19909	-0.33080	-0.33789

H	-2.43854	4.29403	0.18729
H	-1.05386	5.18245	-0.50745
H	-2.39101	4.65561	-1.55232
H	3.10925	1.50032	-1.18485
H	4.94265	0.98592	-2.77123
H	4.62579	-0.81944	-2.54674

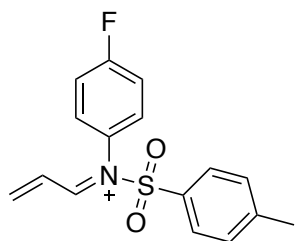


Iminium 24

M06/def2-TZVP Geometry

C	-1.49113	-0.73633	0.62698
C	-2.18986	-1.43695	-0.35084
C	-3.28366	-0.83893	-0.93554
C	-3.69121	0.44225	-0.56076
C	-2.96896	1.11730	0.42136
C	-1.86871	0.54214	1.02032
S	-0.07919	-1.44830	1.32117
O	0.35257	-0.74495	2.47062
O	-0.08535	-2.86441	1.22544
N	1.16522	-0.97882	0.05233
C	1.84176	-1.91710	-0.52012
C	1.28812	0.41835	-0.26055
C	0.72366	0.87928	-1.43792
C	0.79675	2.23355	-1.71170
C	1.41625	3.08980	-0.81983
C	1.98674	2.62473	0.36288
C	1.91087	1.26589	0.63982
C	-4.89860	1.05952	-1.17556
C	2.67654	3.56284	1.29608
C	2.87938	-1.72357	-1.47966
C	3.49673	-2.79098	-1.99214
H	-1.88543	-2.43872	-0.63059
H	-3.84577	-1.37363	-1.69313
H	-3.28140	2.11130	0.72109
H	-1.30864	1.06538	1.78579
H	1.58790	-2.93280	-0.21508
H	0.22432	0.18982	-2.11049
H	0.36248	2.62156	-2.62474
H	1.46355	4.15079	-1.04184

H	2.33032	0.86752	1.55681
H	-5.03213	0.73850	-2.20898
H	-4.85370	2.14817	-1.14761
H	-5.79528	0.75747	-0.62674
H	2.08871	4.46947	1.44846
H	3.64131	3.87409	0.88778
H	2.85979	3.10514	2.26783
H	3.15172	-0.71288	-1.76163
H	4.29856	-2.69282	-2.71330
H	3.21833	-3.79956	-1.70411

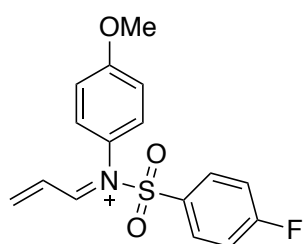


Iminium 25

M06/def2-TZVP Geometry

C	1.35935	-1.05807	0.45623
C	1.91904	0.05869	1.06675
C	3.04577	0.62044	0.50607
C	3.61773	0.09055	-0.64945
C	3.02851	-1.02815	-1.24050
C	1.90412	-1.61007	-0.69875
S	-0.08236	-1.74293	1.11468
O	-0.25733	-3.10059	0.74068
O	-0.35332	-1.24683	2.41210
N	-1.34004	-0.88898	0.07717
C	-2.15876	-1.61055	-0.61336
C	-1.30901	0.54491	0.06599
C	-0.77949	1.18672	-1.04489
C	-0.68975	2.56332	-1.05368
C	-1.12636	3.26458	0.05664
C	-1.65184	2.63182	1.16865
C	-1.74107	1.25353	1.17597
C	4.85689	0.68344	-1.22307
C	-3.22561	-1.11479	-1.41907
C	-3.99650	-1.98185	-2.08089
F	-1.03747	4.57777	0.05314
H	1.47781	0.46659	1.96810
H	3.49978	1.48687	0.97375
H	3.47237	-1.45090	-2.13491

H	1.45987	-2.49060	-1.14808
H	-2.00726	-2.68820	-0.54342
H	-0.42824	0.60334	-1.88981
H	-0.28469	3.10154	-1.90092
H	-1.98523	3.22398	2.01123
H	-2.13769	0.72942	2.03655
H	4.90835	0.54283	-2.30292
H	4.93436	1.74791	-1.00153
H	5.73796	0.19877	-0.79251
H	-3.39761	-0.04543	-1.46472
H	-4.82737	-1.65263	-2.69247
H	-3.82011	-3.05142	-2.02968

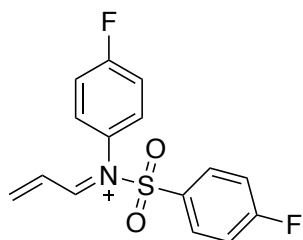


Iminium 26

M06/def2-TZVP Geometry

C	-1.85130	-0.55209	0.50743
C	-2.71554	-0.65857	-0.57841
C	-2.87210	-1.88176	-1.19029
C	-2.15948	-2.96606	-0.70158
C	-1.30144	-2.86952	0.38136
C	-1.14184	-1.64580	0.99333
S	-1.61207	0.99859	1.23632
O	-2.70504	1.87284	1.00050
O	-0.95242	0.88776	2.48338
N	-0.31601	1.66531	0.12903
C	-0.57213	2.74779	-0.52965
C	0.88593	0.89606	-0.00148
C	1.09778	0.18106	-1.17790
C	2.21514	-0.60544	-1.29993
C	3.13466	-0.69246	-0.24834
C	2.90947	0.02473	0.92682
C	1.78102	0.81401	1.04958
C	0.33906	3.42685	-1.39031
C	-0.06312	4.53448	-2.01927
F	-2.30852	-4.13124	-1.28636
O	4.18398	-1.48053	-0.46256
C	5.16089	-1.62060	0.55015

H	-3.27121	0.20567	-0.92259
H	-3.54240	-2.01927	-2.02892
H	-0.78020	-3.75223	0.72851
H	-0.48249	-1.53273	1.84513
H	-1.56898	3.16398	-0.38265
H	0.37253	0.23911	-1.98375
H	2.40786	-1.17404	-2.20111
H	3.61028	-0.02328	1.74893
H	1.59630	1.36432	1.96400
H	1.34400	3.03635	-1.50312
H	0.59981	5.09194	-2.66921
H	-1.07122	4.91892	-1.90258
H	5.63113	-0.66083	0.78241
H	4.72984	-2.04728	1.46041
H	5.91242	-2.30069	0.15794

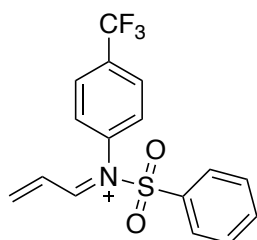


Iminium 27

M06/def2-TZVP Geometry

C	-1.39987	-1.03115	0.41766
C	-1.94910	0.08822	1.03612
C	-3.05920	0.68136	0.47707
C	-3.58680	0.14416	-0.68585
C	-3.04776	-0.97324	-1.30600
C	-1.93978	-1.56912	-0.74739
S	0.02226	-1.74582	1.09115
O	0.27219	-1.26747	2.39909
O	0.17678	-3.10218	0.70512
N	1.30955	-0.90327	0.08897
C	2.14772	-1.63238	-0.57143
C	1.29099	0.53153	0.07590
C	1.69659	1.23836	1.19700
C	1.61921	2.61739	1.18463
C	1.13251	3.25282	0.05635
C	0.72362	2.55317	-1.06578
C	0.80137	1.17587	-1.05190
F	-4.64167	0.71097	-1.21994
F	1.05537	4.56594	0.04822
C	3.24520	-1.14509	-1.33882

C	4.03402	-2.01921	-1.97035
H	-1.51287	0.47589	1.94857
H	-3.52986	1.54640	0.92618
H	-3.51353	-1.36098	-2.20282
H	-1.50497	-2.45531	-1.19438
H	1.98630	-2.70885	-0.50586
H	2.06452	0.71307	2.06960
H	1.93321	3.20843	2.03545
H	0.34976	3.09331	-1.92610
H	0.47360	0.59435	-1.90752
H	3.42576	-0.07700	-1.38068
H	4.88875	-1.69689	-2.55208
H	3.84906	-3.08754	-1.92306

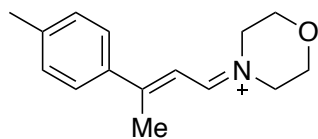


Iminium 28

M06/def2-TZVP Geometry

C	-2.07236	-1.39474	0.20018
C	-1.08688	-2.23873	0.69771
C	-0.76464	-3.36895	-0.02882
C	-1.41531	-3.63415	-1.22406
C	-2.40004	-2.78214	-1.70517
C	-2.73849	-1.64903	-0.99367
S	-2.45250	0.05536	1.06985
O	-3.74897	0.54253	0.76444
O	-1.90329	0.04404	2.37307
N	-1.37110	1.24316	0.17229
C	-1.91839	2.26419	-0.39988
C	0.03327	0.94650	0.13512
C	0.56522	0.42099	-1.03445
C	1.90158	0.08363	-1.06476
C	2.68673	0.26698	0.06584
C	2.14455	0.79274	1.22452
C	0.80336	1.13567	1.26741
C	4.13963	-0.12959	-0.01081
C	-1.22347	3.30233	-1.08554
C	-1.92418	4.29960	-1.63314
F	4.75099	0.52912	-0.98996

F	4.78329	0.11738	1.11797
F	4.25012	-1.42925	-0.27423
H	-0.59620	-2.01292	1.63668
H	-0.00692	-4.04766	0.34164
H	-1.15801	-4.52380	-1.78632
H	-2.91210	-3.01011	-2.63143
H	-3.51805	-0.98105	-1.34051
H	-3.00507	2.31657	-0.32373
H	-0.07098	0.26988	-1.90027
H	2.34090	-0.32803	-1.96605
H	2.76686	0.93698	2.09812
H	0.36029	1.53857	2.16947
H	-0.14117	3.26788	-1.13846
H	-1.43946	5.11575	-2.15455
H	-3.00747	4.33043	-1.57530

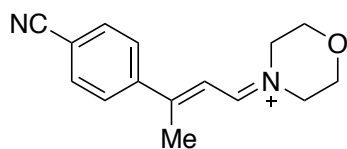


Iminium 29

M06/def2-TZVP Geometry

C	-4.49442	0.63692	0.12130
C	-3.25592	1.23588	0.09552
C	-2.08516	0.47926	-0.05610
C	-2.23342	-0.90805	-0.21235
C	-3.47361	-1.49734	-0.20434
C	-4.63188	-0.74048	-0.02588
C	-5.96856	-1.39156	0.01925
C	-0.78380	1.11855	-0.06402
C	-0.74689	2.59001	-0.29337
C	0.35369	0.37833	0.16132
C	1.64783	0.90208	0.14863
H	1.78874	1.95422	-0.07830
N	2.76482	0.26656	0.39283
C	4.06314	0.94383	0.34393
C	4.98698	0.19727	-0.59775
O	5.10784	-1.14111	-0.20772
C	3.87425	-1.79752	-0.24607
C	2.88710	-1.15603	0.71246
H	-5.38103	1.24703	0.25375
H	-3.20028	2.30989	0.21869
H	-1.36783	-1.53398	-0.39085

H	-3.55947	-2.56859	-0.35061
H	-6.02005	-2.24635	-0.65632
H	-6.17228	-1.76750	1.02641
H	-6.76655	-0.69406	-0.23484
H	-1.17928	3.11081	0.56520
H	0.25082	2.99190	-0.44184
H	-1.34989	2.85811	-1.16183
H	0.23509	-0.67039	0.39654
H	3.91725	1.97685	0.02689
H	4.48539	0.93924	1.35397
H	5.98217	0.64264	-0.57189
H	4.60482	0.26757	-1.62820
H	4.04206	-2.83640	0.04055
H	3.45971	-1.78475	-1.26632
H	3.26072	-1.23558	1.73821
H	1.91760	-1.64471	0.65767

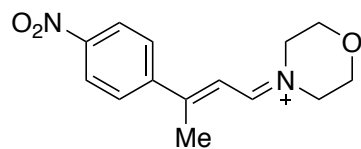


Iminium 30

M06/def2-TZVP Geometry

C	3.38613	-1.16910	-0.59572
C	2.12317	-0.62873	-0.65116
C	1.84026	0.61236	-0.06756
C	2.88393	1.29815	0.56398
C	4.14645	0.75483	0.64179
C	4.40628	-0.48372	0.06162
C	0.50050	1.19019	-0.12634
C	0.39596	2.66923	-0.00612
C	-0.58546	0.36743	-0.25675
C	-1.90728	0.82381	-0.37462
H	-2.09074	1.89285	-0.42692
N	-2.98797	0.09943	-0.44691
C	-4.31562	0.70732	-0.59108
C	-5.22160	0.20785	0.51777
O	-5.28048	-1.18925	0.50961
C	-4.02297	-1.75473	0.73419
C	-3.04752	-1.36227	-0.36236
H	3.59931	-2.12049	-1.06644
H	1.35632	-1.16115	-1.20012
H	2.70655	2.26009	1.02730

H	4.94219	1.28500	1.14954
H	1.12317	3.15917	-0.65513
H	-0.58833	3.06582	-0.23842
H	0.63082	2.97497	1.01756
H	-0.41477	-0.70082	-0.25207
H	-4.21641	1.79292	-0.57257
H	-4.71862	0.40331	-1.56203
H	-6.23310	0.58610	0.36580
H	-4.85875	0.57615	1.49006
H	-4.14169	-2.83880	0.74517
H	-3.62432	-1.44260	1.71205
H	-2.06038	-1.77428	-0.16880
H	-3.40388	-1.73461	-1.32756
N	6.76773	-1.50322	0.18657
C	5.71414	-1.04649	0.13036

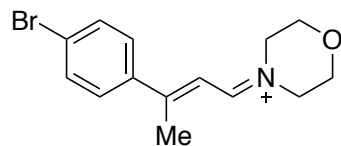


Iminium 31

M06/def2-TZVP Geometry

C	2.99901	-1.00926	-0.62610
C	1.72055	-0.50165	-0.69652
C	1.40109	0.73078	-0.11484
C	2.41431	1.44814	0.52976
C	3.69307	0.94026	0.62264
C	3.96308	-0.28162	0.04252
C	0.04326	1.27061	-0.19053
C	-0.09891	2.74947	-0.12922
C	-1.01590	0.41138	-0.28308
C	-2.35289	0.82419	-0.40908
H	-2.56776	1.88489	-0.49954
N	-3.41040	0.06581	-0.44653
C	-4.75780	0.62726	-0.59897
C	-5.63580	0.14368	0.53937
O	-5.65176	-1.25366	0.58539
C	-4.37542	-1.77212	0.81620
C	-3.42465	-1.39321	-0.30667
H	3.26561	-1.95191	-1.08510
H	0.97265	-1.05156	-1.25442
H	2.20210	2.40416	0.99069
H	4.48269	1.47483	1.13368
H	-1.09305	3.11236	-0.37477

H	0.13066	3.10136	0.88083
H	0.61645	3.23042	-0.79800
H	-0.81141	-0.65017	-0.23874
H	-4.69180	1.71524	-0.62386
H	-5.16082	0.27292	-1.55261
H	-6.65992	0.48526	0.38520
H	-5.27378	0.56036	1.49224
H	-4.46072	-2.85803	0.86990
H	-3.97544	-1.41085	1.77645
H	-2.42324	-1.76807	-0.11112
H	-3.78125	-1.81124	-1.25280
N	5.33961	-0.82931	0.13065
O	6.15670	-0.15753	0.70896
O	5.53090	-1.90418	-0.38180

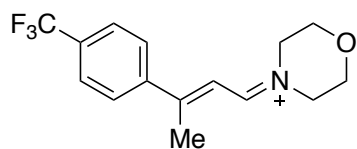


Iminium 32

M06/def2-TZVP Geometry

C	-2.55030	-0.90065	-0.54702
C	-1.25700	-0.43720	-0.58308
C	-0.91641	0.82481	-0.07334
C	-1.94799	1.60546	0.46690
C	-3.24316	1.14352	0.52551
C	-3.54479	-0.11146	0.01709
C	0.44749	1.32286	-0.11106
C	0.64015	2.79197	0.03824
C	1.49787	0.44850	-0.24944
C	2.83689	0.83838	-0.35222
H	3.07627	1.89687	-0.38265
N	3.88441	0.06184	-0.43434
C	5.23865	0.60676	-0.56805
C	6.12338	0.03683	0.52300
O	6.11309	-1.36144	0.48164
C	4.82894	-1.86851	0.69854
C	3.87012	-1.40107	-0.38223
H	-2.80028	-1.86848	-0.96275
H	-0.50726	-1.05547	-1.06117
H	-1.73692	2.58552	0.87506
H	-4.02450	1.75244	0.96218
H	1.65274	3.12945	-0.16199
H	-0.03500	3.33806	-0.62179
H	0.39875	3.09566	1.06071

H	1.27689	-0.61006	-0.26544
H	5.62553	0.31044	-1.54822
H	5.19315	1.69515	-0.52093
H	5.78297	0.39826	1.50599
H	7.15219	0.36736	0.37569
H	4.89417	-2.95710	0.68380
H	4.45092	-1.55994	1.68572
H	2.86421	-1.76600	-0.19015
H	4.20016	-1.77235	-1.35746
Br	-5.30579	-0.74064	0.07696

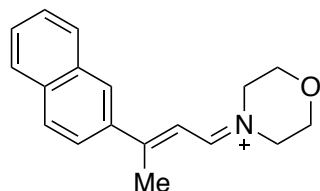


Iminium 33

M06/def2-TZVP Geometry

C	2.63203	-0.84476	0.62440
C	1.33895	-0.38086	0.67551
C	0.98761	0.83674	0.07732
C	1.99026	1.57129	-0.56110
C	3.28480	1.09655	-0.63144
C	3.60636	-0.11039	-0.03876
C	-0.38227	1.33892	0.12876
C	-0.56950	2.80877	-0.00171
C	-1.42142	0.45752	0.26232
C	-2.76578	0.84112	0.37553
H	-3.00742	1.89863	0.42507
N	-3.80622	0.05927	0.44669
C	-5.16484	0.59438	0.58738
C	-6.04032	0.04544	-0.52249
O	-6.02302	-1.35286	-0.51353
C	-4.73585	-1.84910	-0.73488
C	-3.78560	-1.40332	0.36321
H	2.89823	-1.77801	1.10709
H	0.60254	-0.94926	1.23018
H	1.75937	2.51587	-1.03655
H	4.04630	1.66778	-1.14618
H	0.12430	3.34247	0.64932
H	-0.34302	3.12054	-1.02541
H	-1.57645	3.15120	0.21925
H	-1.19084	-0.59946	0.26429
H	-5.55302	0.27083	1.55811
H	-5.12462	1.68375	0.56740
H	-5.69625	0.43216	-1.49448

H	-7.07128	0.36797	-0.37285
H	-4.79551	-2.93800	-0.74556
H	-4.35275	-1.51618	-1.71211
H	-2.77692	-1.76045	0.17152
H	-4.12255	-1.79460	1.32791
C	5.00979	-0.65873	-0.07642
F	5.02292	-1.86235	-0.64188
F	5.83262	0.12399	-0.75602
F	5.48916	-0.79151	1.15663

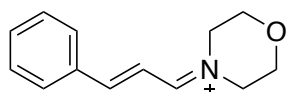


Iminium 34

M06/def2-TZVP Geometry

C	-2.39924	1.03495	0.12012
C	-1.26286	0.34092	-0.26368
C	-1.41223	-1.02879	-0.62566
C	-2.62383	-1.63776	-0.58544
C	0.02545	1.00268	-0.28537
C	0.04140	2.49217	-0.22505
C	1.18332	0.25954	-0.33215
C	2.46683	0.80283	-0.40646
H	2.58140	1.87898	-0.49093
N	3.60414	0.15532	-0.40375
C	4.88661	0.85232	-0.52891
C	5.79624	0.45141	0.61489
O	5.95487	-0.93828	0.65077
C	4.73328	-1.58481	0.86080
C	3.76106	-1.29305	-0.26815
H	-2.33851	2.07848	0.40670
H	-0.56119	-1.59262	-0.98492
H	-2.72220	-2.67557	-0.88460
H	-0.29135	2.83010	0.75982
H	1.02035	2.93003	-0.39546
H	-0.64633	2.91599	-0.95749
H	1.09414	-0.81723	-0.29793
H	5.34086	0.55666	-1.48021
H	4.70977	1.92821	-0.54265
H	5.38244	0.81877	1.56706
H	6.78274	0.89577	0.47765
H	4.92868	-2.65679	0.90829

H	4.28965	-1.27344	1.81941
H	2.79957	-1.76414	-0.07930
H	4.16183	-1.67613	-1.21203
C	-3.65837	0.42615	0.18860
C	-3.78263	-0.94240	-0.17008
C	-5.04645	-1.55053	-0.10849
C	-6.13993	-0.83449	0.29500
C	-6.02029	0.52016	0.65295
C	-4.80593	1.13823	0.60155
H	-5.14116	-2.59479	-0.38489
H	-7.11102	-1.31268	0.34056
H	-6.89842	1.06929	0.96933
H	-4.70387	2.18298	0.87492

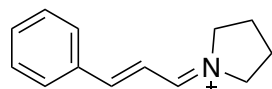


Iminium 35

M06/def2-TZVP Geometry

C	2.93991	1.05268	-0.11750
C	2.63517	-0.31094	0.01098
C	3.68228	-1.22233	0.20508
C	4.98896	-0.78982	0.26923
C	1.30168	-0.81697	-0.04758
C	0.14632	-0.12021	-0.22686
C	-1.06787	-0.82026	-0.26153
H	-1.02020	-1.90212	-0.14838
N	-2.26962	-0.34317	-0.42284
C	-3.45186	-1.21051	-0.43858
C	-4.44798	-0.71954	0.59356
O	-4.77326	0.62110	0.36124
C	-3.65008	1.44592	0.46699
C	-2.60560	1.07443	-0.57082
H	2.14905	1.77788	-0.26902
H	3.45211	-2.27780	0.30475
H	5.79112	-1.50110	0.41933
H	0.16301	0.95549	-0.34839
H	-3.89662	-1.15376	-1.43696
H	-3.14439	-2.23855	-0.24538
H	-4.03142	-0.84839	1.60471
H	-5.36735	-1.30226	0.52654
H	-3.97592	2.47430	0.30662
H	-3.21078	1.37735	1.47443
H	-1.71400	1.68805	-0.46585
H	-3.01367	1.21519	-1.57638

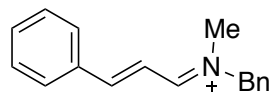
C	4.24420	1.48086	-0.05312
C	5.26966	0.56118	0.14023
H	6.29589	0.90513	0.18999
H	4.47499	2.53398	-0.15304
H	1.21285	-1.89705	0.06645



Iminium 36

M06/def2-TZVP Geometry

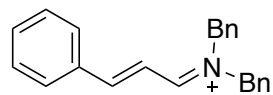
C	-2.59415	1.06236	0.02103
C	-2.31039	-0.31138	-0.00739
C	-3.37579	-1.22196	-0.00920
C	-4.68034	-0.77902	0.01648
C	-0.97970	-0.82821	-0.03477
C	0.19118	-0.13545	-0.03849
C	1.40518	-0.83787	-0.06587
H	1.37023	-1.92623	-0.08087
N	2.59247	-0.31415	-0.07091
C	3.84104	-1.09987	-0.08061
C	4.87431	-0.10694	0.40635
C	4.39029	1.19972	-0.20521
C	2.88355	1.13045	-0.03344
H	-1.78812	1.78670	0.02289
H	-3.16151	-2.28522	-0.03121
H	-5.49683	-1.48987	0.01479
H	0.20323	0.94803	-0.01707
H	3.72602	-1.98847	0.54014
H	4.04675	-1.41479	-1.10859
H	2.32380	1.64599	-0.81560
H	2.56149	1.52262	0.93647
C	-3.89642	1.50098	0.04665
C	-4.94043	0.58191	0.04437
H	-5.96486	0.93414	0.06449
H	-4.11105	2.56201	0.06848
H	-0.90668	-1.91532	-0.05582
H	5.88280	-0.37926	0.10059
H	4.85757	-0.04976	1.49788
H	4.81428	2.08358	0.26775
H	4.64556	1.23669	-1.26721



Iminium 37

M06/def2-TZVP Geometry

C	-3.87843	0.75706	-0.00001
C	-3.00510	-0.34049	-0.00000
C	-3.54514	-1.63329	-0.00001
C	-4.90972	-1.82666	-0.00002
C	-1.58277	-0.20163	0.00001
C	-0.85100	0.94431	0.00000
C	0.55102	0.85643	0.00002
H	1.00655	-0.13159	0.00003
N	1.38202	1.85629	0.00001
C	2.85823	1.68553	0.00000
C	0.91456	3.23778	-0.00000
H	-3.48606	1.76723	-0.00000
H	-2.87387	-2.48556	0.00000
H	-5.31729	-2.82961	-0.00003
H	-1.33422	1.91403	-0.00002
H	3.22502	2.22128	0.88109
H	0.31657	3.43950	-0.88993
H	0.31647	3.43948	0.88986
C	-5.23906	0.56112	-0.00002
C	-5.75632	-0.72977	-0.00003
H	-6.82968	-0.87751	-0.00004
H	-5.90932	1.41151	-0.00003
H	-1.02682	-1.13875	0.00003
H	1.77511	3.90205	0.00006
H	3.22501	2.22128	-0.88109
C	4.14389	-2.38058	0.00001
C	3.94030	-1.71994	1.20062
C	3.53031	-0.39858	1.20025
C	3.32131	0.27050	0.00001
C	3.53030	-0.39858	-1.20023
C	3.94029	-1.71995	-1.20060
H	4.47354	-3.41247	0.00001
H	4.11261	-2.23226	2.13922
H	3.38173	0.12505	2.14000
H	3.38172	0.12504	-2.13999
H	4.11260	-2.23227	-2.13919

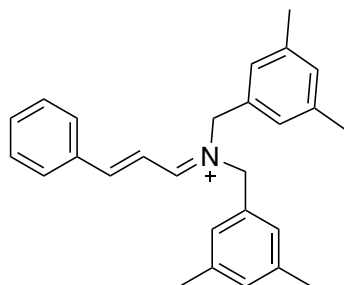


Iminium 38

M06/def2-TZVP Geometry

C	4.69513	1.05791	0.39700
C	3.74466	0.12646	-0.03896
C	4.14851	-1.19791	-0.25966
C	5.45564	-1.56936	-0.04952
C	2.40026	0.57394	-0.23997
C	1.33019	-0.15120	-0.65590
C	0.08586	0.49265	-0.79029
H	0.03937	1.54852	-0.52763
N	-1.04094	-0.02003	-1.18388
C	-2.28778	0.78309	-1.26925
C	-1.21474	-1.42527	-1.57016
H	4.38809	2.08413	0.56904
H	3.43308	-1.93829	-0.59801
H	5.76216	-2.59350	-0.22173
H	1.42826	-1.20789	-0.87325
H	-3.08873	0.10711	-0.95556
H	-1.78519	-1.43251	-2.50303
C	6.00514	0.68294	0.60633
C	6.38534	-0.63045	0.38315
H	7.41396	-0.92919	0.54614
H	6.73222	1.41102	0.94299
H	2.22864	1.62947	-0.03129
H	-0.23654	-1.85065	-1.79381
H	-2.44758	1.01243	-2.32775
C	-2.25647	4.29735	1.14790
C	-2.43079	3.05109	1.73145
C	-2.44501	1.91641	0.94300
C	-2.28268	2.01813	-0.43502
C	-2.10729	3.26797	-1.01215
C	-2.09656	4.40627	-0.22220
H	-2.25433	5.18748	1.76528
H	-2.56795	2.96774	2.80271
H	-2.59288	0.93760	1.39210
H	-1.99169	3.35183	-2.08843
H	-1.97058	5.37993	-0.67967
C	-3.26753	-3.67063	1.43809
C	-2.13408	-2.94467	1.76911
C	-1.47185	-2.21540	0.79896
C	-1.93879	-2.20438	-0.51036
C	-3.07827	-2.92632	-0.83303
C	-3.73839	-3.66163	0.13736

H	-3.78472	-4.24335	2.19813
H	-1.76323	-2.95150	2.78690
H	-0.58369	-1.64943	1.06629
H	-3.44955	-2.91745	-1.85312
H	-4.62551	-4.22519	-0.12444

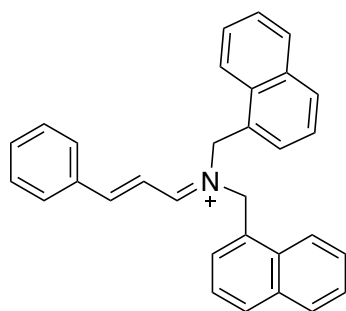


Iminium 39

M06/def2-TZVP Geometry

C	5.22295	0.20595	0.39491
C	4.16250	-0.56047	-0.10272
C	4.37099	-1.92543	-0.34311
C	5.59699	-2.49585	-0.09175
C	2.90931	0.09045	-0.34345
C	1.76181	-0.45517	-0.81852
C	0.63333	0.37268	-0.98162
H	0.73372	1.41785	-0.69179
N	-0.53866	0.04407	-1.43122
C	-1.64691	1.02835	-1.53521
C	-0.90685	-1.31023	-1.86133
H	5.06745	1.26320	0.58226
H	3.56702	-2.54103	-0.72938
H	5.75206	-3.55093	-0.27962
H	1.70795	-1.50989	-1.05957
H	-2.55044	0.47412	-1.26441
H	-1.42980	-1.21067	-2.81649
C	6.45132	-0.36809	0.64556
C	6.63844	-1.71895	0.40246
H	7.60215	-2.17391	0.59777
H	7.26478	0.23419	1.02995
H	2.89004	1.15517	-0.11311
H	0.00450	-1.87574	-2.05494
H	-1.73178	1.30078	-2.59213
C	-1.13930	4.42010	0.96485
C	-0.92874	4.56369	-0.39748
C	-1.09907	3.44521	-1.20971
C	-1.48234	2.22971	-0.66906
C	-1.69308	2.11644	0.70102
C	-1.52529	3.20965	1.53537

H	-1.00519	5.28372	1.61136
C	-0.56107	5.88569	-0.98661
H	-0.93870	3.53301	-2.28143
H	-1.99785	1.15851	1.11790
C	-1.77539	3.11302	3.00438
C	-3.40372	-3.25171	0.98798
C	-3.83119	-3.16117	-0.32613
C	-3.00682	-2.51252	-1.24258
C	-1.78758	-1.98943	-0.85311
C	-1.38199	-2.09600	0.47279
C	-2.18490	-2.72669	1.40924
H	-4.04112	-3.74518	1.71713
C	-5.13028	-3.75377	-0.76237
H	-3.32819	-2.42117	-2.27711
H	-0.42862	-1.67839	0.78889
C	-1.76538	-2.85396	2.83694
H	-1.63942	-3.90280	3.11571
H	-0.82204	-2.34173	3.02881
H	-2.52028	-2.43808	3.50793
H	-4.97150	-4.72153	-1.24558
H	-5.80039	-3.91636	0.08182
H	-5.63875	-3.11433	-1.48596
H	-1.87139	2.07685	3.33016
H	-0.97054	3.57940	3.57576
H	-2.69835	3.63175	3.27550
H	0.07877	5.77191	-1.86302
H	-1.45494	6.42631	-1.30923
H	-0.04505	6.51747	-0.26307



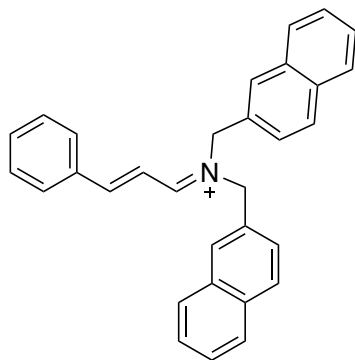
Iminium 40

M06/def2-TZVP Geometry

C	-4.67891	-1.76619	-0.34470
C	-4.38008	-0.41788	-0.10523
C	-5.37424	0.40770	0.43334
C	-6.62561	-0.09299	0.72400

C	-3.09971	0.15843	-0.38748
C	-2.00440	-0.45133	-0.90741
C	-0.83803	0.31381	-1.10722
H	-0.89343	1.37154	-0.85425
N	0.31546	-0.07298	-1.56012
C	1.42740	0.89082	-1.78198
C	0.61500	-1.45694	-1.98530
H	-3.92748	-2.42686	-0.76108
H	-5.14833	1.45218	0.62050
H	-7.38720	0.55437	1.14002
H	-2.03240	-1.50102	-1.17181
H	1.57698	0.93579	-2.86609
H	-0.24702	-2.08019	-1.75376
C	-5.92792	-2.26323	-0.05423
C	-6.90259	-1.42824	0.48018
H	-7.88474	-1.82559	0.70676
H	-6.15320	-3.30562	-0.24193
H	-3.00768	1.21801	-0.15127
H	0.72041	-1.43602	-3.07428
H	2.32100	0.42416	-1.36170
C	0.80288	4.84697	-0.26724
C	0.68297	4.58741	-1.60004
C	0.88407	3.28197	-2.07467
C	1.20697	2.25494	-1.22582
H	0.65265	5.85128	0.11446
H	0.79458	3.08341	-3.13824
C	4.27647	-2.94734	-0.31837
C	4.17335	-2.68606	-1.65175
C	2.96353	-2.20296	-2.17292
C	1.86890	-2.00278	-1.37356
H	5.20817	-3.30918	0.10293
H	2.89429	-1.97833	-3.23316
H	5.01864	-2.83967	-2.31064
H	0.43920	5.38029	-2.29596
C	1.94081	-2.29664	0.01560
C	3.17633	-2.76031	0.54445
C	3.27798	-3.03277	1.92421
C	2.20850	-2.86771	2.75484
C	0.98111	-2.42834	2.23392
C	0.85146	-2.14985	0.90242
H	4.22830	-3.38406	2.31147
H	2.29883	-3.08432	3.81219
H	0.12913	-2.31399	2.89357
H	-0.11127	-1.81561	0.53315
C	1.34209	2.50108	0.16980
C	1.13073	3.82313	0.64663

C	1.25883	4.08690	2.02572
C	1.57683	3.09253	2.90401
C	1.78527	1.78541	2.43601
C	1.67148	1.49598	1.10522
H	1.10170	5.10215	2.37392
H	1.67502	3.30833	3.96087
H	2.04725	0.99934	3.13464
H	1.84947	0.47737	0.77587

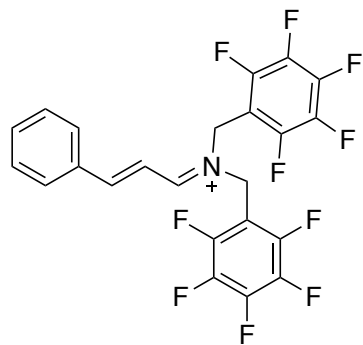


Iminium 41

M06/def2-TZVP Geometry

C	-4.77767	-2.99056	0.58053
C	-3.48048	-3.10587	0.06638
C	-2.92659	-4.38425	-0.08789
C	-3.64901	-5.50107	0.26160
C	-2.77945	-1.90625	-0.27986
C	-1.52754	-1.78688	-0.79015
C	-1.02812	-0.49943	-1.06581
H	-1.67453	0.34683	-0.83517
N	0.12808	-0.17662	-1.56031
C	0.49993	1.24319	-1.79617
C	1.17587	-1.14517	-1.91490
H	-5.21133	-2.00352	0.70172
H	-1.92483	-4.50144	-0.48445
H	-3.21604	-6.48609	0.14003
H	-0.92027	-2.66387	-0.97829
H	0.28198	1.46750	-2.84496
H	0.72212	-2.13238	-2.00164
C	-5.50003	-4.11182	0.92965
C	-4.93592	-5.36699	0.77024
H	-5.50031	-6.25068	1.04304
H	-6.50254	-4.01129	1.32588
H	-3.33169	-0.98275	-0.10890
H	1.54442	-0.87105	-2.90700

H	1.58563	1.28110	-1.66784
C	-1.11917	3.07777	-1.33150
C	-0.17154	2.20294	-0.87655
H	-1.39063	3.09045	-2.38409
C	3.02151	-1.39611	1.36408
C	2.01848	-1.40894	0.44147
C	2.29123	-1.12426	-0.91468
H	1.00265	-1.63915	0.75020
H	2.81243	-1.61876	2.40506
C	3.56929	-0.82898	-1.30051
C	0.18264	2.19926	0.49213
C	-0.41531	3.06281	1.35907
H	3.78737	-0.60632	-2.34210
H	0.94529	1.50677	0.83950
H	-0.13762	3.06844	2.40778
C	-1.39382	3.97974	0.91426
C	-1.75076	3.98971	-0.45925
C	-2.72078	4.90723	-0.90903
C	-3.31120	5.77606	-0.03701
C	-2.95789	5.76678	1.32350
C	-2.02079	4.88909	1.78827
H	-2.98667	4.91413	-1.96089
H	-4.05364	6.48055	-0.39189
H	-3.43215	6.46426	2.00332
H	-1.74219	4.88178	2.83662
C	4.35063	-1.10264	0.98972
C	4.63035	-0.81555	-0.37163
C	5.95492	-0.52214	-0.75198
C	6.95683	-0.51416	0.17490
C	6.68018	-0.79862	1.52369
C	5.40651	-1.08608	1.92203
H	6.16444	-0.30485	-1.79403
H	7.97274	-0.28912	-0.12632
H	7.48605	-0.78954	2.24756
H	5.18892	-1.30757	2.96141

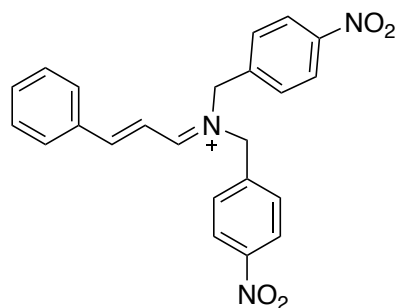


Iminium 42

M06/def2-TZVP Geometry

C	4.03530	-3.99991	-1.12586
C	3.43286	-2.93719	-0.43707
C	4.05647	-2.43525	0.71673
C	5.23586	-2.98436	1.15925
C	2.20874	-2.41358	-0.94568
C	1.44491	-1.41360	-0.42029
C	0.26821	-1.04665	-1.07957
H	0.00118	-1.59872	-1.97835
N	-0.57388	-0.10785	-0.73665
C	-1.82410	0.08653	-1.49615
C	-0.37239	0.74232	0.45280
H	3.55735	-4.38854	-2.01882
H	3.61507	-1.60894	1.26234
H	5.71554	-2.59449	2.04816
H	1.73321	-0.92467	0.50053
H	-1.74743	-0.51199	-2.40474
H	-1.31538	1.26384	0.62159
C	5.21648	-4.54865	-0.67771
C	5.81589	-4.04103	0.46444
H	6.74591	-4.46885	0.81954
H	5.67413	-5.37001	-1.21416
H	1.85187	-2.87684	-1.86518
H	-0.20322	0.10187	1.31936
H	-1.88692	1.13337	-1.78896
C	-3.30047	-1.64327	-0.45271
C	-3.02872	-0.30604	-0.70278
F	-2.46259	-2.56347	-0.91188
C	1.66061	3.73467	-0.70444
C	0.66688	2.78116	-0.59104
C	0.74446	1.73401	0.31582
F	-0.39815	2.88184	-1.37259
F	1.55532	4.70921	-1.57344
C	1.86702	1.68643	1.12847

C	-3.92316	0.63377	-0.21218
C	-5.05377	0.26111	0.49447
F	1.99397	0.71652	2.02717
F	-3.70140	1.92141	-0.41563
F	-5.88535	1.16667	0.94753
C	-5.29809	-1.08408	0.72597
C	-4.41708	-2.04684	0.25170
C	2.77487	3.65321	0.11849
C	2.87951	2.62468	1.04114
F	3.93100	2.54153	1.82103
F	3.72427	4.54519	0.02323
F	-4.64979	-3.31817	0.47177
F	-6.35905	-1.44803	1.39530

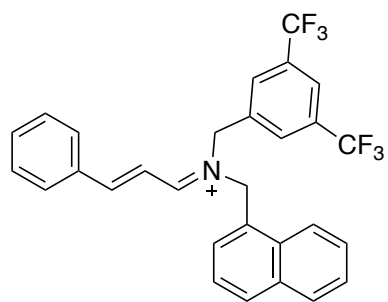


Iminium 43

M06/def2-TZVP Geometry

C	-5.08456	-1.91523	-0.69477
C	-3.84993	-2.27937	-0.13895
C	-3.52389	-3.64141	-0.04702
C	-4.40361	-4.59644	-0.49668
C	-2.98004	-1.24097	0.30872
C	-1.74509	-1.36219	0.87073
C	-1.05501	-0.19908	1.24121
H	-1.54167	0.75350	1.03827
N	0.12166	-0.10353	1.79446
C	0.72960	1.20723	2.12604
C	0.95146	-1.25566	2.15750
H	-5.34122	-0.86371	-0.76775
H	-2.57674	-3.94952	0.38001
H	-4.14871	-5.64621	-0.42403
H	-1.29992	-2.33840	1.02057
H	1.80874	1.06958	2.01110
H	1.32013	-1.08261	3.17225
C	-5.96441	-2.87541	-1.14432
C	-5.62385	-4.21519	-1.04533
H	-6.31311	-4.97333	-1.39765

H	-6.91549	-2.58507	-1.57213
H	-3.36374	-0.22929	0.17988
H	0.32234	-2.14484	2.19953
H	0.53671	1.40276	3.18555
C	-0.57847	3.31600	1.77769
C	0.25962	2.33475	1.26687
C	2.93157	-1.66932	-1.03859
C	1.87887	-1.48516	-0.16470
C	2.10173	-1.43684	1.20769
C	3.39256	-1.57119	1.69889
C	0.66990	2.39861	-0.06181
C	0.24374	3.42738	-0.87633
C	-0.59450	4.38746	-0.34105
C	-1.01073	4.35585	0.97262
C	4.20437	-1.80627	-0.51991
C	4.45588	-1.76232	0.83467
H	3.57103	-1.53059	2.76825
H	5.47097	-1.87146	1.19297
H	2.78669	-1.71424	-2.10984
H	0.87326	-1.38018	-0.56063
H	1.33806	1.63709	-0.45436
H	0.55215	3.50688	-1.91033
H	-1.65901	5.13748	1.34598
H	-0.88856	3.27528	2.81660
N	-1.06384	5.49113	-1.21329
O	-0.68437	5.48121	-2.35855
O	-1.79387	6.31088	-0.71315
N	5.33807	-2.00275	-1.45405
O	5.07758	-2.02241	-2.63246
O	6.43387	-2.12697	-0.96621



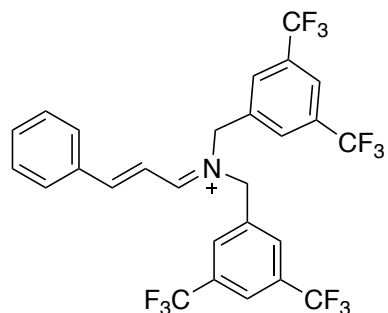
Iminium 44

M06/def2-TZVP Geometry

C	3.98653	-3.27682	-0.85824
C	4.38617	-1.96776	-0.55229
C	5.67135	-1.75713	-0.03607
C	6.53029	-2.81549	0.16840

C	3.53928	-0.83199	-0.74216
C	2.26830	-0.80565	-1.22422
C	1.60894	0.43156	-1.32486
H	2.15229	1.31854	-1.00277
N	0.40340	0.66367	-1.75491
C	-0.18284	2.03111	-1.78670
C	-0.50617	-0.37866	-2.23715
H	2.99755	-3.46715	-1.25839
H	5.98500	-0.74641	0.20262
H	7.52160	-2.64256	0.56768
H	1.76982	-1.72257	-1.51553
H	-1.17824	1.93715	-1.33988
H	-0.97437	-0.00069	-3.14970
C	4.84508	-4.33055	-0.65268
C	6.11721	-4.10170	-0.13971
H	6.78937	-4.93634	0.01994
H	4.53169	-5.33947	-0.88985
H	3.97777	0.12479	-0.46071
H	0.07858	-1.25350	-2.52170
H	-0.32951	2.27540	-2.84314
C	1.33723	3.96793	-1.89433
C	0.62846	3.08595	-1.11901
C	-3.87038	-0.97535	-0.61333
C	-2.90156	-0.64150	-1.54619
C	-1.55800	-0.72553	-1.22194
C	-1.19660	-1.13984	0.05171
C	2.16748	5.10862	0.03585
C	2.11076	4.98815	-1.32081
C	-3.50942	-1.38698	0.65558
C	-2.16643	-1.46443	0.98269
H	-0.14963	-1.20639	0.33562
C	-1.71267	-1.88650	2.35311
C	-5.31580	-0.86270	-1.02147
H	-3.20470	-0.31562	-2.53689
H	2.65132	5.67593	-1.95872
H	1.28820	3.88259	-2.97549
H	2.75784	5.89442	0.49495
C	0.66941	3.19184	0.29974
C	1.45833	4.22442	0.87586
C	1.51215	4.35042	2.27895
C	0.82276	3.49504	3.08739
C	0.04383	2.47290	2.52271
C	-0.03028	2.32322	1.16586
H	2.11275	5.14805	2.70276
H	0.86878	3.60346	4.16396
H	-0.50826	1.80085	3.16794

H	-0.65417	1.53204	0.76074
H	-4.26721	-1.64309	1.38428
F	-5.56663	-1.63394	-2.07630
F	-6.13823	-1.21639	-0.04809
F	-5.60482	0.38976	-1.37145
F	-2.72064	-2.20788	3.14328
F	-0.89212	-2.93295	2.28073
F	-1.02877	-0.89868	2.94031

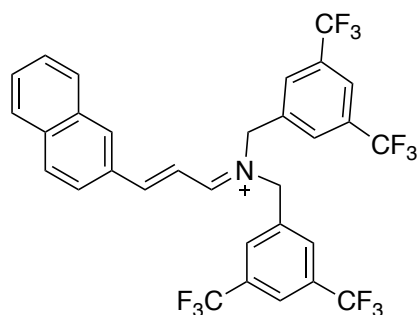


Iminium 45

M06/def2-TZVP Geometry

C	-6.13994	-0.29712	-1.24202
C	-5.99983	-1.01713	-0.04489
C	-7.12092	-1.18176	0.78177
C	-8.34015	-0.64778	0.42757
C	-4.76474	-1.59128	0.37457
C	-3.56109	-1.55677	-0.26489
C	-2.46156	-2.19249	0.32569
H	-2.62796	-2.68380	1.28296
N	-1.24042	-2.27753	-0.12957
C	-0.20777	-3.01914	0.62133
C	-0.81582	-1.68756	-1.40756
H	-5.28898	-0.15420	-1.89755
H	-7.01694	-1.73669	1.70811
H	-9.20037	-0.77935	1.07140
H	-3.45182	-1.04106	-1.21151
H	0.05228	-3.90566	0.03516
H	-0.08354	-2.36991	-1.84550
C	-7.35753	0.23451	-1.59166
C	-8.45802	0.05983	-0.75849
H	-9.41532	0.48186	-1.04038
H	-7.46205	0.79014	-2.51500
H	-4.80042	-2.11965	1.32696
H	-1.67579	-1.68162	-2.07995
H	-0.66611	-3.35741	1.55309

C	0.94738	-1.10642	1.74976
C	1.01301	-2.19070	0.88075
C	-0.28242	1.92773	-0.39781
C	-0.85912	0.67762	-0.54204
C	-0.21533	-0.31440	-1.26238
C	1.00752	-0.03163	-1.85269
C	3.24092	-0.57527	1.27024
C	2.05323	-0.30627	1.94074
C	0.93607	2.20900	-0.98481
C	1.57468	1.22325	-1.71828
H	1.53073	-0.79662	-2.41743
C	2.93709	1.48818	-2.30361
C	-1.02436	2.95512	0.41315
H	-1.81242	0.48680	-0.05864
H	0.02320	-0.88005	2.27342
H	4.10473	0.06257	1.41618
C	2.19819	-2.46702	0.22856
C	3.30904	-1.65556	0.41774
C	4.56113	-1.97942	-0.35268
F	4.97576	-3.21351	-0.08036
H	1.39004	3.18448	-0.86476
F	-2.17997	3.27200	-0.17356
F	-1.32509	2.47020	1.62035
F	-0.33004	4.06497	0.57875
F	3.10505	2.76783	-2.59618
F	3.88846	1.14736	-1.42830
F	3.14021	0.77967	-3.40624
F	5.54638	-1.14261	-0.08608
F	4.31793	-1.92933	-1.66572
H	2.26643	-3.31540	-0.44708
C	1.99752	0.89394	2.84800
F	3.04774	0.93644	3.65455
F	2.00210	2.02016	2.12924
F	0.90197	0.89899	3.59589

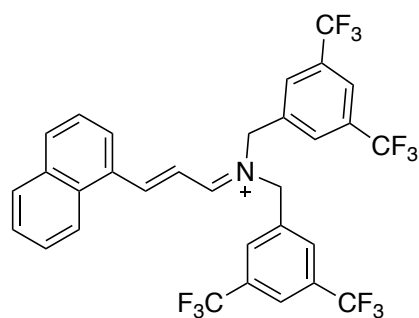


Iminium 46

M06/def2-TZVP Geometry

C	-5.29833	-0.20845	-1.32459
C	-5.17031	-1.00728	-0.15275
C	-6.29096	-1.22085	0.63986
C	-3.94868	-1.60140	0.25197
C	-2.73308	-1.52991	-0.37222
C	-1.64216	-2.19539	0.18990
H	-1.81525	-2.73653	1.11858
N	-0.41376	-2.25986	-0.25978
C	0.60968	-3.03920	0.46032
C	0.01954	-1.61150	-1.50429
H	-4.43576	-0.02811	-1.95435
H	-6.20196	-1.82812	1.53630
H	-2.61717	-0.96113	-1.28705
H	0.87637	-3.89656	-0.16532
H	0.74996	-2.27560	-1.97301
C	-6.49531	0.33191	-1.65707
H	-6.59285	0.94144	-2.54865
H	-3.99577	-2.18258	1.17226
H	-0.83741	-1.56689	-2.17931
H	0.14371	-3.42329	1.37035
C	1.75357	-1.17542	1.68043
C	1.82952	-2.22700	0.77249
C	2.43312	1.29336	-1.65973
C	1.85650	0.05202	-1.86120
C	0.62820	-0.25063	-1.29191
C	-0.01054	0.70810	-0.52365
C	4.05518	-0.63280	1.25461
C	2.85738	-0.38488	1.91580
C	1.79928	2.24517	-0.87864
C	0.57643	1.94392	-0.31145
H	-0.96659	0.49873	-0.05341
C	-0.15297	2.92821	0.56141
C	3.80309	1.57716	-2.21699
H	2.37844	-0.68982	-2.45746

H	0.82081	-0.96409	2.19486
H	4.91659	0.00002	1.43405
C	3.02345	-2.48142	0.12816
C	4.13385	-1.68139	0.36481
C	5.39492	-1.97767	-0.40107
F	6.38127	-1.15994	-0.08313
H	2.26177	3.20858	-0.70536
F	4.02253	0.90772	-3.34071
F	3.97539	2.86655	-2.46263
F	4.74249	1.20636	-1.34057
F	0.54473	4.02855	0.77383
F	-1.31762	3.27542	0.01133
F	-0.43368	2.38133	1.74696
F	5.17152	-1.86717	-1.71389
F	5.79959	-3.22537	-0.17908
H	3.09898	-3.30234	-0.57984
C	2.79544	0.78245	2.86406
F	3.77810	0.73090	3.75264
F	2.92430	1.93205	2.19629
F	1.64518	0.82727	3.52291
C	-7.53565	-0.67546	0.31687
C	-7.64735	0.12036	-0.85750
C	-8.89481	0.66973	-1.18485
C	-9.98407	0.44215	-0.38620
C	-9.87676	-0.34338	0.77419
C	-8.67695	-0.89173	1.12004
H	-8.98413	1.27698	-2.07865
H	-10.94297	0.87221	-0.64964
H	-10.75118	-0.50985	1.39074
H	-8.58075	-1.49958	2.01309



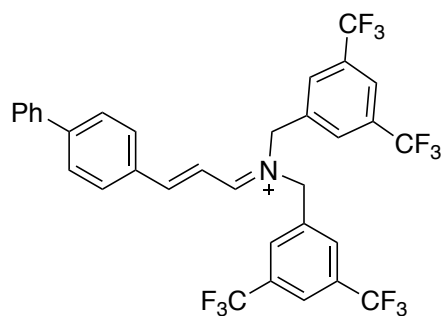
Iminium 47

M06/def2-TZVP Geometry

C	-5.19243	0.70788	-1.61797
C	-5.28225	-0.36741	-0.73555
C	-4.13305	-1.14498	-0.44036

C	-2.87719	-1.04587	-0.97868
C	-1.87705	-1.90469	-0.52161
H	-2.14863	-2.61686	0.25562
N	-0.62671	-1.97054	-0.91000
C	0.29242	-2.95963	-0.32020
C	-0.06485	-1.10689	-1.95621
H	-4.24126	0.94073	-2.08114
H	-2.65262	-0.31184	-1.74296
H	0.56260	-3.67379	-1.10416
H	0.65846	-1.70843	-2.51220
C	-6.28232	1.50908	-1.91219
H	-6.17622	2.34056	-2.59672
H	-4.25354	-1.91801	0.31383
H	-0.86492	-0.85850	-2.65654
H	-0.26375	-3.50276	0.44699
C	2.75316	-2.51448	-0.35175
C	1.52461	-2.32302	0.24793
C	0.59611	2.08243	-0.01577
C	-0.04041	0.96049	-0.51803
C	0.60444	0.13080	-1.41999
C	1.89212	0.45005	-1.82517
C	3.78491	-1.03727	1.23126
C	3.88134	-1.86788	0.13633
C	1.87966	2.39838	-0.41720
C	2.52170	1.57799	-1.32972
H	2.41660	-0.18992	-2.52747
C	3.94592	1.86910	-1.72395
C	-0.15670	2.93709	0.96679
H	-1.04409	0.73356	-0.17204
H	2.84380	-3.16422	-1.21806
H	4.66244	-0.52822	1.61192
C	1.42977	-1.49357	1.36081
C	2.55098	-0.85552	1.84530
C	2.46662	0.07662	3.02428
F	1.29774	-0.01390	3.64543
H	2.37961	3.27164	-0.01778
F	-0.61425	2.19713	1.97931
F	0.58772	3.90413	1.46949
F	-1.22143	3.49384	0.38538
F	4.20862	3.16628	-1.68943
F	4.79031	1.26571	-0.88183
F	4.21606	1.42349	-2.94385
F	2.61627	1.34356	2.62763
F	3.42251	-0.17558	3.90695
H	0.47013	-1.33515	1.84399
C	5.18650	-2.08441	-0.58107

F	6.18279	-1.42010	-0.02525
F	5.50558	-3.37584	-0.59943
F	5.08316	-1.68956	-1.85317
C	-7.49384	1.24209	-1.32250
H	-8.35502	1.86442	-1.54287
C	-6.54830	-0.66174	-0.11478
C	-7.65804	0.17231	-0.42738
C	-8.91610	-0.07846	0.15886
C	-9.08734	-1.11711	1.02443
C	-7.99878	-1.94502	1.33110
C	-6.76619	-1.72558	0.77709
H	-9.74364	0.57398	-0.09665
H	-10.05444	-1.30682	1.47256
H	-8.13434	-2.77324	2.01623
H	-5.96236	-2.40057	1.04175



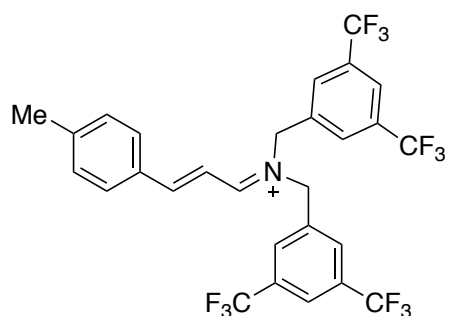
Iminium 48

M06/def2-TZVP Geometry

C	4.85101	-0.73176	-0.72664
C	4.56172	-1.51163	0.40812
C	3.27184	-2.01608	0.69874
C	2.11663	-1.85120	-0.01880
C	0.93979	-2.43604	0.44748
H	0.99908	-2.99860	1.37759
N	-0.25343	-2.39943	-0.09481
C	-1.38331	-3.11034	0.53028
C	-0.53786	-1.70568	-1.35684
H	4.06510	-0.47761	-1.42835
H	2.11370	-1.26737	-0.93170
H	-1.02595	-3.51619	1.47915
H	0.36717	-1.72782	-1.96747
C	6.11876	-0.27236	-0.95396
H	6.31123	0.34975	-1.81922
H	3.19969	-2.60682	1.61166
H	-1.28519	-2.29993	-1.88843
H	-1.64501	-3.95425	-0.11568
C	-3.71508	-2.40872	-0.02917

C	-2.57642	-2.22612	0.73057
C	-0.89492	1.85687	-0.11297
C	-0.40054	0.57879	-0.30989
C	-1.04252	-0.29965	-1.16579
C	-2.17821	0.12656	-1.84068
C	-4.74448	-0.50651	1.00835
C	-4.79530	-1.54768	0.10627
C	-2.02591	2.27979	-0.78112
C	-2.66076	1.40890	-1.65136
H	-2.70281	-0.54977	-2.50811
C	-3.93915	1.84447	-2.31692
C	-0.17460	2.74596	0.86215
H	0.48217	0.27255	0.24310
H	-3.76888	-3.22300	-0.74668
H	-5.58485	0.16895	1.11231
C	-2.53089	-1.18506	1.65160
C	-3.60662	-0.33251	1.78704
C	-3.54432	0.83239	2.73896
F	-2.62796	0.65038	3.68115
H	-2.42086	3.27479	-0.61814
F	-0.78053	3.90603	1.03306
F	-0.07795	2.14950	2.05321
F	1.07173	2.98689	0.45036
F	-4.97262	1.66457	-1.48791
F	-3.90803	3.12970	-2.63716
F	-4.18458	1.14965	-3.41878
F	-4.71007	1.03993	3.33144
F	-3.22609	1.95296	2.08138
H	-1.64285	-1.03117	2.25810
C	-5.98805	-1.76528	-0.78530
F	-6.45148	-3.00594	-0.66302
F	-6.97379	-0.92732	-0.52184
F	-5.63776	-1.60268	-2.06498
C	7.17040	-0.55703	-0.06542
C	5.61379	-1.79734	1.29529
C	6.88187	-1.33146	1.06560
H	5.41249	-2.40571	2.17089
H	7.67793	-1.59077	1.75223
C	11.10016	0.89197	-0.79044
C	10.26242	0.59665	-1.85367
C	8.98337	0.13433	-1.61939
C	8.52130	-0.05805	-0.31537
C	9.38106	0.23697	0.74511
C	10.65412	0.71454	0.50929
H	12.10174	1.26104	-0.97493
H	10.61079	0.72346	-2.87135

H	8.34765	-0.11656	-2.46077
H	9.03626	0.12709	1.76685
H	11.30176	0.95486	1.34348

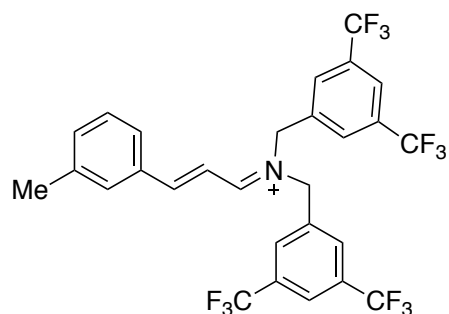


Iminium 49

M06/def2-TZVP Geometry

C	-5.89318	-0.39668	-1.07598
C	-5.71338	-1.14215	0.10341
C	-4.46770	-1.70452	0.48571
C	-3.27403	-1.64147	-0.17739
C	-2.15459	-2.26286	0.38189
H	-2.29262	-2.76992	1.33538
N	-0.93765	-2.31725	-0.09612
C	0.12184	-3.04558	0.62711
C	-0.55051	-1.70745	-1.37546
H	-5.05968	-0.22706	-1.74757
H	-3.19229	-1.10895	-1.11753
H	0.38057	-3.92912	0.03552
H	0.19096	-2.36742	-1.83225
C	-7.12019	0.12448	-1.38611
H	-7.24994	0.69947	-2.29666
H	-4.47574	-2.24998	1.42911
H	-1.42205	-1.71789	-2.03311
H	-0.30805	-3.39019	1.57011
C	2.51519	-2.47617	0.18905
C	1.33883	-2.20242	0.85715
C	1.75275	1.26970	-1.71446
C	1.21459	0.00375	-1.85522
C	0.01804	-0.32057	-1.23038
C	-0.62542	0.64091	-0.47041
C	3.55778	-0.55917	1.18483
C	3.62283	-1.65378	0.35087
C	1.11468	2.22503	-0.94004
C	-0.07461	1.90246	-0.31852
H	-1.55539	0.41589	0.04262
C	-0.80312	2.88789	0.55346
C	3.08900	1.60041	-2.32502

H	1.74284	-0.74035	-2.44301
H	2.57976	-3.33231	-0.47699
H	4.41616	0.09157	1.30480
C	1.27893	-1.10810	1.71451
C	2.37863	-0.29282	1.87255
C	2.32850	0.91993	2.76319
F	3.36001	0.94783	3.59480
H	1.55266	3.20723	-0.81272
F	4.05806	1.44930	-1.41679
F	3.37324	0.80934	-3.34989
F	3.13337	2.85559	-2.74636
F	-2.00277	3.17335	0.04382
F	-1.01259	2.37043	1.76666
F	-0.13963	4.01919	0.70050
F	1.21551	0.96058	3.48359
F	2.37772	2.03722	2.03187
H	0.36156	-0.88421	2.25086
C	4.86287	-1.97860	-0.43766
F	5.86276	-1.16120	-0.16436
F	5.26365	-3.22354	-0.19657
F	4.60612	-1.89625	-1.74655
C	-8.22360	-0.06909	-0.54443
C	-6.82064	-1.33368	0.94336
C	-8.04987	-0.80740	0.62346
H	-6.69672	-1.90601	1.85677
H	-8.89524	-0.96453	1.28335
C	-9.54294	0.51154	-0.90600
H	-10.31152	0.26899	-0.17377
H	-9.47505	1.59963	-0.98581
H	-9.86995	0.14793	-1.88342



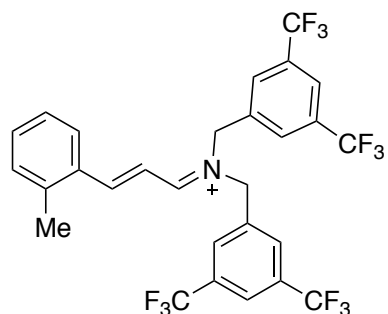
Iminium 50

M06/def2-TZVP Geometry

C	-6.84691	-1.42744	1.05397
C	-5.77276	-1.15781	0.19641
C	-4.51300	-1.75026	0.49537
C	-3.34228	-1.63412	-0.19608

C	-2.20805	-2.30539	0.27409
N	-1.01058	-2.32864	-0.24930
C	-0.66175	-1.61830	-1.48811
C	0.07089	-3.11032	0.38052
C	-8.08567	-0.87634	0.80555
C	-0.67491	0.66022	-0.41436
C	-0.06303	-0.25742	-1.25026
C	2.27774	-0.45444	1.89281
C	1.19582	-1.27455	1.65630
C	1.27327	-2.27065	0.68819
C	2.44848	-2.44258	-0.01554
C	1.09911	2.23326	-0.78900
C	-0.09273	1.89501	-0.18022
C	3.45475	-0.61687	1.17080
C	3.53669	-1.61290	0.22220
C	4.77537	-1.81461	-0.60924
C	2.20340	0.65821	2.90487
C	1.13427	0.08361	-1.86367
C	1.70692	1.32110	-1.63653
C	3.05081	1.65282	-2.22969
F	3.13842	2.93465	-2.55106
F	2.16200	1.84376	2.29008
F	1.12220	0.56370	3.66717
F	3.26680	0.66090	3.69548
F	5.21903	-3.06368	-0.49957
F	4.49934	-1.60943	-1.90058
F	5.75188	-0.99618	-0.26456
F	4.01747	1.39573	-1.34212
F	3.30328	0.93431	-3.31415
C	-0.78336	2.82397	0.77981
F	-0.91344	2.24145	1.97445
F	-0.13050	3.95855	0.94553
F	-2.01516	3.11242	0.35530
C	-8.26064	-0.05520	-0.29329
C	-5.97781	-0.32038	-0.91271
C	-7.21046	0.23776	-1.17073
C	-7.44312	1.13117	-2.34270
H	-6.69403	-2.07222	1.91247
H	-4.49502	-2.37078	1.39095
H	-3.28729	-1.02670	-1.09156
H	-2.31851	-2.88683	1.18798
H	-1.55760	-1.56157	-2.10928
H	0.05052	-2.24867	-2.02598
H	0.33745	-3.91913	-0.30636
H	-0.34161	-3.56297	1.28480
H	-8.91770	-1.08344	1.46653

H	-1.60428	0.42029	0.09345
H	0.27893	-1.13101	2.22046
H	2.52599	-3.22049	-0.77040
H	1.56129	3.19359	-0.59646
H	4.29846	0.03907	1.35063
H	1.63359	-0.62577	-2.51529
H	-9.23674	0.37873	-0.48685
H	-5.15600	-0.09912	-1.58577
H	-8.21799	0.72421	-2.99596
H	-7.78499	2.11688	-2.01972
H	-6.53834	1.26566	-2.93495

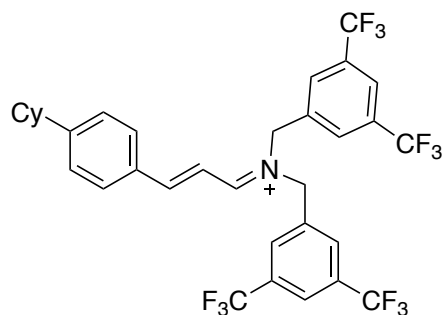


Iminium 51

M06/def2-TZVP Geometry

C	-5.86506	0.10417	-1.46282
C	-5.83537	-0.75173	-0.34654
C	-4.63347	-1.40935	0.03822
C	-3.40804	-1.35099	-0.56376
C	-2.35021	-2.08207	-0.01368
N	-1.11748	-2.16520	-0.44245
C	-0.63548	-1.46777	-1.64323
C	-0.13401	-3.01275	0.25864
C	-7.01773	0.74390	-1.83799
C	1.25588	0.15755	-1.86887
C	0.00434	-0.13697	-1.34772
C	2.14634	-0.49823	1.89793
C	1.02849	-1.24539	1.59758
C	1.09978	-2.25425	0.64194
C	2.30310	-2.51267	0.01697
C	1.23211	2.30053	-0.77925
C	1.86133	1.36965	-1.58868
C	3.35454	-0.74992	1.25737
C	3.42861	-1.75770	0.32120
C	4.69998	-2.05022	-0.42936
C	2.08775	0.62989	2.89285
C	-0.62919	0.80176	-0.55090

C	-0.01510	2.00859	-0.26258
C	-0.74476	2.97194	0.63313
F	-0.03127	4.04799	0.90625
F	2.27568	1.80062	2.27770
F	0.91616	0.68536	3.51264
F	3.03580	0.51001	3.81132
F	5.05910	-3.32123	-0.27238
F	4.51421	-1.85514	-1.73838
F	5.70227	-1.28511	-0.03939
F	-1.88897	3.36465	0.07039
F	-1.06515	2.38317	1.78806
C	3.25575	1.63909	-2.09020
F	4.15549	1.19474	-1.20592
F	3.49024	1.02139	-3.23996
F	3.47342	2.93315	-2.26271
C	-8.17664	0.53807	-1.09860
C	-7.01920	-0.95722	0.40484
C	-8.16975	-0.29959	0.00226
H	-4.96195	0.26766	-2.03849
H	-4.69598	-2.03785	0.92392
H	-3.24900	-0.74634	-1.44834
H	-2.56043	-2.66213	0.88336
H	-1.47393	-1.36624	-2.33500
H	0.08791	-2.12919	-2.12609
H	0.12246	-3.84237	-0.40714
H	-0.63380	-3.43098	1.13507
H	-7.02560	1.40144	-2.69765
H	1.77358	-0.56794	-2.48851
H	0.08806	-1.03066	2.09640
H	2.37501	-3.30004	-0.72853
H	1.71680	3.23989	-0.54504
H	4.22754	-0.15058	1.48834
H	-1.60386	0.59875	-0.11759
H	-9.09477	1.03769	-1.38451
C	-7.06700	-1.85020	1.60169
H	-9.08321	-0.44733	0.56668
H	-8.06911	-1.86307	2.02695
H	-6.80655	-2.88209	1.35360
H	-6.38544	-1.51723	2.38841

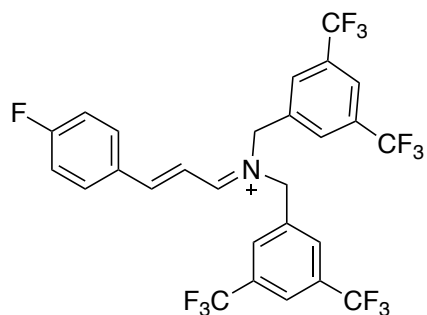


Iminium 52

M06/def2-TZVP Geometry

C	-5.35350	-2.05817	1.40295
C	-4.34764	-1.68265	0.49890
C	-3.03937	-2.19425	0.68962
C	-1.92088	-1.95645	-0.06157
C	-0.71632	-2.55752	0.30758
N	0.45142	-2.45520	-0.27635
C	0.67658	-1.65112	-1.48475
C	1.62042	-3.18440	0.24757
C	-6.63639	-1.58550	1.26576
C	0.51032	0.55612	-0.28399
C	1.16456	-0.25628	-1.19501
C	3.73996	-0.46057	1.76536
C	2.70012	-1.33872	1.54965
C	2.77986	-2.27664	0.52515
C	3.91568	-2.33038	-0.25762
C	2.10859	2.31005	-0.64965
C	0.98413	1.82736	-0.00885
C	4.87615	-0.50492	0.96560
C	4.96039	-1.44105	-0.04162
C	6.15430	-1.51762	-0.95491
C	3.66421	0.58584	2.84497
C	2.29257	0.22938	-1.83997
C	2.75688	1.50470	-1.57099
C	4.02394	1.98857	-2.22570
F	4.03837	3.30637	-2.35165
F	4.77366	0.60998	3.56973
F	3.51424	1.79928	2.30717
F	2.64116	0.38032	3.66415
F	5.77997	-1.30414	-2.21982
F	7.08166	-0.62996	-0.64733
F	6.70445	-2.72805	-0.91119
F	5.08491	1.64410	-1.48882
F	4.18656	1.45519	-3.42924
C	0.23574	2.65251	1.00166
F	-0.99805	2.92052	0.56931

F	0.10485	1.98253	2.14886
F	0.83590	3.79885	1.26268
C	-6.97394	-0.71996	0.22608
C	-4.68982	-0.81059	-0.55072
C	-5.97067	-0.34446	-0.67912
H	-5.10566	-2.72947	2.21864
H	-2.92078	-2.85543	1.54781
H	-1.96508	-1.30201	-0.92401
H	-0.72932	-3.19500	1.19005
H	-0.25028	-1.63983	-2.06174
H	1.41324	-2.18454	-2.09041
H	1.90018	-3.94073	-0.49218
H	1.29879	-3.70614	1.15154
H	-7.40199	-1.88389	1.97309
H	-0.36897	0.20323	0.24622
H	1.81349	-1.28679	2.17479
H	3.99504	-3.06194	-1.05729
H	2.48278	3.30169	-0.42887
H	5.68640	0.19481	1.13312
H	2.82358	-0.39332	-2.55292
H	-6.21362	0.32747	-1.49412
H	-3.93858	-0.49869	-1.26711
C	-10.45653	-0.24434	-1.32597
C	-9.02156	-0.72731	-1.21277
C	-8.37225	-0.21536	0.07704
C	-8.44962	1.31211	0.14045
C	-9.88748	1.78605	0.02451
C	-10.53671	1.26985	-1.24728
H	-11.04865	-0.68259	-0.51268
H	-10.89707	-0.60664	-2.25795
H	-8.44601	-0.36334	-2.07400
H	-8.97350	-1.82012	-1.24370
H	-8.95886	-0.61015	0.91807
H	-7.99418	1.66921	1.06900
H	-7.86139	1.73917	-0.68210
H	-10.45514	1.42960	0.89332
H	-9.92229	2.87752	0.06023
H	-10.02484	1.70424	-2.11592
H	-11.57651	1.59954	-1.30514

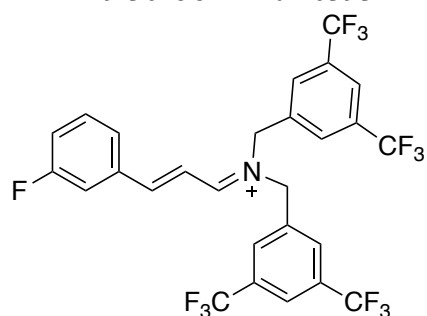


Iminium 53

M06/def2-TZVP Geometry

C	5.90277	-0.35042	-1.09718
C	5.73025	-1.10095	0.07941
C	4.48419	-1.66947	0.45965
C	3.29138	-1.60709	-0.20122
C	2.17478	-2.24298	0.35304
N	0.96088	-2.30450	-0.12715
C	0.56739	-1.68431	-1.40037
C	-0.09411	-3.04897	0.58822
C	7.12492	0.17837	-1.41894
C	-1.22881	0.00090	-1.84783
C	-0.02066	-0.30745	-1.24016
C	-3.58879	-1.63553	0.34617
C	-2.48513	-2.45785	0.16193
C	-1.30927	-2.21052	0.84195
C	-1.24643	-1.14459	1.73357
C	-1.14701	2.22461	-0.93820
C	-1.78329	1.26007	-1.70139
C	-3.52302	-0.57294	1.22084
C	-2.34501	-0.33326	1.91899
C	-2.29083	0.84841	2.85030
C	-4.82989	-1.92779	-0.45410
C	0.62078	0.66339	-0.48948
C	0.05642	1.91772	-0.33331
C	0.79512	2.92161	0.50930
F	1.96223	3.23986	-0.05414
F	-5.26417	-3.16210	-0.21554
F	-5.81004	-1.08482	-0.18838
F	-4.56134	-1.85358	-1.76107
F	-2.27189	1.98842	2.15381
F	-3.35309	0.88685	3.64108
F	-1.20718	0.82682	3.61524
F	0.10831	4.03408	0.68736
F	1.07425	2.40993	1.71055
C	-3.13018	1.55389	-2.30879
F	-3.32301	0.86338	-3.42461

F	-4.10341	1.21682	-1.45664
F	-3.27230	2.83989	-2.58723
C	8.19485	-0.04168	-0.55913
C	6.83842	-1.29748	0.92000
C	8.06962	-0.77403	0.60974
H	5.06631	-0.17984	-1.76422
H	4.49545	-2.22114	1.39922
H	3.20447	-1.06843	-1.13735
H	2.31679	-2.75723	1.30212
H	-0.16368	-2.34949	-1.86605
H	1.44004	-1.67477	-2.05633
H	0.34203	-3.41233	1.52119
H	-0.35415	-3.91989	-0.02099
H	7.28102	0.76009	-2.31828
H	-1.75079	-0.74774	-2.43518
H	-2.55132	-3.29162	-0.53188
H	-0.32942	-0.94056	2.27859
H	-1.59149	3.20333	-0.80910
H	-4.38069	0.07414	1.36228
H	1.56198	0.45177	0.00869
H	8.93355	-0.91596	1.24588
H	6.71465	-1.87409	1.83024
F	9.36258	0.46393	-0.86896

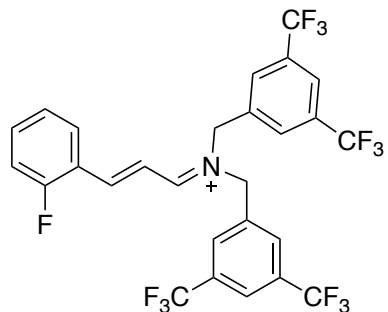


Iminium 54

M06/def2-TZVP Geometry

C	-6.86033	-1.40154	1.03340
C	-5.77253	-1.15224	0.18715
C	-4.51288	-1.73911	0.51702
C	-3.33908	-1.63343	-0.16403
C	-2.20366	-2.29258	0.33074
N	-1.00407	-2.31829	-0.18061
C	-0.64442	-1.62530	-1.42771
C	0.07326	-3.09386	0.46806
C	-8.09969	-0.85851	0.76094
C	-0.69524	0.66892	-0.38941
C	-0.06293	-0.25447	-1.20473
C	2.34010	-0.43833	1.88930

C	1.24255	-1.24731	1.68830
C	1.28896	-2.26159	0.73722
C	2.44807	-2.46201	0.01436
C	1.04980	2.26750	-0.79173
C	-0.13759	1.91817	-0.17824
C	3.50064	-0.62962	1.14817
C	3.55090	-1.64265	0.21558
C	4.77105	-1.87929	-0.63382
C	2.30225	0.69060	2.88499
C	1.12935	0.09634	-1.82089
C	1.67657	1.35088	-1.61903
C	3.00814	1.68850	-2.23747
F	3.13324	2.98817	-2.45228
F	3.38671	0.69742	3.64573
F	2.25215	1.86612	2.25226
F	1.24163	0.61578	3.67819
F	5.21626	-3.12332	-0.48265
F	4.46545	-1.72765	-1.92593
F	5.75476	-1.04862	-0.34464
F	4.00087	1.31794	-1.42221
F	3.18470	1.05729	-3.39033
C	-0.86469	2.86765	0.73485
F	-1.11287	2.28617	1.91113
F	-0.18141	3.97359	0.96040
F	-2.04574	3.20708	0.21611
C	-8.27516	-0.06006	-0.35448
C	-5.95308	-0.34233	-0.94289
C	-7.19420	0.18534	-1.19016
H	-6.71947	-2.02695	1.90753
H	-4.50689	-2.33967	1.42577
H	-3.27637	-1.04452	-1.07140
H	-2.32123	-2.85842	1.25350
H	-1.53231	-1.58765	-2.06165
H	0.08039	-2.25853	-1.94454
H	0.32179	-3.92740	-0.19557
H	-0.33874	-3.51091	1.38943
H	-8.93678	-1.05468	1.41846
H	-1.62400	0.42372	0.11669
H	0.33940	-1.08204	2.26848
H	2.50164	-3.25564	-0.72605
H	1.48998	3.24160	-0.61976
H	4.35739	0.01590	1.30194
H	1.64582	-0.61537	-2.45713
F	-7.36989	0.94833	-2.25147
H	-5.14672	-0.11486	-1.62882
H	-9.23519	0.38079	-0.59413

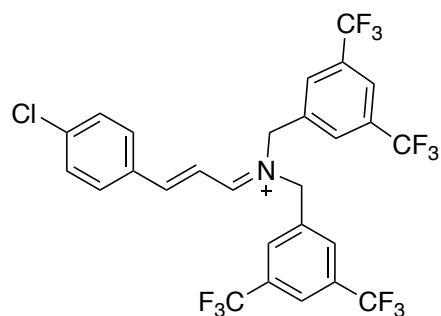


Iminium 55

M06/def2-TZVP Geometry

C	6.94259	-1.12745	1.02016
C	5.86209	-0.97731	0.13102
C	4.60705	-1.54592	0.49060
C	3.41904	-1.53610	-0.17850
C	2.31770	-2.17910	0.40707
N	1.10826	-2.28319	-0.07111
C	0.70230	-1.71254	-1.36523
C	0.06505	-3.01644	0.67360
C	8.18131	-0.60396	0.74279
C	0.70120	0.66115	-0.52074
C	0.08621	-0.34363	-1.24767
C	-3.44150	-1.62688	0.45643
C	-2.33826	-2.45120	0.27669
C	-1.14997	-2.17642	0.92337
C	-1.07346	-1.08145	1.77785
C	-1.10007	2.16821	-1.01776
C	0.10596	1.90516	-0.39887
C	-3.36113	-0.53313	1.29062
C	-2.17037	-0.26679	1.95735
C	-2.10057	0.94397	2.85006
C	-4.70078	-1.95730	-0.29950
C	-1.12623	-0.08009	-1.86825
C	-1.70908	1.16956	-1.75929
C	-3.06303	1.41756	-2.36991
F	-3.26565	0.65875	-3.43829
F	-5.67413	-1.10009	-0.05505
F	-4.46293	-1.95238	-1.61397
F	-5.13010	-3.17681	0.01386
F	-2.10056	2.06197	2.11938
F	-3.14635	1.00284	3.66170
F	-1.00104	0.94915	3.59207
F	-4.02330	1.12985	-1.48519
F	-3.21579	2.68345	-2.72525

C	0.79897	2.93312	0.45244
F	0.96279	2.46916	1.69449
F	2.01626	3.20005	-0.02293
F	0.12820	4.06712	0.52395
C	8.37895	0.09202	-0.44347
C	6.11194	-0.26697	-1.05424
C	7.34330	0.26287	-1.34739
H	6.77592	-1.67200	1.94321
H	4.61738	-2.06027	1.45124
H	3.32090	-1.03872	-1.13259
H	2.47064	-2.65440	1.37483
H	-0.01619	-2.40751	-1.80620
H	1.57458	-1.70659	-2.02134
H	0.51475	-3.35710	1.60874
H	-0.19735	-3.90135	0.08632
H	8.99692	-0.73164	1.44215
H	1.64450	0.48586	-0.01257
H	-2.41522	-3.30815	-0.38706
H	-0.14667	-0.85709	2.29781
H	-1.56967	3.13829	-0.91394
H	-4.21830	0.11586	1.42688
H	-1.62959	-0.85660	-2.43534
F	5.12967	-0.09780	-1.92631
H	9.35297	0.50879	-0.66967
H	7.47764	0.80211	-2.27635



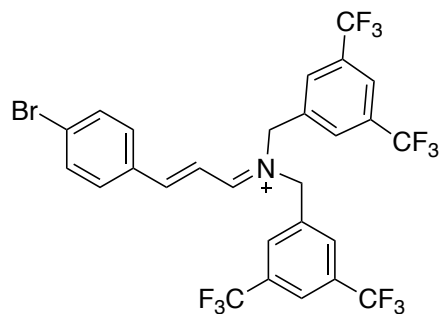
Iminium 56

M06/def2-TZVP Geometry

C	6.53569	-1.46802	1.02541
C	5.43983	-1.22800	0.18162
C	4.18044	-1.78834	0.53021
C	2.99887	-1.68908	-0.14596
C	1.86150	-2.31347	0.37850
N	0.65332	-2.33623	-0.11935
C	0.29331	-1.68227	-1.38558
C	-0.42749	-3.07387	0.56395

C	7.77735	-0.95238	0.74392
C	-1.43916	0.07114	-1.83101
C	-0.25357	-0.29089	-1.20623
C	-2.69483	-0.35032	1.85557
C	-1.59619	-1.16685	1.69296
C	-1.64143	-2.22635	0.79230
C	-2.80213	-2.46446	0.08361
C	-1.29997	2.26975	-0.86724
C	-1.95347	1.34387	-1.66422
C	-3.85643	-0.57935	1.12671
C	-3.90701	-1.63965	0.24824
C	-5.13029	-1.92422	-0.58120
C	-2.65540	0.82466	2.79630
C	0.40381	0.64025	-0.42080
C	-0.12050	1.91003	-0.24697
C	0.63094	2.86479	0.63988
F	0.00357	4.01572	0.79065
F	-1.61358	0.76695	3.61551
F	-2.56702	1.96772	2.11013
F	-3.75507	0.88983	3.53194
F	-6.12862	-1.10691	-0.30260
F	-5.54784	-3.17280	-0.39389
F	-4.84110	-1.79852	-1.87965
F	0.81565	2.33127	1.84972
F	1.84299	3.11549	0.14048
C	-3.27751	1.71333	-2.27993
F	-3.55378	0.96656	-3.33962
F	-4.26145	1.53526	-1.39308
F	-3.30306	2.98448	-2.65086
C	7.94200	-0.17828	-0.39811
C	5.63810	-0.44118	-0.96586
C	6.87221	0.07941	-1.25480
H	6.39588	-2.07239	1.91528
H	4.17010	-2.36432	1.45505
H	2.93578	-1.12705	-1.07021
H	1.97886	-2.85153	1.31767
H	-0.45258	-2.31643	-1.87047
H	1.17337	-1.68822	-2.03180
H	-0.01907	-3.44802	1.50516
H	-0.68122	-3.93804	-0.05757
H	8.62285	-1.13738	1.39363
H	-1.97575	-0.64734	-2.44252
H	-0.69283	-0.97305	2.26393
H	-2.85643	-3.29515	-0.61484
H	-1.71675	3.25892	-0.72384
H	-4.71458	0.07061	1.25099

H	1.32653	0.38623	0.09175
H	4.81316	-0.23290	-1.63680
Cl	9.48002	0.47206	-0.76178
H	7.03107	0.68794	-2.13574

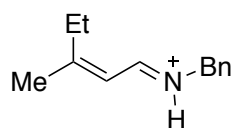


Iminium 57

M06/def2-TZVP Geometry

C	5.95448	-1.59032	1.18977
C	4.88242	-1.33435	0.32084
C	3.60677	-1.87549	0.64047
C	2.44197	-1.75409	-0.06063
C	1.28394	-2.36462	0.43418
N	0.08670	-2.36465	-0.09017
C	-0.23552	-1.69256	-1.35709
C	-1.01886	-3.09441	0.56158
C	7.21052	-1.09351	0.93592
C	-1.92743	0.09435	-1.82567
C	-0.76476	-0.29462	-1.17454
C	-3.28220	-0.35449	1.82448
C	-2.19050	-1.18370	1.68069
C	-2.22750	-2.23416	0.76910
C	-3.37312	-2.45001	0.02939
C	-1.78348	2.27560	-0.82412
C	-2.42854	1.37155	-1.65220
C	-4.42858	-0.56191	1.06570
C	-4.47088	-1.61223	0.17484
C	-5.67476	-1.86842	-0.69152
C	-3.24920	0.81351	2.77405
C	-0.11456	0.61551	-0.35900
C	-0.62496	1.89019	-0.18022
C	0.11818	2.82266	0.73669
F	-0.50033	3.97762	0.89342
F	-2.22675	0.73748	3.61582
F	-3.13078	1.95974	2.09725
F	-4.36425	0.88836	3.48514
F	-6.67080	-1.04409	-0.42558

F	-6.11151	-3.11495	-0.53776
F	-5.34918	-1.72338	-1.97955
F	1.34243	3.06846	0.26560
F	0.27302	2.26818	1.94125
C	-3.73185	1.76805	-2.29462
F	-3.73500	3.04683	-2.63917
F	-3.98758	1.04662	-3.37676
F	-4.74060	1.58189	-1.43767
C	7.41461	-0.32422	-0.20265
C	5.11908	-0.55260	-0.82248
C	6.36843	-0.05219	-1.08327
H	5.78493	-2.19124	2.07691
H	3.56724	-2.45467	1.56253
H	2.40787	-1.18572	-0.98251
H	1.37256	-2.91192	1.37116
H	-0.98053	-2.30987	-1.86453
H	0.65816	-1.70578	-1.98422
H	-0.63698	-3.48132	1.50877
H	-1.26831	-3.95025	-0.07305
H	8.03416	-1.29343	1.60917
H	-2.45648	-0.60589	-2.46423
H	-1.29839	-1.00621	2.27424
H	-3.42050	-3.27266	-0.67900
H	-2.19015	3.26823	-0.67605
H	-5.28177	0.09686	1.17659
H	0.79077	0.34062	0.17342
H	4.31343	-0.33291	-1.51304
Br	9.11472	0.35947	-0.56279
H	6.55130	0.55124	-1.96317



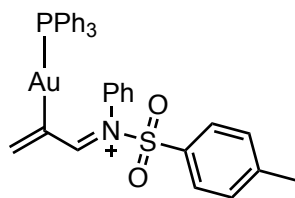
Iminium 58

M06/def2-TZVP Geometry

N	-0.03030	1.81924	0.15224
C	0.63549	0.72706	-0.03455
C	-1.50263	1.95568	0.24932
C	-2.22057	0.65689	0.11540
C	-2.61618	0.20180	-1.13671
C	-3.25688	-1.01797	-1.26397
C	-3.50400	-1.78937	-0.14012
C	-3.11367	-1.34124	1.11138
C	-2.47322	-0.12149	1.23881

C	2.05403	0.65207	-0.11859
C	2.55061	-0.58907	-0.32523
C	2.85447	1.90475	0.01721
C	3.95628	-1.00838	-0.45347
C	4.27617	-2.18263	0.46516
H	0.49432	2.68352	0.24345
H	0.04424	-0.18139	-0.13015
H	-1.80049	2.66038	-0.53152
H	-1.70628	2.42819	1.21385
H	-2.43402	0.81443	-2.01473
H	-3.57457	-1.36220	-2.24050
H	-4.01359	-2.74015	-0.23879
H	-3.31955	-1.93811	1.99138
H	-2.17915	0.23831	2.22042
H	1.82590	-1.40014	-0.40167
H	2.66394	2.39804	0.97518
H	3.92292	1.71375	-0.03684
H	2.61661	2.61669	-0.77900
H	4.64449	-0.17916	-0.28352
H	4.10451	-1.32522	-1.49485
H	5.30360	-2.51156	0.31619
H	4.15957	-1.90721	1.51413
H	3.62023	-3.03160	0.26346

Cartesian coordinates of reaction components for predicting gold catalyzed dearomatization



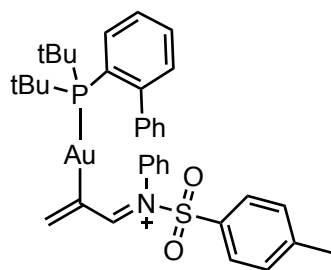
Gold intermediate 1

M06/def2-TZVP Geometry

C	-0.78726	-3.36224	1.99169
C	-0.87123	-2.35379	1.09910
C	-2.15110	-2.30669	0.47226
N	-2.64408	-1.34165	-0.25559
C	-2.04894	-0.04627	-0.42177
S	-4.24057	-1.58517	-1.05450
C	-1.45892	0.29780	-1.62572
C	-0.93089	1.56918	-1.76987

C	-1.00820	2.47895	-0.72829
C	-1.60993	2.12370	0.46934
C	-2.13472	0.85478	0.62892
O	-3.98505	-1.30323	-2.41971
O	-4.65383	-2.86264	-0.59186
C	-5.16151	-0.31168	-0.31958
C	-5.71594	-0.52044	0.93748
C	-6.40709	0.51023	1.53592
C	-6.55600	1.74249	0.89939
C	-5.98725	1.92055	-0.35904
C	-5.28756	0.90437	-0.97658
C	-7.34035	2.83402	1.54254
P	2.64308	0.16630	0.05459
C	2.45291	0.89794	-1.59627
C	2.95417	1.55296	1.17609
C	2.13466	0.04327	-2.64987
C	1.97010	0.54163	-3.92787
C	2.10815	1.90247	-4.16349
C	2.41717	2.75724	-3.12003
C	2.59283	2.25820	-1.83788
C	4.22445	2.10081	1.32439
C	4.41404	3.19752	2.14617
C	3.33993	3.75449	2.82117
C	2.07375	3.21145	2.68005
C	1.88156	2.11076	1.86416
H	-1.62547	-4.02653	2.20565
H	0.11591	-3.55613	2.55980
H	-1.40827	-0.42555	-2.43053
H	-0.44887	1.84582	-2.70040
H	-0.59133	3.47201	-0.85009
H	-1.67117	2.83761	1.28218
H	-2.61170	0.55448	1.55595
H	-5.61458	-1.48249	1.42639
H	-6.85203	0.36117	2.51362
H	-6.09918	2.87452	-0.86219
H	-4.84392	1.04206	-1.95527
H	-7.03392	3.81634	1.18290
H	-8.40367	2.72090	1.31310
H	-7.24284	2.81177	2.62850
H	2.02099	-1.02164	-2.46463
H	1.73436	-0.13084	-4.74410
H	1.97894	2.29426	-5.16538
H	2.53196	3.81902	-3.30324
H	2.83927	2.93421	-1.02607
H	5.06922	1.66638	0.79989
H	5.40576	3.61761	2.26257

H	3.49295	4.61088	3.46697
H	1.23582	3.63929	3.21781
H	0.89309	1.67170	1.76225
H	3.65377	-1.92898	1.71774
C	6.34906	-1.24694	-0.95465
C	6.57035	-2.19729	0.02750
C	5.60439	-2.43951	0.99087
C	4.41566	-1.73433	0.96851
C	4.18860	-0.77470	-0.01365
C	5.16275	-0.53403	-0.97683
H	7.10337	-1.05887	-1.70914
H	7.49877	-2.75551	0.04048
H	5.77565	-3.18535	1.75757
H	4.99531	0.21005	-1.74840
H	-2.81819	-3.16763	0.56047
Au	0.76401	-1.12526	0.63083



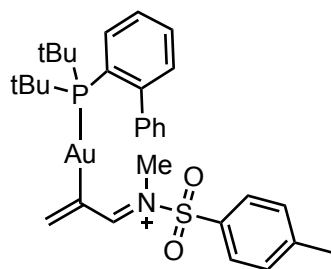
Gold intermediate 2

M06/def2-TZVP Geometry

C	-0.77987	0.29683	-2.04263
C	-0.59405	1.10770	-3.10725
C	-2.10129	-0.22738	-2.01280
N	-2.72818	-0.77808	-1.00676
C	-2.29536	-0.76248	0.35947
S	-4.39220	-1.41273	-1.28162
O	-4.36227	-2.72526	-0.74783
O	-4.63259	-1.14481	-2.65537
C	-5.30152	-0.34595	-0.25643
C	-5.61891	0.92394	-0.72273
C	-6.29791	1.78570	0.11062
C	-6.66702	1.39971	1.39918
C	-6.33238	0.12144	1.83763
C	-5.64897	-0.75746	1.02217
C	-7.43697	2.32840	2.27401
C	-2.24546	0.45701	1.01908

C	-1.97816	0.47996	2.37505
C	-1.77103	-0.70680	3.06032
C	-1.80247	-1.91701	2.38670
C	-2.06638	-1.95367	1.02872
P	2.89288	-0.80389	0.23803
C	4.01557	0.56869	0.70868
C	2.55043	-1.76540	1.81682
C	3.83282	-1.79304	-1.07342
C	2.84090	-2.68616	-1.81906
C	4.37723	-0.76065	-2.05920
C	4.97102	-2.67574	-0.57915
C	1.72105	-0.81938	2.68115
C	3.75759	-2.20946	2.63317
C	1.71330	-2.98983	1.46223
C	3.70958	1.92405	0.50221
C	4.69284	2.88162	0.75581
C	5.94442	2.54026	1.22374
C	6.24135	1.20999	1.45427
C	5.28782	0.24755	1.19329
C	2.40677	2.47417	0.04907
C	1.30764	2.51692	0.90215
C	0.15086	3.17990	0.52792
C	0.07073	3.80428	-0.70510
C	1.15704	3.76410	-1.56376
C	2.31694	3.10866	-1.18716
H	-1.39048	1.33733	-3.81658
H	0.35667	1.59292	-3.30028
H	-2.69366	-0.21336	-2.93054
H	-5.34706	1.22006	-1.72958
H	-6.56005	2.77745	-0.24136
H	-6.61729	-0.18868	2.83686
H	-5.38976	-1.75263	1.36236
H	-8.50759	2.24092	2.06857
H	-7.29012	2.10190	3.33011
H	-7.16072	3.36838	2.09668
H	-2.43762	1.37204	0.46819
H	-1.94589	1.42630	2.90173
H	-1.57494	-0.68737	4.12576
H	-1.62715	-2.84244	2.92183
H	-2.11619	-2.89279	0.49244
H	3.38135	-3.22249	-2.60468
H	2.04627	-2.10799	-2.29539
H	2.37648	-3.43315	-1.17397
H	3.59372	-0.08038	-2.40923
H	5.18414	-0.16221	-1.63264
H	4.77345	-1.28470	-2.93376

H	5.43531	-3.15267	-1.44775
H	4.61923	-3.47716	0.07321
H	5.75814	-2.12342	-0.06723
H	0.81493	-0.48543	2.16897
H	1.41851	-1.34345	3.59383
H	2.29677	0.06052	2.98101
H	4.44027	-2.85337	2.07858
H	4.31771	-1.36337	3.03180
H	3.39506	-2.78544	3.49032
H	2.29954	-3.74919	0.94068
H	1.34429	-3.44503	2.38674
H	0.84725	-2.73406	0.84453
H	4.44554	3.92446	0.59028
H	6.68142	3.31110	1.41390
H	7.21454	0.91736	1.82908
H	5.55248	-0.78595	1.36370
H	1.37491	2.05300	1.88085
H	-0.68542	3.22643	1.21671
H	-0.82876	4.33719	-0.99034
H	1.10913	4.26349	-2.52480
H	3.17791	3.09948	-1.84822
Au	0.84920	-0.16325	-0.80079



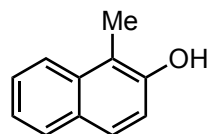
Gold intermediate 3

M06/def2-TZVP Geometry

C	-0.86394	1.38979	2.05446
C	-0.65097	1.91399	3.23725
C	-1.71576	1.25565	0.98816
N	-2.64544	0.29077	0.85305
S	-3.05193	-0.20612	-0.74745
O	-2.50049	-1.51245	-0.89804
O	-2.63751	0.87643	-1.57570
C	-4.79073	-0.30495	-0.67506
C	-5.53540	0.86877	-0.65831
C	-6.90860	0.78445	-0.61791

C	-7.55567	-0.45210	-0.59943
C	-6.78534	-1.60867	-0.62019
C	-5.40495	-1.54681	-0.65773
C	-9.04476	-0.51552	-0.57745
P	2.35876	-1.07781	0.00870
C	3.58238	-0.14986	-0.98329
C	3.28102	-1.84689	1.46365
C	1.55945	-2.31263	-1.15847
C	2.53330	-3.19447	-1.92989
C	0.59462	-3.19124	-0.37066
C	0.77140	-1.47706	-2.16555
C	4.09924	-3.09481	1.15650
C	2.26300	-2.20822	2.54583
C	4.19366	-0.75248	2.01211
C	3.45614	1.21632	-1.27833
C	4.46464	1.84133	-2.01065
C	5.57591	1.15468	-2.45458
C	5.69972	-0.19359	-2.17313
C	4.71295	-0.82923	-1.44845
C	2.32205	2.09469	-0.88672
C	1.21110	2.22722	-1.71361
C	0.22127	3.15223	-1.42030
C	0.33065	3.95479	-0.29612
C	1.43041	3.82605	0.53730
C	2.42315	2.90689	0.24034
H	-1.40383	2.52498	3.72827
H	0.28066	1.76973	3.77153
H	-1.61314	1.92943	0.13765
H	-5.03806	1.83143	-0.68793
H	-7.50223	1.69232	-0.60649
H	-7.27670	-2.57515	-0.61068
H	-4.80447	-2.44794	-0.68556
H	-9.45720	-0.17785	-1.53172
H	-9.45541	0.13867	0.19405
H	-9.40448	-1.52816	-0.39818
H	1.94916	-3.88040	-2.55048
H	3.16705	-3.80296	-1.28444
H	3.16784	-2.61600	-2.60209
H	-0.11331	-2.60285	0.21894
H	0.00815	-3.78590	-1.07675
H	1.11574	-3.88710	0.29018
H	0.26737	-2.15358	-2.86178
H	1.42499	-0.82491	-2.75075
H	-0.00058	-0.86796	-1.68920
H	3.47540	-3.92888	0.83079
H	4.87981	-2.92971	0.41494

H	4.60024	-3.40945	2.07684
H	1.53050	-2.94370	2.21008
H	2.79913	-2.64103	3.39539
H	1.72222	-1.33000	2.90806
H	3.64688	0.17749	2.20005
H	4.61063	-1.08820	2.96587
H	5.02496	-0.52880	1.34209
H	4.35662	2.89746	-2.23209
H	6.34154	1.67095	-3.02097
H	6.56203	-0.75236	-2.51555
H	4.83122	-1.88385	-1.24097
H	1.13379	1.61453	-2.60564
H	-0.63096	3.25150	-2.08288
H	-0.43381	4.69105	-0.07588
H	1.52456	4.45518	1.41457
H	3.29952	2.82323	0.87562
C	-2.82842	-0.69629	1.90490
H	-1.94735	-1.34424	1.97719
H	-2.97831	-0.18688	2.85505
H	-3.70570	-1.30289	1.68678
Au	0.64896	0.26833	0.94425

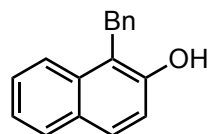


Naphthol 29

M06-2X/def2-TZVP Geometry

C	2.44977	0.48213	0.00000
C	2.50429	1.84703	0.00000
C	1.30744	2.59321	0.00000
C	0.09283	1.96462	0.00000
C	0.00000	0.54904	0.00000
C	1.20861	-0.19642	0.00000
C	1.13970	-1.60893	0.00000
C	-0.06688	-2.24006	0.00000
C	-1.26638	-1.49159	0.00000
C	-1.25841	-0.11842	0.00000
C	-2.54383	0.65814	0.00000
O	-2.46927	-2.13880	0.00000
H	-0.12089	-3.32353	0.00000
H	3.36016	-0.10591	0.00000
H	3.45846	2.35717	0.00000
H	1.35242	3.67481	0.00000
H	-0.81314	2.55541	0.00000

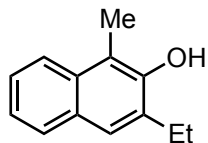
H	2.05846	-2.18253	0.00000
H	-3.39915	-0.01106	0.00000
H	-2.61120	1.30107	0.88016
H	-2.61120	1.30107	-0.88016
H	-2.32256	-3.08861	0.00000



Naphthol 30

M06-2X/def2-TZVP Geometry

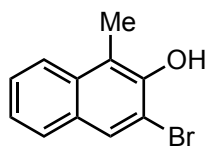
C	-3.83738	-0.34341	0.56548
C	-3.94623	-1.64907	0.17993
C	-2.86056	-2.27438	-0.46524
C	-1.70725	-1.58496	-0.72116
C	-1.56262	-0.22353	-0.34545
C	-2.65527	0.39414	0.32350
C	-2.53610	1.74024	0.74564
C	-1.38322	2.43369	0.54387
C	-0.29869	1.81688	-0.11595
C	-0.37751	0.52961	-0.59615
C	0.79659	-0.01710	-1.36955
O	0.81237	2.58839	-0.26784
H	-1.26174	3.45565	0.87707
H	-4.65788	0.15198	1.07127
H	-4.85412	-2.20508	0.37241
H	-2.93899	-3.31329	-0.75892
H	-0.88930	-2.10138	-1.20397
H	-3.37508	2.20595	1.24827
H	1.08186	0.71011	-2.13553
H	0.50862	-0.91446	-1.91497
H	1.59004	2.03495	-0.40925
C	4.25355	-0.90758	1.04914
C	2.98157	-1.24621	1.49467
C	1.86908	-0.95081	0.72242
C	2.01066	-0.32218	-0.51349
C	3.28876	0.01609	-0.94956
C	4.40499	-0.27303	-0.17405
H	5.12038	-1.13258	1.65648
H	2.85617	-1.73716	2.45114
H	0.87649	-1.20109	1.07947
H	3.41135	0.50839	-1.90838
H	5.39102	0.00042	-0.52683



Naphthol 31

M06-2X/def2-TZVP Geometry

C	1.73932	-1.97257	0.00000
C	3.07319	-1.67432	0.00000
C	3.48753	-0.32689	-0.00000
C	2.56652	0.68499	-0.00000
C	1.17629	0.40786	-0.00000
C	0.76487	-0.94790	0.00000
C	-0.61841	-1.24705	0.00000
C	-1.56395	-0.26331	0.00000
C	-1.12712	1.09488	-0.00000
C	0.19955	1.44410	-0.00000
C	0.61518	2.88757	-0.00000
O	-2.05188	2.10155	-0.00000
C	-3.04725	-0.54682	0.00000
H	1.40585	-3.00389	0.00000
H	3.81099	-2.46585	0.00000
H	4.54436	-0.09246	-0.00000
H	2.90315	1.71295	-0.00000
H	-0.91395	-2.28874	0.00000
H	1.21965	3.11808	0.87989
H	-0.25143	3.54163	0.00000
H	-2.93981	1.73549	0.00000
H	1.21965	3.11809	-0.87989
H	-3.49962	-0.06854	0.87747
H	-3.49962	-0.06854	-0.87747
C	-3.43032	-2.01898	0.00000
H	-4.51425	-2.12680	0.00000
H	-3.04117	-2.52663	-0.88303
H	-3.04117	-2.52663	0.88303

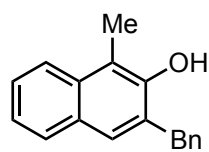


Naphthol 32

M06-2X/def2-TZVP Geometry

C	2.26323	-1.97796	-0.00000
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C	3.59488	-1.67616	0.00000
C	4.00693	-0.32693	0.00000
C	3.08656	0.68417	0.00000
C	1.69537	0.40717	0.00000
C	1.28864	-0.95190	-0.00000
C	-0.09082	-1.25585	-0.00000
C	-1.00195	-0.24701	-0.00000
C	-0.61177	1.11825	0.00000
C	0.72423	1.44707	0.00000
C	1.14417	2.88941	0.00000
O	-1.53044	2.11257	0.00000
Br	-2.85848	-0.65524	-0.00000
H	1.93044	-3.00908	-0.00000
H	4.33421	-2.46604	0.00000
H	5.06339	-0.09145	0.00000
H	3.42299	1.71187	0.00000
H	-0.41519	-2.28794	-0.00000
H	1.74866	3.11671	0.88041
H	0.27925	3.54538	-0.00000
H	-2.41886	1.73518	0.00000
H	1.74866	3.11671	-0.88041

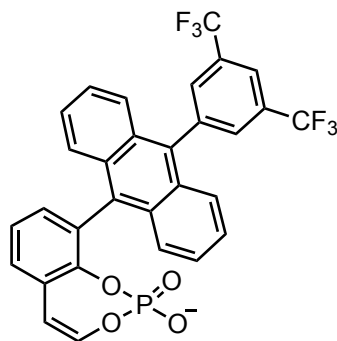


Naphthol 33

M06-2X/def2-TZVP Geometry

C	3.21571	-1.88923	-0.09570
C	4.44984	-1.52163	0.36214
C	4.70008	-0.17377	0.69072
C	3.71841	0.76996	0.55694
C	2.42737	0.42083	0.08702
C	2.18242	-0.93557	-0.24415
C	0.90322	-1.30069	-0.72494
C	-0.09277	-0.38088	-0.87683
C	0.16359	0.97524	-0.51753
C	1.38752	1.38572	-0.04984
C	1.62821	2.82387	0.31006
O	-0.81566	1.91389	-0.68061
H	3.00885	-2.92115	-0.35461
H	5.23487	-2.25823	0.47172
H	5.67903	0.11565	1.05084
H	3.93014	1.79959	0.81166

H	0.72155	-2.33662	-0.99048
H	1.95964	2.91411	1.34653
H	0.72228	3.40914	0.18604
H	-1.68741	1.50517	-0.62031
H	2.40714	3.25869	-0.32024
C	-1.44228	-0.76513	-1.42505
H	-1.64566	-0.19053	-2.33342
H	-1.40899	-1.81562	-1.72185
C	-4.72073	-0.20552	1.32133
C	-3.50435	-0.69815	1.77663
C	-2.44686	-0.87067	0.89643
C	-2.59052	-0.56054	-0.45477
C	-3.81227	-0.06112	-0.89980
C	-4.87217	0.11469	-0.01946
H	-5.54344	-0.06643	2.01029
H	-3.37740	-0.94402	2.82302
H	-1.49440	-1.24217	1.25624
H	-3.93328	0.19174	-1.94728
H	-5.81415	0.50497	-0.38249

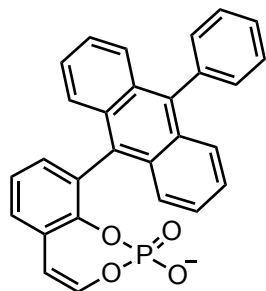


9-Anthryl-3,5-(CF₃)₂-C₆H₃

M06-2X/def2-TZVP Geometry

C	-5.81327	-2.12872	0.48174
C	-5.47735	-0.96139	-0.19425
C	-4.13557	-0.55695	-0.19742
C	-3.14354	-1.31902	0.41101
C	-3.51902	-2.47897	1.09028
C	-4.84751	-2.86592	1.15478
C	-6.39869	-0.35237	-1.16353
C	-6.70744	0.94412	-1.28435
O	-3.84082	0.64226	-0.76886
O	-6.02537	2.00505	-0.85394
P	-4.54801	1.99479	-0.08322
O	-4.81168	1.68660	1.33647

O	-3.81892	3.15830	-0.58857
C	-1.70051	-0.96398	0.29780
C	-1.13930	0.04236	1.09581
C	-0.89204	-1.67995	-0.59852
C	-1.94623	0.79956	1.99738
C	0.26377	0.32550	1.01551
C	0.51109	-1.39680	-0.68801
C	-1.43788	-2.68451	-1.45903
C	-1.40205	1.77865	2.76484
C	0.79779	1.33783	1.87232
C	1.06849	-0.40129	0.12557
C	1.29148	-2.13137	-1.63733
C	-0.65820	-3.36492	-2.33815
C	-0.00886	2.04076	2.71057
C	0.73083	-3.08226	-2.42817
C	2.52264	-0.10478	0.03700
C	3.46496	-1.00922	0.50987
C	4.82379	-0.72981	0.41821
C	5.26867	0.45276	-0.14170
C	4.32737	1.35929	-0.61325
C	2.97215	1.09058	-0.52780
C	4.81402	2.66096	-1.18514
C	5.80182	-1.75551	0.91479
F	5.17585	3.51883	-0.21829
F	5.89581	2.48682	-1.95953
F	3.88940	3.27183	-1.92527
F	5.80367	-2.85177	0.14144
F	7.05740	-1.29414	0.93842
F	5.50783	-2.16552	2.15495
H	-6.84338	-2.46560	0.46444
H	-2.74947	-3.07356	1.56830
H	-5.12530	-3.76020	1.69781
H	-7.11325	-1.03387	-1.61127
H	-7.54938	1.23892	-1.90367
H	-3.01414	0.62683	2.03016
H	-2.49905	-2.88461	-1.40386
H	-2.04205	2.36843	3.40733
H	1.85930	1.54458	1.85048
H	2.34633	-1.91176	-1.73348
H	-1.09602	-4.11461	-2.98455
H	0.41558	2.81232	3.34121
H	1.34246	-3.61962	-3.14208
H	3.13109	-1.94095	0.95124
H	6.32576	0.66788	-0.21491
H	2.24777	1.80417	-0.89990

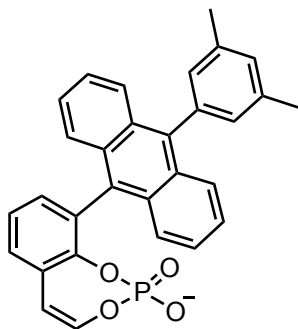


9-Anthryl-Ph

M06-2X/def2-TZVP Geometry

C	-4.28785	-1.10927	1.93767
C	-4.01169	-0.78535	0.61364
C	-2.67848	-0.57205	0.23327
C	-1.64527	-0.63640	1.16907
C	-1.95908	-0.93495	2.49191
C	-3.27154	-1.16620	2.88005
C	-5.03568	-0.81693	-0.44331
C	-5.21681	0.25043	-1.21904
O	-2.41364	-0.29168	-1.06174
O	-4.38485	1.30943	-1.16466
P	-2.79957	1.21039	-1.67970
O	-2.08486	2.23568	-0.90231
O	-2.77331	1.05572	-3.13870
C	-0.22540	-0.42558	0.77085
C	0.50350	-1.48500	0.21331
C	0.39799	0.80626	1.00526
C	-0.10830	-2.74696	-0.06306
C	1.89176	-1.31665	-0.09904
C	1.79435	0.96748	0.72377
C	-0.33391	1.92436	1.51294
C	0.59542	-3.76679	-0.61840
C	2.59118	-2.41433	-0.69391
C	2.52286	-0.09474	0.17124
C	2.40783	2.22228	1.03525
C	0.28503	3.10229	1.77642
C	1.96808	-3.59522	-0.94285
C	1.68012	3.24660	1.55008
C	3.96708	0.08065	-0.14574
C	4.95083	-0.50111	0.65104
C	6.29637	-0.33777	0.35111
C	6.67768	0.41169	-0.75354
C	5.70531	0.99594	-1.55431
C	4.36073	0.83154	-1.25186
H	-5.31396	-1.30666	2.22618

H	-1.15621	-0.98172	3.21824
H	-3.49800	-1.39854	3.91288
H	-5.75562	-1.62509	-0.46359
H	-6.01271	0.31976	-1.95473
H	-1.15794	-2.86993	0.16759
H	-1.40338	1.82802	1.62982
H	0.10840	-4.71017	-0.82986
H	3.63302	-2.28671	-0.95608
H	3.46710	2.34555	0.85387
H	-0.29068	3.94612	2.13311
H	2.51592	-4.40952	-1.40076
H	2.16290	4.18998	1.77484
H	4.64900	-1.08723	1.51086
H	7.04797	-0.79542	0.98229
H	7.72661	0.53966	-0.98925
H	5.99329	1.58041	-2.41910
H	3.59838	1.28698	-1.87240



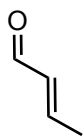
9-Anthryl-3,5-Me-C₆H₃

M06-2X/def2-TZVP Geometry

C	4.67265	1.95617	1.08855
C	4.37828	1.02469	0.09955
C	3.05104	0.59578	-0.03814
C	2.03013	1.11814	0.75008
C	2.36580	2.04218	1.74082
C	3.68003	2.43566	1.93322
C	5.32353	0.75394	-0.99275
C	5.67803	-0.44032	-1.48154
O	2.80174	-0.39576	-0.93699
O	5.03317	-1.60246	-1.38690
P	3.55201	-1.86455	-0.66554
O	3.80193	-1.97796	0.78503
O	2.86924	-2.85416	-1.50000
C	0.59852	0.77129	0.52094
C	0.06282	-0.43724	0.98640

C	-0.22914	1.69421	-0.13646
C	0.88548	-1.40388	1.64034
C	-1.33104	-0.72196	0.80820
C	-1.62302	1.40916	-0.31945
C	0.28440	2.92314	-0.66069
C	0.36395	-2.57691	2.08268
C	-1.84057	-1.95707	1.31811
C	-2.15712	0.20599	0.15844
C	-2.42875	2.36794	-1.01299
C	-0.51756	3.80776	-1.30769
C	-1.02057	-2.85143	1.92972
C	-1.89911	3.52555	-1.48567
C	-3.60215	-0.09676	-0.03952
C	-4.57191	0.50571	0.75912
C	-5.92198	0.22879	0.58297
C	-6.29532	-0.66434	-0.41862
C	-5.35021	-1.27919	-1.23093
C	-4.00370	-0.98709	-1.02834
C	-6.95811	0.85513	1.47688
C	-5.76117	-2.23140	-2.32111
H	5.69093	2.31594	1.18241
H	1.57426	2.44847	2.35945
H	3.92506	3.14250	2.71577
H	6.01457	1.55953	-1.21448
H	6.53128	-0.51337	-2.14962
H	1.94792	-1.22144	1.73710
H	1.33893	3.13105	-0.54128
H	1.01677	-3.31072	2.53663
H	-2.89452	-2.17306	1.20493
H	-3.47748	2.14974	-1.16553
H	-0.10285	4.72672	-1.70232
H	-1.42427	-3.78678	2.29821
H	-2.52759	4.23349	-2.01181
H	-4.25822	1.20277	1.52866
H	-7.34785	-0.88447	-0.56761
H	-3.24799	-1.45894	-1.64725
H	-6.62265	1.82322	1.84835
H	-7.90153	0.99651	0.94877
H	-7.15641	0.21983	2.34336
H	-5.20031	-3.16466	-2.25495
H	-6.82404	-2.46445	-2.26234
H	-5.56208	-1.80289	-3.30540

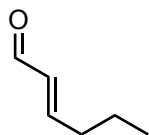
Cartesian coordinates of reaction components relevant to secondary amine catalysis



Carbonyl 1

M06-2X/def2-TZVP Geometry

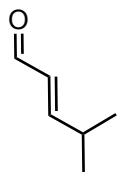
C	2.41641	-0.16193	-0.00000
C	1.03252	0.38970	-0.00000
C	-0.08691	-0.32977	-0.00000
C	-1.39907	0.33121	0.00000
O	-2.45235	-0.24995	0.00000
H	2.96630	0.18771	0.87644
H	2.41221	-1.25048	-0.00000
H	2.96630	0.18771	-0.87644
H	0.94032	1.47431	0.00000
H	-0.08178	-1.41435	-0.00000
H	-1.36230	1.43943	-0.00000



Carbonyl 2

M06-2X/def2-TZVP Geometry

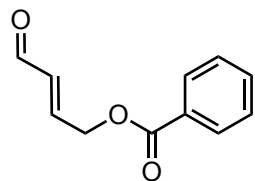
C	-1.21212	0.86488	0.00001
C	0.27982	0.92963	0.00000
C	1.12099	-0.10267	-0.00000
C	2.57214	0.12765	-0.00000
O	3.39918	-0.74609	-0.00001
C	-1.81271	-0.53309	-0.00000
H	-1.57688	1.42542	0.86887
H	-1.57689	1.42543	-0.86885
H	0.71059	1.92970	0.00001
H	0.79206	-1.13504	-0.00001
H	2.87449	1.19457	0.00000
C	-3.33529	-0.49628	0.00000
H	-1.45560	-1.08037	-0.87608
H	-1.45559	-1.08038	0.87607
H	-3.75626	-1.50133	-0.00000
H	-3.71319	0.02500	0.88144
H	-3.71319	0.02501	-0.88143



Carbonyl 3

M06-2X/def2-TZVP Geometry

C	-1.53323	-0.04218	-0.40727
C	-0.10080	-0.47952	-0.40165
C	0.95717	0.23318	-0.02003
C	2.30105	-0.36098	-0.05682
O	3.30620	0.21244	0.27209
C	-2.35974	-1.00072	0.45782
C	-1.73095	1.40210	0.03008
H	-1.88634	-0.14702	-1.44029
H	0.07351	-1.50314	-0.73279
H	0.88824	1.25734	0.32686
H	2.33820	-1.40844	-0.41865
H	-2.24004	-2.03533	0.13396
H	-2.04557	-0.93271	1.50103
H	-3.41857	-0.74643	0.40250
H	-2.78564	1.67193	-0.02618
H	-1.40482	1.53963	1.06331
H	-1.16951	2.09333	-0.59921

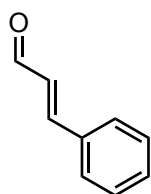


Carbonyl 4

M06-2X/def2-TZVP Geometry

C	-1.58709	-1.69284	0.00001
C	-2.89474	-0.98658	0.00001
C	-3.07535	0.32964	0.00001
C	-4.43719	0.88652	0.00001
O	-4.68468	2.06273	0.00000
O	-0.53134	-0.74468	0.00000
H	-1.50101	-2.34173	-0.87642
H	-3.76369	-1.64055	0.00002
H	-2.24990	1.02961	-0.00000
H	-5.25118	0.13385	0.00002
H	-1.50100	-2.34173	0.87644
C	0.70923	-1.26751	0.00001

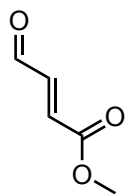
O	0.91205	-2.45109	0.00002
C	3.82012	1.63789	-0.00002
C	4.11850	0.28081	-0.00001
C	3.09468	-0.65157	0.00000
C	1.77006	-0.22555	-0.00000
C	1.47040	1.13330	-0.00002
C	2.49838	2.06326	-0.00003
H	4.62074	2.36632	-0.00003
H	5.14912	-0.04823	-0.00000
H	3.29949	-1.71388	0.00001
H	0.43890	1.45614	-0.00002
H	2.26827	3.12035	-0.00003



Carbonyl 5

M06-2X/def2-TZVP Geometry

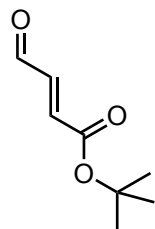
C	-0.93462	-0.58745	0.00006
C	-1.97789	0.24678	0.00004
C	-3.34379	-0.28799	0.00012
O	-4.33780	0.39081	0.00012
H	-1.14957	-1.65434	0.00013
H	-1.88298	1.32573	-0.00003
H	-3.41186	-1.39446	0.00018
C	3.22242	0.32711	-0.00012
C	2.29272	1.36178	-0.00008
C	0.93848	1.08212	-0.00002
C	0.48674	-0.24077	0.00000
C	1.43017	-1.26904	-0.00004
C	2.78821	-0.98979	-0.00010
H	4.28127	0.55031	-0.00017
H	2.62877	2.39037	-0.00009
H	0.22640	1.89677	0.00002
H	1.08988	-2.29779	-0.00002
H	3.50583	-1.79958	-0.00014



Carbonyl 6

M06-2X/def2-TZVP Geometry

C	-0.32987	-0.48556	-0.00000
C	-1.44372	0.23688	-0.00004
C	-2.76582	-0.42325	-0.00006
O	-3.80563	0.17611	-0.00009
H	-0.35071	-1.56941	0.00001
H	-1.41373	1.32057	-0.00005
H	-2.74119	-1.52999	-0.00005
C	1.00581	0.16924	0.00002
O	1.19057	1.35454	0.00001
O	1.98378	-0.74163	0.00006
C	3.30843	-0.20935	0.00008
H	3.97350	-1.06691	0.00010
H	3.46670	0.40291	-0.88633
H	3.46666	0.40292	0.88649

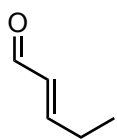


Carbonyl 7

M06-2X/def2-TZVP Geometry

C	-1.42774	0.45949	-0.00008
C	-2.57768	-0.20403	-0.00026
C	-3.86309	0.52332	-0.00029
O	-4.93378	-0.01965	-0.00045
H	-1.39399	1.54301	0.00004
H	-2.60285	-1.28782	-0.00037
H	-3.78036	1.62741	-0.00017
C	-0.12348	-0.26543	-0.00003
O	-0.02630	-1.46283	-0.00015
O	0.88534	0.60377	0.00014
C	2.27412	0.14859	0.00022
C	2.55939	-0.65012	-1.26396

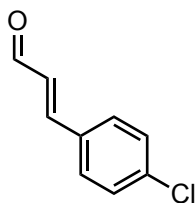
H	3.63001	-0.85103	-1.32046
H	2.02497	-1.59676	-1.26644
H	2.27374	-0.07343	-2.14483
C	2.55917	-0.65038	1.26428
H	2.27336	-0.07386	2.14522
H	2.02476	-1.59702	1.26648
H	3.62978	-0.85128	1.32093
C	3.05840	1.45089	0.00042
H	2.81817	2.03912	0.88622
H	4.12736	1.23810	0.00049
H	2.81832	2.03930	-0.88531



Carbonyl 8

M06-2X/def2-TZVP Geometry

C	0.42529	0.80619	0.00001
C	-0.52128	-0.13023	-0.00000
C	-1.93998	0.25253	-0.00000
O	-2.85459	-0.52898	-0.00002
H	0.10546	1.84694	0.00003
H	-0.30351	-1.19168	-0.00002
H	-2.12792	1.34539	0.00002
C	1.90204	0.58031	0.00001
H	2.32122	1.09909	-0.86846
H	2.32121	1.09907	0.86851
C	2.33205	-0.87790	-0.00001
H	3.41834	-0.95656	-0.00001
H	1.95662	-1.39789	0.88219
H	1.95662	-1.39786	-0.88222

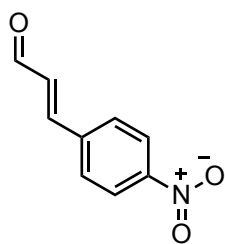


Carbonyl 9

M06-2X/def2-TZVP Geometry

C	-1.89438	0.60050	-0.00007
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C	-2.88335	-0.29723	0.00003
C	-4.28070	0.15112	0.00001
O	-5.22871	-0.58994	0.00012
H	-2.17472	1.65193	-0.00016
H	-2.72206	-1.36835	0.00014
H	-4.41864	1.25093	-0.00012
C	2.29867	-0.05394	-0.00001
C	1.44644	-1.15159	0.00005
C	0.08010	-0.94888	0.00003
C	-0.45536	0.34246	-0.00005
C	0.42520	1.42472	-0.00011
C	1.79739	1.23724	-0.00009
H	-0.57644	-1.80872	0.00007
H	0.02739	2.43235	-0.00017
H	2.47562	2.07897	-0.00013
Cl	4.00910	-0.30550	0.00003
H	1.85981	-2.15056	0.00011

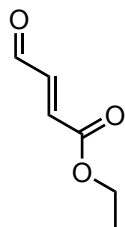


Carbonyl 10

M06-2X/def2-TZVP Geometry

C	2.18706	0.61427	-0.00001
C	3.16417	-0.29422	0.00003
C	4.57063	0.13704	0.00007
O	5.50330	-0.62101	0.00019
H	2.47519	1.66313	-0.00003
H	2.99204	-1.36363	0.00006
H	4.72556	1.23399	-0.00000
C	-1.98872	-0.01199	-0.00003
C	-1.16079	-1.12269	-0.00000
C	0.20605	-0.92728	0.00000
C	0.74374	0.36396	-0.00002
C	-0.12536	1.45687	-0.00006
C	-1.49805	1.27918	-0.00006
H	0.85985	-1.78838	0.00003
H	0.28275	2.45970	-0.00008
H	-2.18303	2.11406	-0.00009
H	-1.59438	-2.11177	0.00002
N	-3.45032	-0.21635	-0.00004
O	-4.15031	0.76953	-0.00004

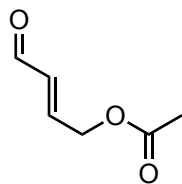
O -3.85275 -1.35646 -0.00004



Carbonyl 11

M06-2X/def2-TZVP Geometry

C	-0.80965	-0.39341	-0.00004
C	-1.99521	0.20413	-0.00005
C	-3.23782	-0.59507	-0.00013
O	-4.33681	-0.11243	-0.00014
H	-0.71361	-1.47326	-0.00010
H	-2.08234	1.28473	0.00000
H	-3.09328	-1.69268	-0.00018
C	0.44845	0.40179	0.00003
O	0.50034	1.60073	0.00009
O	1.51824	-0.39753	0.00003
C	2.79143	0.26704	0.00009
H	2.84664	0.90795	0.88091
H	2.84669	0.90802	-0.88067
C	3.86020	-0.79726	0.00008
H	4.84442	-0.32951	0.00013
H	3.77645	-1.42740	0.88486
H	3.77650	-1.42733	-0.88474

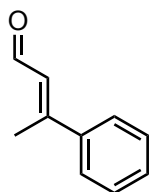


Carbonyl 12

M06-2X/def2-TZVP Geometry

C	0.74483	-0.80684	-0.13181
C	1.79577	-0.14988	0.34719
C	2.96677	0.12582	-0.50574
O	3.94778	0.70443	-0.12456
H	0.73918	-1.13736	-1.16813
H	1.84380	0.20660	1.37133
H	2.88455	-0.23966	-1.54792
O	-1.66070	-0.96185	-0.07393
C	-2.22368	0.26953	-0.18127

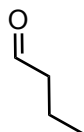
O	-3.15686	0.40373	-0.91095
C	-0.46666	-1.17069	0.66643
H	-0.45395	-2.24201	0.87456
H	-0.48218	-0.64533	1.62243
C	-1.65194	1.38371	0.65860
H	-2.18040	2.29540	0.40100
H	-1.79925	1.17054	1.71846
H	-0.58410	1.51144	0.48336



Carbonyl 13

M06-2X/def2-TZVP Geometry

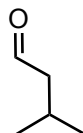
C	0.83795	0.51247	0.12717
C	1.77889	-0.41044	-0.13017
C	3.22926	-0.20367	-0.07967
O	4.01940	-1.07643	-0.34445
H	1.49352	-1.41255	-0.42795
H	3.59615	0.79437	0.21335
C	-3.30710	-0.54584	-0.10817
C	-2.36768	-1.48754	0.29079
C	-1.02807	-1.14579	0.37009
C	-0.59768	0.14522	0.05369
C	-1.55615	1.08783	-0.32372
C	-2.89624	0.74303	-0.41418
H	-4.35372	-0.81339	-0.17087
H	-2.68086	-2.49050	0.54992
H	-0.30889	-1.87980	0.70909
H	-1.25512	2.09818	-0.56672
H	-3.62098	1.48523	-0.72254
C	1.13706	1.94693	0.46814
H	0.50417	2.27616	1.29276
H	2.17411	2.11036	0.74109
H	0.91487	2.59021	-0.38628



Carbonyl 14

M06-2X/def2-TZVP Geometry

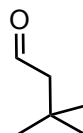
C	0.09436	0.74489	0.00001
C	-0.82502	-0.46422	0.00029
C	1.55824	0.40367	0.00052
O	1.99393	-0.71386	-0.00028
C	-2.29500	-0.06587	-0.00020
H	-0.08813	1.38741	-0.87011
H	-0.08850	1.38811	0.86953
H	-0.59788	-1.08223	-0.87015
H	-0.59827	-1.08152	0.87134
H	2.24914	1.27056	-0.00109
H	-2.94242	-0.94253	0.00002
H	-2.54061	0.53051	0.88068
H	-2.54022	0.52979	-0.88167



Carbonyl 15

M06-2X/def2-TZVP Geometry

C	-0.30105	-0.84502	0.40766
C	0.72625	0.04054	-0.28689
C	-1.73518	-0.44180	0.19881
O	-2.10113	0.43139	-0.53810
C	2.09733	-0.62723	-0.27017
H	-0.11916	-0.88750	1.48893
H	-0.22747	-1.88511	0.06459
H	0.40454	0.16675	-1.32410
C	0.78723	1.41890	0.36530
H	-2.47834	-1.03184	0.77206
H	2.07733	-1.59728	-0.76997
H	2.43503	-0.78517	0.75763
H	2.83943	-0.00413	-0.77109
H	1.50826	2.05675	-0.14774
H	-0.18271	1.91371	0.33795
H	1.10462	1.33041	1.40825

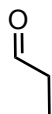


Carbonyl 16

M06-2X/def2-TZVP Geometry

C	-0.40515	1.04688	-0.00002
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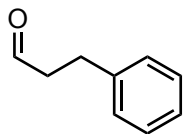
C	0.69955	-0.01434	-0.00003
C	-1.83950	0.59219	0.00006
O	-2.22845	-0.54284	0.00011
C	0.60721	-0.88593	1.25455
H	-0.29862	1.70921	-0.86949
H	-0.29856	1.70926	0.86942
C	0.60718	-0.88593	-1.25460
C	2.04338	0.71842	-0.00005
H	-2.57320	1.42476	0.00005
H	-0.32269	-1.45175	1.27533
H	0.66287	-0.27277	2.15764
H	1.44033	-1.59144	1.27962
H	2.86675	0.00160	-0.00005
H	2.14716	1.35106	-0.88474
H	2.14718	1.35107	0.88464
H	1.44031	-1.59144	-1.27970
H	-0.32272	-1.45177	-1.27536
H	0.66281	-0.27278	-2.15770



Carbonyl 17

M06-2X/def2-TZVP Geometry

C	0.54453	0.73360	0.00006
C	1.42491	-0.50264	0.00002
C	-0.92592	0.42155	-0.00012
O	-1.38259	-0.68757	-0.00001
H	0.73548	1.37233	-0.86933
H	0.73530	1.37213	0.86963
H	-1.59970	1.30134	0.00003
H	1.22507	-1.11632	-0.87731
H	1.22489	-1.11650	0.87718
H	2.47861	-0.22748	0.00016

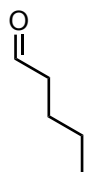


Carbonyl 18

M06-2X/def2-TZVP Geometry

C	1.81424	-0.00003	0.73104
C	1.03276	0.00004	-0.57842
C	3.30495	-0.00003	0.54121

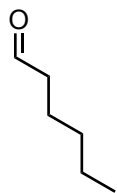
O	3.85039	0.00002	-0.52705
H	1.55715	-0.86996	1.34624
H	1.55716	0.86985	1.34632
H	3.90321	-0.00008	1.47411
H	1.32192	-0.87391	-1.16399
H	1.32192	0.87406	-1.16390
C	-3.19486	-0.00002	0.22092
C	-2.51032	1.19949	0.08237
C	-1.14990	1.19657	-0.19123
C	-0.45192	0.00002	-0.33136
C	-1.14987	-1.19655	-0.19129
C	-2.51029	-1.19951	0.08231
H	-4.25650	-0.00004	0.43035
H	-3.03769	2.13952	0.18248
H	-0.62065	2.13621	-0.30540
H	-0.62060	-2.13617	-0.30551
H	-3.03764	-2.13956	0.18238



Carbonyl 19

M06-2X/def2-TZVP Geometry

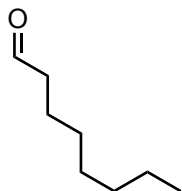
C	-1.02609	1.03921	0.07811
C	0.35036	0.70925	-0.47754
C	-1.94969	-0.14501	0.17816
O	-1.69652	-1.24460	-0.22914
C	1.21906	-0.06670	0.50737
H	-1.54927	1.77794	-0.54044
H	-0.96256	1.49262	1.07405
H	0.23163	0.12330	-1.39227
H	0.85818	1.63641	-0.75516
H	-2.93001	0.05945	0.65346
H	0.70296	-0.98543	0.79310
C	2.58511	-0.40402	-0.07481
H	1.34268	0.52605	1.41913
H	2.48139	-1.02364	-0.96725
H	3.12329	0.50239	-0.35984
H	3.20141	-0.94861	0.64064



Carbonyl 20

M06-2X/def2-TZVP Geometry

C	1.71210	-0.91578	0.29957
C	0.37744	-0.94595	-0.42881
C	2.41032	0.41659	0.25050
O	2.03346	1.36197	-0.38460
H	1.60423	-1.19301	1.35451
H	2.42023	-1.64187	-0.11701
H	3.34455	0.48234	0.84348
H	0.50972	-0.51907	-1.42592
H	0.06546	-1.98454	-0.56383
C	-0.71756	-0.18026	0.30585
H	-0.85761	-0.61539	1.30196
C	-2.04657	-0.19401	-0.43883
H	-0.39777	0.85445	0.45475
C	-3.14141	0.55943	0.30515
H	-2.35766	-1.23007	-0.60384
H	-1.90363	0.24643	-1.42957
H	-2.85957	1.60316	0.45554
H	-4.08396	0.54248	-0.24252
H	-3.31757	0.11917	1.28863

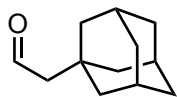


Carbonyl 21

M06-2X/def2-TZVP Geometry

C	2.98264	-0.74533	0.36427
C	1.66068	-0.98889	-0.34694
C	3.51043	0.65668	0.21955
O	3.01820	1.50344	-0.47317
H	2.91179	-0.96217	1.43634
H	3.77457	-1.40477	-0.01015
H	4.43043	0.87703	0.79736
H	1.73683	-0.61586	-1.37111
H	1.47997	-2.06476	-0.41047

C	0.48051	-0.31758	0.34744
H	0.39778	-0.70108	1.37062
C	-0.83708	-0.54366	-0.38253
H	0.67106	0.75584	0.42591
C	-2.02541	0.11024	0.31064
H	-1.02071	-1.61946	-0.47900
H	-0.75361	-0.15372	-1.40227
H	-2.11039	-0.27903	1.33119
H	-1.84034	1.18529	0.40837
C	-3.34388	-0.10832	-0.42135
C	-4.52265	0.55119	0.28272
H	-3.25724	0.28180	-1.43963
H	-3.52651	-1.18256	-0.51934
H	-5.45668	0.38544	-0.25478
H	-4.64284	0.15542	1.29313
H	-4.37108	1.62909	0.36641

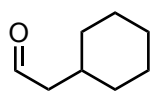


Carbonyl 22

M06-2X/def2-TZVP Geometry

C	2.03325	1.08440	0.00001
C	3.20816	0.14380	-0.00000
O	3.16553	-1.05537	-0.00000
H	2.17351	1.74133	-0.86947
H	2.17351	1.74127	0.86953
H	4.19172	0.65812	-0.00006
C	-1.07042	-0.88062	-1.25341
C	0.36927	-0.35354	-1.25407
C	0.62403	0.50119	-0.00001
C	-0.37930	1.66899	0.00034
C	-1.82050	1.15077	0.00036
C	-2.05135	0.29628	-1.25100
H	0.54255	0.25632	-2.14824
H	1.07275	-1.18724	-1.28019
H	-0.20758	2.29624	0.88221
H	-0.20774	2.29664	-0.88127
C	-2.05112	0.29571	1.25137
H	-2.50996	1.99856	0.00062
H	-1.91024	0.90342	-2.15025
H	-3.08096	-0.07301	-1.26559
H	-3.08073	-0.07358	1.26598
C	-1.07019	-0.88119	1.25306
H	-1.90984	0.90243	2.15088
H	-1.22950	-1.49120	2.14534

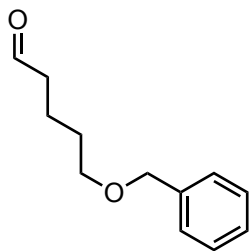
C	-1.29567	-1.73529	-0.00035
C	0.36949	-0.35412	1.25370
H	-1.22990	-1.49022	-2.14594
H	-2.31353	-2.13634	-0.00035
H	-0.60810	-2.58565	-0.00061
H	1.07299	-1.18782	1.27931
H	0.54294	0.25534	2.14812



Carbonyl 23

M06-2X/def2-TZVP Geometry

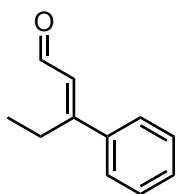
C	1.59121	0.88143	0.45456
C	2.81196	0.08671	0.07841
O	2.82281	-0.82669	-0.69945
H	1.78712	1.90969	0.12297
H	1.55303	0.93762	1.54948
H	3.75389	0.41331	0.56346
C	-2.15711	0.88599	-0.52808
C	-0.83050	1.39828	0.02670
C	0.28182	0.35845	-0.11604
C	-0.13316	-0.95616	0.54933
C	-1.45705	-1.47342	-0.00734
C	-2.56140	-0.42908	0.13422
H	-2.05451	0.72682	-1.60680
H	-2.93752	1.63739	-0.39236
H	-0.95277	1.64181	1.08946
H	-0.54140	2.32451	-0.47743
H	0.43634	0.15927	-1.18261
H	0.65256	-1.70134	0.41753
H	-0.24098	-0.78101	1.62744
H	-1.32645	-1.71942	-1.06634
H	-1.74062	-2.39851	0.49827
H	-2.75192	-0.25058	1.19826
H	-3.49391	-0.79927	-0.29627



Carbonyl 24

M06-2X/def2-TZVP Geometry

C	2.30402	1.23097	1.07796
C	1.46594	1.86586	-0.04040
O	1.83781	1.86975	-1.21382
H	1.63124	0.69348	1.74576
H	2.71335	2.05679	1.65810
H	0.52917	2.31928	0.28463
C	3.45963	0.29774	0.63190
C	3.07207	-1.18728	0.42701
H	3.93752	0.68099	-0.27272
H	4.24201	0.34101	1.39129
C	1.99061	-1.46395	-0.63002
H	2.75405	-1.61998	1.37635
H	3.97045	-1.73586	0.14270
O	0.72777	-1.10342	-0.08905
H	2.21614	-0.90995	-1.54383
H	1.97862	-2.52499	-0.88568
C	-0.33378	-1.11968	-1.03744
H	-0.52867	-2.13868	-1.37565
H	-0.06455	-0.51848	-1.90906
C	-3.93067	0.48056	0.71281
C	-3.66412	0.69105	-0.63859
C	-2.50001	0.17324	-1.20123
C	-1.60221	-0.55130	-0.41113
C	-1.87975	-0.76076	0.94382
C	-3.04368	-0.24348	1.50683
H	-4.83423	0.88177	1.14908
H	-4.35728	1.25317	-1.24792
H	-2.29600	0.33943	-2.24951
H	-1.18827	-1.32209	1.55660
H	-3.25655	-0.40432	2.55374

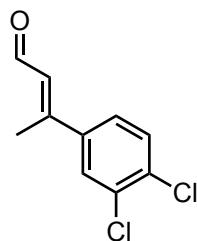


Carbonyl 25

M06-2X/def2-TZVP Geometry

C	-1.65413	-0.77232	-0.21584
C	-3.11569	-0.65207	-0.21498
O	-3.84755	-1.61133	-0.21634
H	-3.54569	0.36400	-0.20184
C	-0.77810	0.24524	-0.21673
C	-1.16219	1.70189	-0.23806
H	-1.29651	-1.79608	-0.21486

C	3.40708	-0.64225	0.02385
C	2.95720	0.35929	-0.82482
C	1.60541	0.65894	-0.89672
C	0.67549	-0.05112	-0.13544
C	1.14218	-1.05355	0.71707
C	2.49458	-1.34556	0.79774
H	4.46313	-0.87008	0.08510
H	3.66110	0.90993	-1.43518
H	1.27359	1.43536	-1.57330
H	0.43584	-1.59014	1.33763
H	2.83680	-2.12007	1.47172
C	-0.87720	2.37005	1.10944
H	-0.58754	2.20776	-1.01630
H	-2.20853	1.82923	-0.50340
H	-1.47018	1.90579	1.89833
H	0.17542	2.27312	1.37699
H	-1.12476	3.43058	1.07267

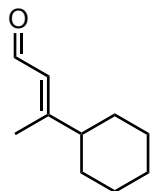


Carbonyl 26

M06-2X/def2-TZVP Geometry

C	-3.11345	-0.41385	-0.19058
C	-4.55678	-0.14718	-0.18995
O	-5.36181	-0.95352	-0.58463
H	-4.90007	0.83023	0.18787
C	-2.15217	0.43194	0.21166
C	-2.40838	1.83413	0.69163
H	-2.85607	-1.39121	-0.58148
C	1.95735	-0.77795	0.06484
C	0.95765	-1.71869	0.27795
C	-0.36727	-1.33353	0.32858
C	-0.73183	0.00558	0.16796
C	0.27977	0.94331	-0.02321
C	1.61141	0.56081	-0.08452
Cl	3.59798	-1.28974	0.00709
H	1.23723	-2.75440	0.41288
H	-1.12471	-2.07980	0.52499
H	0.05008	1.99255	-0.14378
Cl	2.81414	1.76680	-0.34131

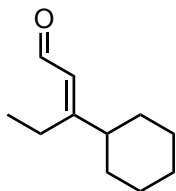
H	-2.10854	2.55465	-0.07282
H	-3.45225	2.01699	0.92231
H	-1.81503	2.04165	1.58268



Carbonyl 27

M06-2X/def2-TZVP Geometry

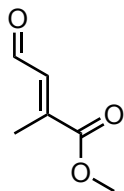
C	2.05699	-0.34446	-0.37004
C	3.47293	-0.10737	-0.07429
O	4.36486	-0.72459	-0.60343
H	3.71526	0.67663	0.66385
C	1.01523	0.29828	0.17542
C	1.13379	1.40087	1.18913
H	1.88503	-1.12075	-1.10873
H	0.40504	1.26217	1.98926
H	2.11945	1.47096	1.63779
H	0.90586	2.36021	0.71836
C	-2.64832	0.67358	-1.04576
C	-1.26095	1.12010	-0.59083
C	-0.38721	-0.08770	-0.22919
C	-1.07425	-0.92612	0.86195
C	-2.46642	-1.36791	0.41550
C	-3.33129	-0.17158	0.02673
H	-2.55407	0.08459	-1.96404
H	-3.25922	1.54444	-1.29045
H	-1.36817	1.76731	0.28581
H	-0.77228	1.71177	-1.36900
H	-0.30910	-0.72059	-1.11958
H	-0.45409	-1.79278	1.09976
H	-1.16373	-0.33250	1.77772
H	-2.36961	-2.03701	-0.44587
H	-2.94639	-1.94319	1.20941
H	-3.50650	0.44798	0.91299
H	-4.30934	-0.50863	-0.32148



Carbonyl 28

M06-2X/def2-TZVP Geometry

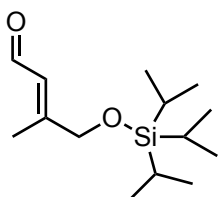
C	1.59212	-0.85421	-0.09632
C	3.03647	-0.92507	-0.33722
O	3.66000	-1.95790	-0.31656
H	3.56034	0.02692	-0.53887
C	0.87504	0.27744	-0.10088
C	1.48078	1.64385	-0.31873
H	1.13018	-1.81219	0.10908
H	0.71075	2.30898	-0.71468
C	2.01240	2.22165	0.99621
H	2.27832	1.61709	-1.05984
C	-2.65704	-0.76230	1.17309
C	-1.16014	-0.91804	0.91304
C	-0.61214	0.28752	0.15144
C	-1.37404	0.44544	-1.17813
C	-2.87542	0.58937	-0.93960
C	-3.42524	-0.58507	-0.13448
H	-2.82425	0.11116	1.81245
H	-3.03289	-1.62915	1.71944
H	-1.00186	-1.82481	0.32082
H	-0.61379	-1.04850	1.84980
H	-0.82308	1.18551	0.75003
H	-0.99621	1.30313	-1.73829
H	-1.17851	-0.44344	-1.78723
H	-3.06274	1.52026	-0.39375
H	-3.39700	0.67316	-1.89499
H	-3.33371	-1.50036	-0.72885
H	-4.48889	-0.44243	0.06507
H	1.23249	2.23477	1.75940
H	2.36736	3.24279	0.85720
H	2.83680	1.61695	1.37521



Carbonyl 29

M06-2X/def2-TZVP Geometry

C	1.17838	-0.41441	-0.00006
C	2.64614	-0.27061	-0.00010
O	3.38192	-1.22327	-0.00020
H	3.06093	0.75066	-0.00005
C	0.30625	0.59788	0.00003
C	0.61403	2.06211	0.00009
H	0.82430	-1.43741	-0.00010
H	0.15730	2.53142	-0.87204
H	1.67846	2.27096	0.00007
H	0.15735	2.53133	0.87229
C	-1.16767	0.30621	0.00007
O	-1.99950	1.17388	0.00014
O	-1.46136	-0.99489	-0.00001
C	-2.85467	-1.30292	0.00003
H	-3.33162	-0.88798	0.88657
H	-2.91831	-2.38634	-0.00004
H	-3.33168	-0.88787	-0.88644

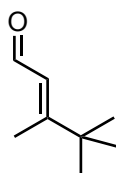


Carbonyl 30

M06-2X/def2-TZVP Geometry

C	-2.98805	-0.18783	-0.46104
C	-4.35724	-0.71177	-0.42117
O	-4.64995	-1.81272	-0.81703
H	-5.14120	-0.05568	-0.00402
C	-2.60686	1.01384	-0.02027
C	-3.48581	2.05972	0.59874
H	-2.24760	-0.85441	-0.88595
H	-4.54376	1.82419	0.55009
H	-3.32787	3.02030	0.10296
H	-3.21421	2.19669	1.64868
C	-1.16378	1.43723	-0.10414

H	-1.11511	2.34628	-0.71949
H	-0.84350	1.73468	0.90622
O	-0.33262	0.45535	-0.64385
Si	1.16954	0.01720	-0.07497
C	1.07463	-0.12047	1.80362
C	1.54814	-1.57681	-0.99344
C	2.42664	1.33677	-0.55825
C	2.38275	1.57182	-2.07264
C	2.22458	2.65696	0.19196
H	3.41900	0.94903	-0.29895
H	2.94508	3.40829	-0.14182
H	1.22732	3.06709	0.00867
H	2.34475	2.54149	1.27036
H	3.12081	2.31921	-2.37465
H	2.58213	0.65962	-2.63829
H	1.39832	1.93577	-2.37744
C	2.36038	-0.71724	2.38721
H	1.00065	0.91211	2.16734
C	-0.15881	-0.87480	2.31153
H	2.46584	-1.76620	2.10008
H	3.25423	-0.18853	2.04716
H	2.34807	-0.68012	3.47937
H	-0.23065	-0.80535	3.40022
H	-1.08775	-0.48705	1.88783
H	-0.10790	-1.93396	2.05640
C	0.72972	-2.77148	-0.49407
H	1.22327	-1.35821	-2.01865
C	3.04017	-1.92308	-1.03459
H	3.43475	-2.10882	-0.03283
H	3.20671	-2.83041	-1.62084
H	3.63746	-1.12667	-1.48148
H	0.83789	-3.62343	-1.16975
H	1.07571	-3.09455	0.49069
H	-0.33427	-2.54032	-0.41589

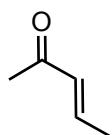


Carbonyl 31

M06-2X/def2-TZVP Geometry

C	-1.21277	-0.37247	-0.00121
C	-2.59450	0.12347	0.00311
O	-3.54938	-0.61418	-0.00863
H	-2.75085	1.21543	0.01019

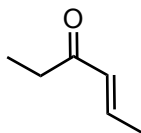
C	-0.10561	0.38278	0.00459
C	-0.14682	1.88924	0.00284
H	-1.15370	-1.45267	-0.02275
H	-1.09079	2.28960	0.35796
H	0.64524	2.30258	0.62610
H	0.01896	2.26420	-1.00979
C	1.28853	-0.23870	-0.00343
C	1.94561	-0.00627	1.36766
C	1.26228	-1.74392	-0.26764
C	2.14158	0.42896	-1.09267
H	3.12726	-0.03807	-1.12178
H	1.68049	0.31061	-2.07544
H	2.28469	1.49323	-0.90568
H	2.28548	-2.11980	-0.30999
H	0.74513	-2.28508	0.52555
H	0.77631	-1.97411	-1.21712
H	2.94139	-0.45376	1.37398
H	2.05882	1.05300	1.59799
H	1.35675	-0.47027	2.16029



Carbonyl 43

M06-2X/def2-TZVP Geometry

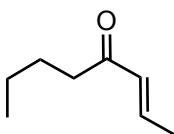
O	1.98134	-1.08067	-0.00002
C	1.14485	-0.20754	0.00001
C	-0.29378	-0.56636	-0.00002
C	1.53971	1.25151	0.00004
C	-1.29205	0.31223	0.00000
C	-2.74006	-0.04707	-0.00002
H	-0.48712	-1.63420	-0.00005
H	1.14056	1.75632	0.88106
H	2.62389	1.31877	0.00003
H	1.14055	1.75636	-0.88094
H	-1.06131	1.37404	0.00004
H	-3.23881	0.37198	-0.87667
H	-2.88173	-1.12653	-0.00006
H	-3.23883	0.37193	0.87664



Carbonyl 44

M06-2X/def2-TZVP Geometry

O	-0.68049	1.36132	0.00001
C	-0.52304	0.16341	0.00000
C	0.82914	-0.46109	-0.00000
C	-1.69268	-0.79673	-0.00000
C	1.93081	0.28166	-0.00000
C	3.32443	-0.24479	-0.00001
H	0.88379	-1.54533	-0.00001
H	-1.57625	-1.45145	0.87041
C	-3.04029	-0.10074	0.00000
H	-1.57625	-1.45144	-0.87042
H	1.79876	1.36066	0.00001
H	3.86802	0.11649	0.87585
H	3.34457	-1.33369	-0.00001
H	3.86802	0.11650	-0.87586
H	-3.85210	-0.82725	0.00000
H	-3.14242	0.53728	0.87683
H	-3.14243	0.53729	-0.87682

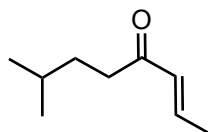


Carbonyl 45

M06-2X/def2-TZVP Geometry

O	-0.20727	-0.99628	-0.76780
C	-0.47982	0.08581	-0.30353
C	-1.86410	0.44270	0.11403
C	0.55964	1.17508	-0.13312
C	-2.86226	-0.42761	0.00508
C	-4.27685	-0.16863	0.39367
H	-2.02985	1.43899	0.51190
H	0.47609	1.56602	0.88721
C	1.97929	0.72686	-0.43797
H	0.24934	1.99909	-0.78607
H	-2.62175	-1.40685	-0.40099
H	-4.60143	-0.88648	1.15033
H	-4.40992	0.83841	0.78641
H	-4.93792	-0.30061	-0.46584
C	2.55590	-0.19081	0.63522

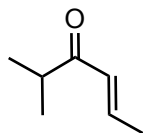
H	1.98641	0.20566	-1.39816
H	2.62052	1.60598	-0.54394
C	3.96733	-0.65306	0.29883
H	2.55931	0.33759	1.59387
H	1.90169	-1.05701	0.75138
H	4.64115	0.19866	0.18387
H	4.37371	-1.29890	1.07752
H	3.97596	-1.21235	-0.63837



Carbonyl 46

M06-2X/def2-TZVP Geometry

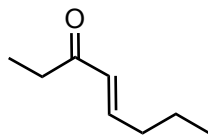
O	-0.57224	-1.36407	-0.19212
C	-0.79595	-0.29561	0.32689
C	-2.14274	0.33888	0.28362
C	0.26711	0.47038	1.08761
C	-3.15795	-0.24258	-0.34641
C	-4.53844	0.30812	-0.44660
H	-2.26674	1.29388	0.78459
H	-0.07127	0.50379	2.12997
C	1.65650	-0.13850	0.98807
H	0.24567	1.51107	0.75051
H	-2.95959	-1.19768	-0.82610
H	-5.25914	-0.39117	-0.01671
H	-4.62993	1.26457	0.06617
H	-4.81997	0.44241	-1.49344
C	2.31670	-0.00337	-0.38731
H	2.30804	0.32658	1.73500
H	1.58374	-1.19860	1.24066
C	2.61443	1.45242	-0.73705
C	3.60098	-0.82545	-0.42379
H	1.62780	-0.41190	-1.13146
H	3.11088	1.52335	-1.70617
H	1.71154	2.06210	-0.78893
H	3.27853	1.89584	0.01051
H	4.08684	-0.75713	-1.39842
H	4.30779	-0.46260	0.32797
H	3.39998	-1.87764	-0.21736



Carbonyl 47

M06-2X/def2-TZVP Geometry

O	-0.30822	-1.50573	0.53736
C	-0.25845	-0.42215	0.00447
C	1.03534	0.26670	-0.26524
C	-1.51436	0.33028	-0.40139
C	2.19280	-0.27714	0.09574
C	3.53627	0.32278	-0.13790
H	1.00354	1.22439	-0.77521
H	-1.33769	0.73010	-1.40608
C	-2.73184	-0.57841	-0.40815
C	-1.70112	1.51392	0.55673
H	2.15041	-1.23871	0.60095
H	4.15468	-0.34966	-0.73675
H	3.46681	1.28222	-0.64859
H	4.05935	0.46665	0.81019
H	-2.59258	-1.42077	-1.08499
H	-2.90350	-0.98435	0.58877
H	-3.61826	-0.02310	-0.71686
H	-2.57242	2.10016	0.26369
H	-1.86247	1.14785	1.57238
H	-0.83399	2.17517	0.56812

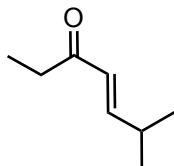


Carbonyl 48

M06-2X/def2-TZVP Geometry

O	-2.06516	1.36473	0.00000
C	-1.62533	0.23940	0.00000
C	-0.16314	-0.04643	-0.00000
C	-2.53247	-0.97213	-0.00000
C	0.72453	0.94344	0.00000
C	2.21136	0.80512	0.00000
H	0.14029	-1.08745	-0.00000
H	-2.26327	-1.58017	-0.87040
C	-4.00727	-0.61794	0.00000
H	0.32615	1.95520	0.00000
C	2.74986	-0.61774	-0.00000
H	2.60263	1.34839	-0.86841
H	2.60263	1.34839	0.86841

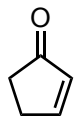
H	-4.25872	-0.02264	-0.87678
H	-4.62230	-1.51718	-0.00000
H	-4.25872	-0.02264	0.87678
H	-2.26327	-1.58017	0.87040
C	4.27271	-0.65006	-0.00000
H	2.36898	-1.14884	0.87632
H	2.36898	-1.14884	-0.87633
H	4.67337	-0.14561	-0.88121
H	4.67337	-0.14561	0.88121
H	4.64958	-1.67266	-0.00000



Carbonyl 49

M06-2X/def2-TZVP Geometry

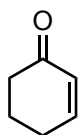
O	-1.66569	-1.37551	-0.30412
C	-1.42749	-0.21152	-0.08519
C	-0.04087	0.33493	-0.09127
C	-2.52604	0.78592	0.21316
C	1.00138	-0.45192	-0.34011
C	2.44582	-0.05710	-0.36242
H	0.07680	1.39329	0.11309
H	-2.29432	1.24593	1.17985
C	-3.91304	0.17222	0.20411
H	0.78642	-1.50131	-0.53252
C	3.22082	-0.91288	0.64617
H	2.82131	-0.31115	-1.36115
C	2.68377	1.42620	-0.11841
H	-3.98567	-0.62282	0.94506
H	-4.67113	0.92359	0.42240
H	-4.12988	-0.27113	-0.76685
H	-2.43799	1.59556	-0.51932
H	2.88553	-0.69400	1.66180
H	3.07101	-1.97728	0.46257
H	4.28902	-0.70162	0.58558
H	3.74825	1.65397	-0.17960
H	2.16244	2.04304	-0.85140
H	2.33763	1.71292	0.87726



Carbonyl 50

M06-2X/def2-TZVP Geometry

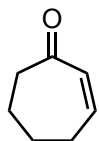
C	1.46939	-0.61752	0.00001
C	0.05016	-1.19562	0.00001
C	-0.88044	0.01602	0.00000
C	-0.02475	1.22638	-0.00001
C	1.25841	0.87391	-0.00001
O	-2.08255	-0.01994	-0.00000
H	2.04799	-0.92170	0.87461
H	2.04799	-0.92172	-0.87458
H	-0.16642	-1.80439	-0.87743
H	-0.16642	-1.80438	0.87746
H	-0.43091	2.22706	-0.00002
H	2.09156	1.56560	-0.00002



Carbonyl 51

M06-2X/def2-TZVP Geometry

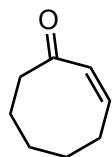
C	-1.80539	0.08111	0.12647
C	-1.05557	-1.15761	-0.35288
C	0.32724	-1.23146	0.28719
C	1.13502	0.02174	0.02086
C	0.37203	1.28919	-0.04875
C	-0.95835	1.31505	0.02861
O	2.33786	0.00222	-0.09092
H	-2.72392	0.22386	-0.44603
H	-2.11824	-0.04602	1.17009
H	-1.62703	-2.05943	-0.13126
H	-0.94484	-1.10494	-1.43928
H	0.22664	-1.31526	1.37570
H	0.90514	-2.08866	-0.05491
H	0.96124	2.19322	-0.13966
H	-1.47172	2.27139	0.02370



Carbonyl 52

M06-2X/def2-TZVP Geometry

C	-0.53339	-1.65878	-0.04015
C	0.61216	-1.02742	0.76284
C	1.30209	0.10333	0.03256
C	0.62477	1.42768	0.01486
C	-0.68614	1.63037	0.13906
O	2.38974	-0.03604	-0.47644
H	-1.08705	-2.31559	0.63435
H	-0.11421	-2.29137	-0.82415
H	0.21732	-0.63145	1.70188
H	1.36588	-1.77797	0.99588
H	1.29521	2.26671	-0.13117
C	-1.48988	-0.64435	-0.66837
H	-2.43206	-1.14407	-0.89889
C	-1.76664	0.58391	0.20713
H	-1.08162	-0.29326	-1.61904
H	-1.03095	2.65971	0.12684
H	-1.92795	0.27690	1.24755
H	-2.70037	1.05040	-0.10932

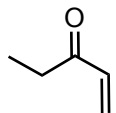


Carbonyl 53

M06-2X/def2-TZVP Geometry

C	-0.04225	-1.78941	0.15210
C	0.90665	-0.85469	0.93084
C	1.50081	0.22632	0.05349
C	0.75313	1.48057	-0.23277
C	-0.52963	1.76657	0.00108
O	2.59677	0.07907	-0.43968
H	0.58143	-2.49953	-0.39401
H	-0.62467	-2.37253	0.87053
H	0.40949	-0.40163	1.78585
H	1.74544	-1.43818	1.30839
H	1.36814	2.21327	-0.74364
C	-0.98192	-1.12828	-0.85798
H	-0.86430	2.74107	-0.34287
C	-1.59567	0.91100	0.62751

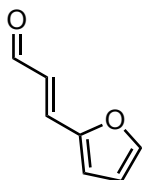
C	-2.07695	-0.24076	-0.27468
H	-2.45387	1.54225	0.85963
H	-1.25725	0.50725	1.57983
H	-1.46630	-1.92050	-1.43328
H	-0.39278	-0.55751	-1.57998
H	-2.65613	0.17926	-1.10074
H	-2.76832	-0.85366	0.31025



Carbonyl 55

M06-2X/def2-TZVP Geometry

C	-2.22999	-0.78171	-0.00001
C	-1.56191	0.36399	-0.00001
C	-0.07663	0.47816	0.00000
C	0.75803	-0.78638	0.00000
O	0.43301	1.57337	0.00000
C	2.24894	-0.49814	0.00001
H	-3.31208	-0.80106	-0.00002
H	-1.72550	-1.74013	-0.00001
H	-2.07583	1.31855	-0.00001
H	0.47098	-1.38013	0.87276
H	0.47098	-1.38013	-0.87276
H	2.81882	-1.42656	0.00001
H	2.52896	0.08352	-0.87697
H	2.52896	0.08352	0.87699

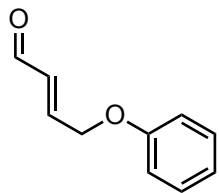


Carbonyl 56

M06-2X/def2-TZVP Geometry

C	1.60055	-0.20477	-0.00001
C	0.59083	0.67306	0.00003
C	2.98464	0.27503	0.00001
O	3.95288	-0.44036	-0.00003
C	-0.80705	0.34403	0.00002
O	-1.16882	-0.96458	-0.00004
C	-2.51491	-1.00822	-0.00004
C	-3.03801	0.24183	0.00002
C	-1.92289	1.12701	0.00006
H	1.43760	-1.27530	-0.00006

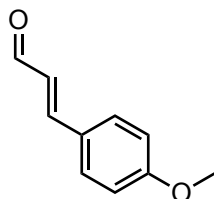
H	0.81130	1.73656	0.00008
H	3.09509	1.37851	0.00005
H	-2.95613	-1.98968	-0.00008
H	-4.08319	0.49765	0.00003
H	-1.93623	2.20398	0.00010



Carbonyl 57

M06-2X/def2-TZVP Geometry

C	-2.83471	0.10735	0.00000
C	-2.19215	-1.05525	-0.00000
C	-4.30591	0.13013	-0.00000
O	-4.96706	1.13390	-0.00000
C	-0.71401	-1.23159	0.00000
H	-2.31379	1.05593	0.00000
H	-2.76421	-1.98011	-0.00000
H	-4.78899	-0.86810	-0.00000
H	-0.41784	-1.81305	0.88328
H	-0.41784	-1.81305	-0.88328
O	-0.08573	0.02231	0.00000
C	4.04431	0.34262	-0.00000
C	3.22139	1.46538	-0.00000
C	1.84702	1.32810	-0.00000
C	1.27608	0.05681	0.00000
C	2.08686	-1.07201	0.00000
C	3.47019	-0.91573	0.00000
H	5.11999	0.45309	-0.00000
H	3.65617	2.45651	-0.00000
H	1.19147	2.18866	-0.00000
H	1.66555	-2.06665	0.00000
H	4.09744	-1.79783	0.00000

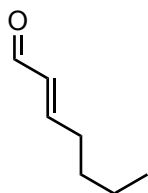


Carbonyl 58

M06-2X/def2-TZVP Geometry

C	2.93708	-0.24166	-0.00012
C	1.89371	0.59535	-0.00009

C	4.30100	0.29083	-0.00019
O	5.29770	-0.38566	-0.00021
H	2.83940	-1.32039	-0.00008
H	2.11367	1.66147	-0.00013
H	4.36831	1.39775	-0.00023
C	-2.27141	-0.29919	0.00010
C	-1.33744	-1.34157	0.00007
C	0.00859	-1.06531	0.00001
C	0.47568	0.25756	-0.00003
C	-0.46810	1.27988	0.00001
C	-1.83193	1.02015	0.00007
O	-3.56886	-0.67169	0.00016
H	-1.70511	-2.35883	0.00009
H	0.71299	-1.88675	-0.00002
H	-0.13003	2.30948	-0.00002
H	-2.53094	1.84321	0.00009
C	-4.54945	0.34352	0.00019
H	-4.46758	0.96942	-0.89202
H	-5.51015	-0.16333	0.00023
H	-4.46751	0.96943	0.89238

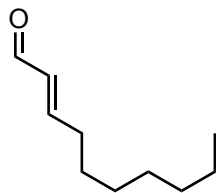


Carbonyl 59

M06-2X/def2-TZVP Geometry

O	4.23591	-0.40535	-0.41265
C	3.21718	-0.33713	0.22376
C	1.96911	0.26087	-0.26920
C	0.88424	0.29615	0.50124
C	-0.44392	0.85238	0.11373
C	-1.54767	-0.20771	0.16190
C	-2.91778	0.35752	-0.19106
C	-4.01189	-0.70100	-0.14731
H	3.16509	-0.73821	1.25618
H	1.98049	0.66511	-1.27566
H	0.95192	-0.13440	1.50004
H	-0.70601	1.66103	0.80460
H	-0.38721	1.28837	-0.88600
H	-1.58256	-0.65013	1.16269
H	-1.29573	-1.01964	-0.52649
H	-2.87576	0.80467	-1.18829
H	-4.98475	-0.28082	-0.40241

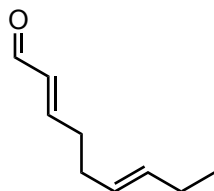
H	-3.16019	1.16964	0.50046
H	-4.08770	-1.14121	0.84868
H	-3.80041	-1.50811	-0.85101



Carbonyl 60

M06-2X/def2-TZVP Geometry

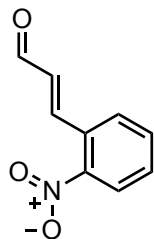
O	-6.06903	-0.67822	-0.51150
C	-5.09578	-0.45565	0.15988
C	-3.85960	0.15524	-0.34687
C	-2.82658	0.36749	0.46533
C	-1.51408	0.95640	0.07298
C	-0.35284	-0.01052	0.32119
C	0.99830	0.59479	-0.03684
C	2.16040	-0.36127	0.20058
C	3.51356	0.24077	-0.15597
C	4.67728	-0.71410	0.08060
H	-5.08037	-0.71048	1.23893
H	-3.83584	0.41959	-1.39857
H	-2.92726	0.07043	1.50901
H	-1.53801	1.25048	-0.97853
H	-1.34284	1.86570	0.65924
H	-0.35101	-0.31165	1.37357
H	-0.51516	-0.92184	-0.26142
H	0.99044	0.90223	-1.08777
H	2.00405	-1.27348	-0.38481
H	3.50773	0.54963	-1.20688
H	3.67052	1.15331	0.42932
H	4.68083	-1.02226	1.13023
H	4.51930	-1.62422	-0.50537
H	1.15307	1.50733	0.54855
H	2.16688	-0.66961	1.25148
C	6.02344	-0.09865	-0.27868
H	6.04966	0.19166	-1.33075
H	6.21223	0.79720	0.31600
H	6.84349	-0.79533	-0.10347



Carbonyl 61

M06-2X/def2-TZVP Geometry

O	-3.22816	-1.87702	-0.24798
C	-2.65439	-0.98666	0.32298
C	-1.99684	0.14218	-0.34839
C	-1.36596	1.07533	0.35970
C	-0.63298	2.24935	-0.19615
C	0.85391	2.23170	0.20543
C	1.57556	1.05422	-0.37318
C	2.09841	0.06185	0.33357
C	2.75508	-1.15472	-0.24066
C	1.98927	-2.42930	0.11665
H	-2.58579	-0.97374	1.42961
H	-2.04352	0.16684	-1.43171
H	-1.35277	0.97269	1.44475
H	-0.72518	2.26396	-1.28413
H	-1.08843	3.16841	0.18391
H	1.31205	3.16209	-0.13942
H	0.93684	2.21664	1.29512
H	1.63211	1.01244	-1.45980
H	2.02692	0.09941	1.42008
H	2.82622	-1.05158	-1.32535
H	3.77762	-1.23180	0.14033
H	0.97619	-2.39350	-0.28606
H	2.48671	-3.31343	-0.28237
H	1.91393	-2.54600	1.19925

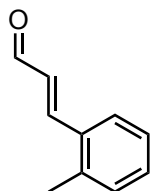


Carbonyl 62

M06-2X/def2-TZVP Geometry

O	-4.68507	0.18676	-0.20904
C	-3.62513	-0.24431	0.15976
C	-2.33490	0.40213	-0.12730

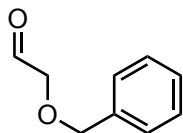
C	-1.20254	-0.12884	0.33335
C	0.12455	0.47566	0.13996
C	0.25092	1.86730	0.14735
C	1.48022	2.48698	0.00260
C	2.63561	1.72957	-0.13290
C	2.55034	0.34863	-0.12202
C	1.30997	-0.25143	0.00422
H	-3.56135	-1.17684	0.75345
H	-2.36277	1.29712	-0.73820
H	-1.25652	-1.05545	0.89298
H	-0.63825	2.46428	0.29927
H	1.53727	3.56739	0.00931
H	3.59837	2.20945	-0.24183
H	3.42598	-0.27626	-0.21895
N	1.28999	-1.72610	-0.04739
O	0.27149	-2.26311	-0.42225
O	2.30023	-2.30629	0.27449



Carbonyl 63

M06-2X/def2-TZVP Geometry

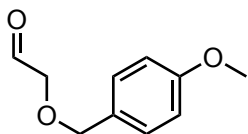
O	4.44867	-0.42922	-0.17152
C	3.43297	0.17244	0.06324
C	2.08544	-0.38453	-0.09812
C	1.01438	0.36022	0.19212
C	-0.38832	-0.05253	0.10025
C	-0.73190	-1.40633	0.12765
C	-2.05097	-1.81136	0.03585
C	-3.05206	-0.85747	-0.08377
C	-2.72276	0.48925	-0.10439
C	-1.40217	0.91493	-0.00906
C	-1.08640	2.38612	-0.04295
H	3.46464	1.21951	0.42651
H	2.02093	-1.39994	-0.47065
H	1.19939	1.37872	0.52350
H	0.04778	-2.14773	0.24597
H	-2.29809	-2.86420	0.06509
H	-4.08850	-1.16076	-0.15529
H	-3.50715	1.23064	-0.19726
H	-1.99533	2.96704	-0.18705
H	-0.62467	2.71700	0.88992
H	-0.39767	2.62912	-0.85354



Carbonyl 79

M06-2X/def2-TZVP Geometry

C	0.89477	0.64672	0.24806
C	-0.28769	1.53522	0.55369
O	-1.48026	0.81273	0.77438
C	1.12012	-0.49339	1.01551
C	2.20894	-1.31007	0.75513
C	3.08935	-0.99216	-0.27265
C	2.87048	0.14093	-1.04080
C	1.77256	0.95301	-0.78329
C	-1.95720	0.16025	-0.37192
C	-3.24755	-0.53655	-0.01396
O	-3.91976	-1.11785	-0.81561
H	-0.11256	2.09352	1.47460
H	-0.42917	2.25790	-0.25940
H	0.42830	-0.73825	1.81271
H	2.37486	-2.19552	1.35512
H	3.94011	-1.62957	-0.47509
H	3.54820	0.39000	-1.84701
H	1.59582	1.83205	-1.39267
H	-1.24698	-0.58913	-0.74415
H	-2.15313	0.86845	-1.18786
H	-3.52808	-0.47227	1.05487

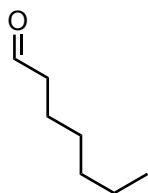


Carbonyl 80

M06-2X/def2-TZVP Geometry

C	-0.10014	1.06809	-0.06948
C	-1.44762	1.71929	-0.24206
O	-2.50747	0.94173	0.28275
C	0.72452	0.80672	-1.14897
C	1.96859	0.20082	-0.98653
C	2.38783	-0.15952	0.28762
C	1.56025	0.09039	1.38623
C	0.33688	0.69724	1.20497

C	-2.69730	-0.27143	-0.39291
C	-3.88108	-0.97411	0.22568
O	-4.34264	-1.98739	-0.21391
O	3.57230	-0.75559	0.56414
C	4.43822	-1.02912	-0.51413
H	-1.49288	2.66408	0.30089
H	-1.62681	1.92651	-1.30442
H	0.39909	1.07723	-2.14725
H	2.58612	0.01366	-1.85260
H	1.90854	-0.20063	2.36827
H	-0.30328	0.88467	2.05922
H	-2.89802	-0.11437	-1.46115
H	-1.82144	-0.92822	-0.31235
H	-4.29314	-0.48169	1.12726
H	4.73066	-0.10994	-1.02895
H	5.31894	-1.49897	-0.08519
H	3.97386	-1.71258	-1.23010

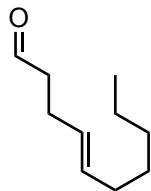


Carbonyl 85

M06-2X/def2-TZVP Geometry

C	2.35456	-0.87750	0.21501
C	2.98310	0.48996	0.20316
O	2.52985	1.44487	-0.36419
C	0.98974	-0.94054	-0.45278
C	-0.10585	-0.27241	0.37121
C	-1.46570	-0.31686	-0.31305
C	-2.57222	0.33317	0.50845
C	-3.92525	0.28675	-0.18964
H	3.07689	-1.54476	-0.26994
H	2.31092	-1.21139	1.25809
H	3.94049	0.57456	0.75540
H	1.05239	-0.45642	-1.43030
H	0.72424	-1.98576	-0.62937
H	-0.17563	-0.76619	1.34701
H	0.16961	0.76809	0.56173
H	-1.39587	0.18366	-1.28454
H	-1.73538	-1.35797	-0.52297
H	-2.64057	-0.16716	1.47901
H	-2.29981	1.37170	0.71705
H	-4.70442	0.75617	0.41140

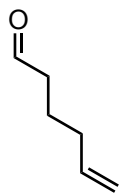
H	-3.88449	0.80531	-1.14941
H	-4.22741	-0.74428	-0.38386



Carbonyl 86

M06-2X/def2-TZVP Geometry

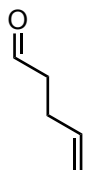
C	-2.87237	-1.00986	-0.57695
C	-1.87150	-1.88837	0.12540
O	-1.28690	-1.58777	1.12881
C	-2.90434	0.42342	-0.05256
C	-1.69228	1.19505	-0.48320
C	-0.74277	1.62825	0.33346
C	0.50297	2.34289	-0.08889
C	1.76900	1.59495	0.34286
C	1.86742	0.19550	-0.25040
C	3.15169	-0.52865	0.13300
C	3.21357	-1.94148	-0.43325
H	-2.65183	-1.04163	-1.64915
H	-3.84471	-1.50408	-0.46375
H	-1.70656	-2.88176	-0.33773
H	-3.80886	0.91129	-0.42363
H	-2.96179	0.40524	1.03656
H	-1.59107	1.37482	-1.55273
H	-0.83957	1.41894	1.39778
H	0.50076	2.46953	-1.17516
H	0.51629	3.34480	0.35081
H	2.64680	2.18011	0.05410
H	1.78854	1.52383	1.43530
H	1.00815	-0.39669	0.07796
H	1.79777	0.26005	-1.34296
H	4.01366	0.04857	-0.21503
H	3.22745	-0.56717	1.22363
H	4.13648	-2.44947	-0.15176
H	2.37598	-2.53893	-0.06771
H	3.15929	-1.92561	-1.52382



Carbonyl 87

M06-2X/def2-TZVP Geometry

C	-0.95642	0.37137	0.98565
C	-1.81592	-0.67023	0.32378
O	-2.04247	-0.72352	-0.85371
C	-0.26861	1.31955	0.01559
C	0.83818	0.64182	-0.80347
C	1.95147	0.12817	0.05635
C	2.29687	-1.14642	0.16629
H	-1.61119	0.91113	1.67946
H	-0.23278	-0.15485	1.61763
H	-2.26501	-1.41609	1.00965
H	0.15684	2.15528	0.57646
H	-1.01206	1.73279	-0.66770
H	1.23795	1.37433	-1.51010
H	0.41253	-0.17353	-1.38992
H	2.49113	0.87364	0.63739
H	3.10741	-1.46375	0.80961
H	1.78146	-1.91628	-0.39787

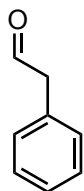


Carbonyl 93

M06-2X/def2-TZVP Geometry

C	0.39078	0.64860	-0.00000
C	1.88865	0.52184	0.00000
O	2.48200	-0.52047	0.00001
C	-2.54767	0.50580	-0.00001
C	-1.82017	-0.60174	-0.00000
C	-0.32403	-0.68778	0.00000
H	0.11614	1.25456	0.87112
H	0.11615	1.25455	-0.87114
H	2.44460	1.48032	0.00001
H	-3.62866	0.46272	-0.00001
H	-2.10201	1.49312	-0.00001
H	-2.33346	-1.55904	0.00000

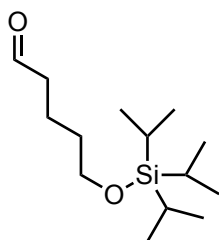
H	0.00290	-1.27139	-0.86531
H	0.00290	-1.27138	0.86531



Carbonyl 94

M06-2X/def2-TZVP Geometry

C	-1.48669	-0.59227	0.69199
C	-2.35976	-0.20524	-0.47957
O	-3.24814	0.59636	-0.42305
C	-0.04592	-0.27476	0.37316
C	0.86113	-1.27529	0.04210
C	2.17371	-0.95973	-0.28390
C	2.59089	0.36283	-0.28495
C	1.68992	1.36939	0.03881
C	0.38000	1.05191	0.36226
H	-1.83605	-0.05258	1.57185
H	-1.60197	-1.66565	0.86282
H	-2.10555	-0.70487	-1.43571
H	0.54061	-2.31053	0.04757
H	2.87050	-1.74914	-0.53430
H	3.61399	0.60977	-0.53635
H	2.00874	2.40361	0.03869
H	-0.32481	1.83750	0.61038

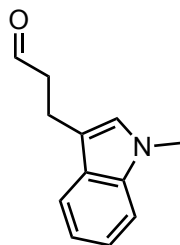


Carbonyl 95

M06-2X/def2-TZVP Geometry

C	-3.33566	-0.10526	-1.06067
C	-2.79976	-1.24730	-0.23507
O	-3.01661	-1.38550	0.93908
C	-1.29955	1.24343	0.81216
C	-2.41807	1.98485	0.09564
C	-3.64742	1.14011	-0.23817

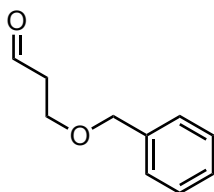
O	-0.61581	0.39287	-0.09791
Si	1.00455	0.03237	0.00871
C	1.95778	1.63970	0.26867
C	1.32456	-1.15149	1.43727
C	1.47550	-0.74484	-1.64626
C	1.53818	2.71818	-0.73357
C	3.47046	1.40274	0.20793
C	0.30454	-1.43565	-2.35109
C	2.66068	-1.70971	-1.51850
C	0.37684	-2.35503	1.37028
C	1.22218	-0.46632	2.80419
H	-2.62885	0.10641	-1.86504
H	-4.24479	-0.49216	-1.53676
H	-2.21131	-2.00521	-0.78490
H	-0.60120	1.96898	1.24403
H	-1.70934	0.64230	1.63038
H	-2.73050	2.82146	0.72590
H	-2.00008	2.41321	-0.82078
H	-4.35880	1.76256	-0.78340
H	-4.13815	0.82792	0.68612
H	1.71781	2.00066	1.27522
H	2.35250	-1.51532	1.31903
H	1.79315	0.09210	-2.28057
H	0.46852	2.93037	-0.68260
H	1.76189	2.41070	-1.75828
H	2.07578	3.65250	-0.55140
H	3.79733	0.63556	0.91425
H	3.77323	1.08455	-0.79318
H	4.02010	2.31957	0.43557
H	0.60508	-1.79132	-3.34025
H	-0.03631	-2.30496	-1.78376
H	-0.54517	-0.76381	-2.47295
H	2.38473	-2.58864	-0.93106
H	2.97943	-2.06186	-2.50285
H	3.52494	-1.25152	-1.03419
H	0.59368	-3.06538	2.17245
H	0.46226	-2.89351	0.42357
H	-0.66382	-2.04086	1.47999
H	1.39323	-1.18443	3.61049
H	0.22745	-0.04065	2.95975
H	1.95132	0.33813	2.91697



Carbonyl 96

M06-2X/def2-TZVP Geometry

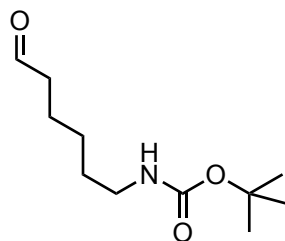
C	2.63154	-1.36501	-0.21945
C	3.39354	-0.27353	-0.92065
O	3.55640	0.83237	-0.48348
C	0.66347	-0.07917	0.65746
C	1.87655	-0.87761	1.01511
C	0.55946	1.27686	0.55406
N	-0.70853	1.63749	0.16174
C	-1.45238	0.49877	-0.00142
C	-0.62324	-0.60510	0.29855
C	-1.19204	2.97858	-0.04793
C	-2.78418	0.34733	-0.38484
C	-3.27919	-0.93937	-0.46809
C	-2.47275	-2.05132	-0.17550
C	-1.15514	-1.89564	0.20630
H	1.95414	-1.82429	-0.94658
H	3.36795	-2.13783	0.03308
H	3.83712	-0.55504	-1.89608
H	1.57984	-1.74079	1.61454
H	2.55124	-0.27711	1.62620
H	1.31569	2.02884	0.71723
H	-1.53895	3.10844	-1.07483
H	-2.01504	3.20585	0.63257
H	-0.38065	3.67843	0.13744
H	-3.40841	1.20325	-0.60871
H	-4.30856	-1.09476	-0.76344
H	-2.89649	-3.04415	-0.25029
H	-0.54314	-2.76096	0.43295



Carbonyl 97

M06-2X/def2-TZVP Geometry

C	-3.24149	1.02041	-0.01187
O	-2.32292	1.77208	-0.17882
C	-3.12053	-0.35695	0.58750
C	-1.69409	-0.84357	0.69806
O	-1.24232	-1.12481	-0.60736
C	0.06338	-1.64608	-0.65337
C	1.14251	-0.64932	-0.29446
C	2.36596	-1.09709	0.19160
C	3.38467	-0.19836	0.47465
C	3.18101	1.16162	0.28560
C	1.95649	1.61413	-0.18728
C	0.94137	0.71413	-0.48095
H	-4.27030	1.32910	-0.28235
H	-3.59628	-0.31626	1.57354
H	-3.71521	-1.05046	-0.01305
H	-1.06810	-0.07904	1.16991
H	-1.64890	-1.75270	1.31076
H	0.14360	-2.52410	0.00163
H	0.20652	-1.98712	-1.68076
H	2.52284	-2.15836	0.35143
H	4.33358	-0.55884	0.85072
H	3.97096	1.86585	0.51238
H	1.78770	2.67414	-0.32742
H	-0.02011	1.06615	-0.83422



Carbonyl 98

M06-2X/def2-TZVP Geometry

C	3.00622	2.14284	-0.13588
O	2.03600	1.86200	-0.78790
C	4.00211	1.14458	0.38828
C	3.61411	-0.29623	0.09885
C	2.45943	-0.77040	0.98157
C	1.76746	-2.03075	0.47133
C	1.07169	-1.83414	-0.87830
N	0.17464	-0.69788	-0.89916
C	-1.06328	-0.79494	-0.35804
O	-1.65351	0.41500	-0.33093
C	-3.00684	0.56525	0.16939
C	-3.07897	0.16800	1.63840

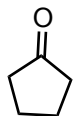
C	-3.98201	-0.23296	-0.68628
C	-3.26245	2.05694	0.01150
O	-1.56137	-1.82911	0.02973
H	3.22068	3.20250	0.10047
H	4.96637	1.41401	-0.05802
H	4.11915	1.33007	1.46240
H	3.33806	-0.36311	-0.95500
H	4.47797	-0.94886	0.24039
H	2.83443	-0.94328	1.99378
H	1.71347	0.02444	1.06264
H	1.01463	-2.34838	1.19572
H	2.48871	-2.84833	0.37654
H	0.48919	-2.72266	-1.11844
H	1.79806	-1.69285	-1.67876
H	0.55283	0.22665	-1.04974
H	-4.06193	0.43023	2.03297
H	-2.91969	-0.89986	1.76452
H	-2.32495	0.71319	2.20872
H	-3.82654	-1.30199	-0.56543
H	-5.00306	0.01350	-0.39066
H	-3.85651	0.03082	-1.73755
H	-2.53727	2.62827	0.59151
H	-3.17445	2.34677	-1.03576
H	-4.26538	2.30187	0.36183



Carbonyl 100

M06-2X/def2-TZVP Geometry

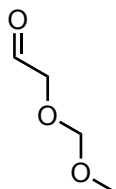
C	0.00001	0.18642	0.00003
O	-0.00032	1.39000	-0.00002
C	-1.28285	-0.61082	0.00130
C	1.28314	-0.61038	-0.00136
H	-1.35080	-1.19601	-0.91817
H	-1.28706	-1.31825	0.83250
H	-2.13604	0.05802	0.07428
H	1.35101	-1.19544	0.91829
H	1.28749	-1.31817	-0.83224
H	2.13617	0.05861	-0.07432



Carbonyl 103

M06-2X/def2-TZVP Geometry

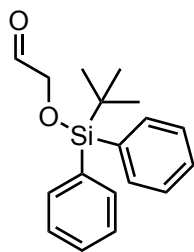
C	0.91929	-0.00000	-0.00002
C	0.02848	1.23031	-0.12722
O	2.11827	-0.00000	-0.00000
C	0.02847	-1.23031	0.12725
C	-1.36914	-0.73104	-0.23853
C	-1.36914	0.73104	0.23852
H	0.41284	2.05067	0.47596
H	0.06987	1.54367	-1.17517
H	0.41283	-2.05070	-0.47588
H	0.06985	-1.54361	1.17522
H	-1.50196	-0.76088	-1.32264
H	-2.16767	-1.32044	0.20843
H	-1.50200	0.76087	1.32262
H	-2.16767	1.32044	-0.20846



Carbonyl 111

M06-2X/def2-TZVP Geometry

C	-1.48890	-0.49948	-0.26250
C	-1.12198	0.96586	-0.13067
O	-2.41358	-0.99012	0.31745
O	0.19721	1.24974	-0.52765
C	1.14828	0.90425	0.43985
O	1.23147	-0.46978	0.64420
C	1.90236	-1.15148	-0.39774
H	-0.86873	-1.07965	-0.97221
H	-1.31964	1.28593	0.89804
H	-1.78235	1.52707	-0.79662
H	0.88031	1.33889	1.40705
H	2.09836	1.31031	0.08149
H	1.44989	-0.93798	-1.36950
H	2.95756	-0.86265	-0.42599
H	1.82529	-2.21558	-0.18803

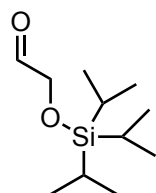


Carbonyl 112

M06-2X/def2-TZVP Geometry

C	2.40999	-1.47713	-2.35094
C	0.96812	-1.03597	-2.28769
O	2.99333	-2.02961	-1.46443
O	0.33928	-1.42947	-1.11537
Si	-0.11280	-0.44223	0.13879
C	1.10564	0.98184	0.22985
C	-1.83175	0.20403	-0.23579
C	-0.12760	-1.55193	1.65644
C	-0.67779	-0.79953	2.87181
C	1.28916	-2.05039	1.96521
C	-1.02996	-2.75523	1.35166
C	-2.52429	-0.27899	-1.34880
C	-3.81173	0.15359	-1.64131
C	-4.43452	1.08068	-0.81890
C	-3.76752	1.57130	0.29644
C	-2.48185	1.13546	0.58206
C	2.47663	0.71088	0.33998
C	3.41064	1.73635	0.37919
C	2.99396	3.05941	0.31084
C	1.64314	3.35024	0.19019
C	0.71168	2.32047	0.14475
H	2.91212	-1.24309	-3.31149
H	0.96441	0.05456	-2.43731
H	0.45782	-1.46992	-3.15740
H	-1.72468	-0.52145	2.73466
H	-0.62070	-1.44060	3.75744
H	-0.10357	0.10694	3.08370
H	1.76053	-2.50371	1.08971
H	1.92795	-1.23945	2.32046
H	1.24511	-2.80495	2.75744
H	-0.64404	-3.33812	0.51365
H	-1.07611	-3.41033	2.22766
H	-2.05024	-2.44502	1.11242
H	-2.05123	-1.01313	-1.99145
H	-4.32920	-0.23510	-2.50923
H	-5.43783	1.41946	-1.04353

H	-4.25068	2.29250	0.94335
H	-1.97811	1.53059	1.45823
H	2.82242	-0.31544	0.37844
H	4.46433	1.50208	0.46222
H	3.72145	3.86051	0.34464
H	1.31332	4.37934	0.12476
H	-0.33640	2.56783	0.02705

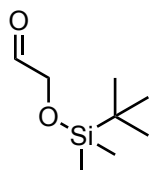


Carbonyl 113

M06-2X/def2-TZVP Geometry

C	-3.40474	-0.16913	0.70597
C	-2.22523	-0.46441	-0.19770
O	-4.53878	-0.16800	0.32486
O	-1.04489	-0.44652	0.55261
Si	0.44223	0.04905	-0.00993
C	0.23181	1.73827	-0.81630
C	1.54588	0.15247	1.51290
C	1.09254	-1.19944	-1.26277
C	1.59081	2.32104	-1.21971
C	-0.52885	2.70944	0.09054
C	3.01998	-0.10262	1.17493
C	1.08648	-0.77122	2.64644
C	0.38949	-1.09364	-2.62036
C	0.98541	-2.62560	-0.71094
H	-3.13165	0.05081	1.75732
H	-2.39221	-1.44323	-0.66150
H	-2.23026	0.28322	-1.00189
H	-0.35606	1.59621	-1.73071
H	1.46021	1.18541	1.87210
H	2.15414	-0.97163	-1.41549
H	1.46973	3.27049	-1.74685
H	2.20502	2.51659	-0.33665
H	2.15203	1.64781	-1.87257
H	-0.66321	3.67737	-0.39879
H	-1.51762	2.33242	0.35983
H	0.01633	2.88857	1.02056
H	3.65039	0.06512	2.05149
H	3.17361	-1.13652	0.85651
H	3.38556	0.54403	0.37458
H	0.05755	-0.56834	2.94088

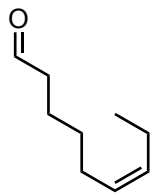
H	1.13871	-1.82040	2.34724
H	1.72772	-0.64753	3.52295
H	0.77484	-1.84396	-3.31556
H	-0.68637	-1.26599	-2.52785
H	0.52927	-0.11379	-3.07995
H	1.36843	-3.35289	-1.43128
H	1.54580	-2.75092	0.21722
H	-0.05522	-2.88448	-0.50023



Carbonyl 114

M06-2X/def2-TZVP Geometry

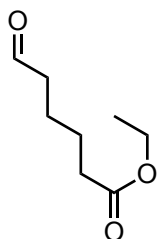
C	3.02486	-0.51888	-0.10476
C	2.30211	0.57886	-0.84935
O	2.48782	-1.46113	0.40033
O	0.94378	0.35475	-0.98252
Si	-0.21976	0.66214	0.16970
C	-1.57505	-0.60357	-0.13220
C	-0.83047	2.41009	-0.09757
C	0.49744	0.53650	1.89113
C	-0.98349	-2.01467	-0.04373
C	-2.17300	-0.39428	-1.52797
C	-2.67496	-0.44348	0.92267
H	4.12526	-0.38813	-0.05401
H	2.54032	1.52393	-0.33486
H	2.76374	0.65316	-1.84158
H	-0.02754	3.12797	0.08678
H	-1.17819	2.55533	-1.12138
H	-1.65034	2.65597	0.58037
H	0.75897	-0.48924	2.14994
H	1.39883	1.14689	1.99240
H	-0.22425	0.90993	2.62105
H	-0.55625	-2.21616	0.94086
H	-1.76748	-2.75718	-0.22670
H	-0.19191	-2.16116	-0.77969
H	-2.65705	0.58088	-1.61910
H	-2.93100	-1.15894	-1.72747
H	-1.40910	-0.46981	-2.30479
H	-3.47357	-1.17055	0.74278
H	-2.29486	-0.61699	1.93233
H	-3.12636	0.55168	0.89541



Carbonyl 116

M06-2X/def2-TZVP Geometry

O	3.24593	0.38031	-1.16072
C	3.36482	0.59465	0.01377
C	2.22775	0.62024	0.99929
C	0.88368	0.21998	0.41192
C	0.79077	-1.27334	0.11700
C	-0.54507	-1.66083	-0.52828
C	-1.70886	-1.44904	0.39474
C	-2.62920	-0.49183	0.33360
C	-2.72999	0.61955	-0.66784
C	-2.70898	1.98991	0.01088
H	4.36493	0.81037	0.44040
H	2.20678	1.63708	1.40892
H	2.50780	-0.02196	1.84238
H	0.08722	0.50227	1.10331
H	0.72038	0.77979	-0.51352
H	1.60534	-1.56191	-0.54986
H	0.92009	-1.83454	1.04893
H	-0.66741	-1.09792	-1.45461
H	-0.50718	-2.71674	-0.80792
H	-1.77612	-2.15810	1.21648
H	-3.39931	-0.48281	1.10182
H	-1.92300	0.56049	-1.39794
H	-3.66651	0.51475	-1.22427
H	-2.83141	2.79231	-0.71697
H	-3.51382	2.07287	0.74335
H	-1.76482	2.14583	0.53478

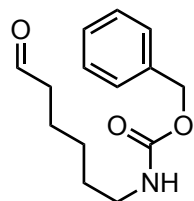


Carbonyl 117

M06-2X/def2-TZVP Geometry

O	-0.59991	1.59932	-0.99818
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C	-1.15187	1.75819	0.05824
C	-2.34053	0.97451	0.53567
C	-2.73177	-0.21387	-0.33616
C	-1.92786	-1.49660	-0.10504
C	-0.48980	-1.47483	-0.61045
C	0.46807	-0.74712	0.29580
O	1.64884	-0.55942	-0.29439
O	0.22726	-0.38124	1.41872
C	2.61527	0.18785	0.45442
C	3.84935	0.31976	-0.40362
H	-0.80321	2.54676	0.75299
H	-3.16126	1.70036	0.59224
H	-2.13612	0.67115	1.56608
H	-3.78185	-0.44089	-0.14340
H	-2.65924	0.07737	-1.38720
H	-1.92791	-1.74200	0.95974
H	-2.44648	-2.30941	-0.61687
H	-0.10344	-2.49342	-0.70734
H	-0.41706	-1.01727	-1.59830
H	2.18285	1.15957	0.69888
H	2.81762	-0.33388	1.39079
H	4.61127	0.88875	0.12908
H	4.25629	-0.66149	-0.64638
H	3.61390	0.83776	-1.33259

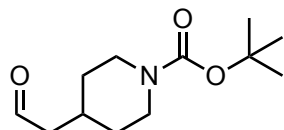


Carbonyl 118

M06-2X/def2-TZVP Geometry

O	0.34664	3.11827	-0.57447
C	1.24668	2.38679	-0.89114
C	2.63459	2.44356	-0.31576
C	3.15306	1.04596	0.02056
C	2.38706	0.40177	1.17193
C	2.91417	-0.98413	1.53616
C	2.65296	-2.04991	0.47366
N	1.24828	-2.37043	0.31213
C	0.46053	-1.77109	-0.60557
O	-0.77641	-2.30478	-0.57855
O	0.81439	-0.89138	-1.36086
C	-1.79051	-1.60331	-1.31699

C	-2.40210	-0.52063	-0.47349
C	-1.92216	0.78311	-0.53921
C	-2.45090	1.77021	0.28145
C	-3.47068	1.45754	1.16944
C	-3.96011	0.15884	1.23731
C	-3.42530	-0.82530	0.42012
H	1.09199	1.59787	-1.65337
H	2.63040	3.10623	0.55101
H	3.27153	2.89535	-1.08433
H	4.21402	1.10620	0.27650
H	3.07029	0.42219	-0.87296
H	2.45481	1.05033	2.04976
H	1.32332	0.33787	0.91923
H	3.99407	-0.92873	1.70652
H	2.46429	-1.31609	2.47550
H	3.02553	-1.73038	-0.49924
H	3.17606	-2.97044	0.73606
H	0.81155	-3.04914	0.91228
H	-1.35185	-1.20030	-2.22786
H	-2.52379	-2.36722	-1.56834
H	-1.12824	1.02713	-1.23321
H	-2.05361	2.77444	0.22085
H	-3.88722	2.22604	1.80800
H	-4.75872	-0.08536	1.92604
H	-3.80307	-1.84016	0.47290

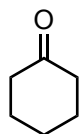


Carbonyl 119

M06-2X/def2-TZVP Geometry

O	-4.87525	-1.46423	-0.60447
C	-4.93982	-0.86248	0.43154
C	-3.95512	0.18468	0.87667
C	-2.75214	0.35892	-0.03700
C	-1.81468	-0.84809	0.02819
C	-0.58719	-0.64324	-0.85357
N	0.08263	0.60052	-0.51075
C	-0.75017	1.78753	-0.58353
C	-1.97874	1.63235	0.30507
C	1.39484	0.72201	-0.17445
O	2.01783	-0.47070	-0.17768
O	1.92999	1.77539	0.09721
C	3.42714	-0.56749	0.16425
C	3.70199	-2.05840	0.03202

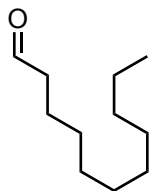
C	3.65930	-0.11156	1.59866
C	4.27272	0.21637	-0.83071
H	-5.77862	-1.04899	1.13123
H	-4.52373	1.11929	0.96657
H	-3.64458	-0.05995	1.89978
H	-3.11996	0.44097	-1.06648
H	-1.48440	-0.99064	1.06304
H	-2.34124	-1.74984	-0.28656
H	-0.90040	-0.59493	-1.90398
H	0.11157	-1.46578	-0.74914
H	-0.14694	2.64155	-0.28990
H	-1.06902	1.93155	-1.62356
H	-2.62155	2.50885	0.19059
H	-1.65742	1.59517	1.35133
H	3.49876	-2.39266	-0.98577
H	4.74597	-2.26628	0.26683
H	3.06978	-2.62327	0.71778
H	3.49011	0.95679	1.70401
H	2.99134	-0.64936	2.27356
H	4.68777	-0.33883	1.88344
H	4.10628	1.28574	-0.73215
H	5.32703	0.00172	-0.64938
H	4.03152	-0.09195	-1.84926



Carbonyl 120

M06-2X/def2-TZVP Geometry

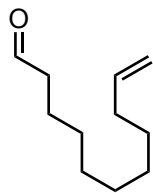
C	1.77283	0.00000	0.09255
C	0.99615	1.25711	-0.28941
C	-0.38826	1.27697	0.37094
C	-1.14600	-0.00000	0.07649
C	-0.38826	-1.27697	0.37094
C	0.99616	-1.25711	-0.28941
O	-2.26250	-0.00000	-0.37572
H	2.74971	0.00000	-0.39397
H	1.95514	0.00000	1.17262
H	1.54943	2.15406	-0.00760
H	0.87384	1.28829	-1.37621
H	-0.26261	1.34330	1.45744
H	-0.99094	2.12249	0.04363
H	-0.26262	-1.34330	1.45744
H	-0.99094	-2.12249	0.04362
H	0.87384	-1.28830	-1.37621
H	1.54944	-2.15405	-0.00759



Carbonyl 125

M06-2X/def2-TZVP Geometry

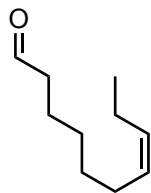
O	4.72726	1.61434	-0.56446
C	5.28702	0.82013	0.13914
C	4.84997	-0.60637	0.33740
C	3.52943	-0.95138	-0.33320
C	2.32647	-0.33397	0.37204
C	1.00860	-0.66210	-0.31749
C	-0.20154	-0.06425	0.38885
C	-1.52018	-0.38513	-0.30338
C	-2.73093	0.21121	0.40343
C	-4.04960	-0.10798	-0.28913
C	-5.26125	0.48727	0.41771
C	-6.57175	0.15996	-0.28637
H	6.20544	1.11302	0.68638
H	5.67215	-1.22757	-0.03723
H	4.81729	-0.79419	1.41680
H	3.55812	-0.60433	-1.36886
H	3.41440	-2.03771	-0.36233
H	2.29212	-0.69183	1.40722
H	2.45162	0.75101	0.41587
H	1.04271	-0.29648	-1.34901
H	0.89074	-1.74953	-0.38053
H	-0.23628	-0.42997	1.42084
H	-0.08117	1.02228	0.45331
H	-1.48583	-0.01764	-1.33454
H	-1.63929	-1.47195	-0.37040
H	-2.76552	-0.15654	1.43466
H	-2.61131	1.29785	0.47092
H	-4.01624	0.26053	-1.32021
H	-4.16976	-1.19472	-0.35785
H	-5.29325	0.11807	1.44705
H	-5.13975	1.57237	0.48536
H	-7.42709	0.59311	0.23287
H	-6.57026	0.54472	-1.30809
H	-6.72437	-0.91973	-0.34065



Carbonyl 126

M06-2X/def2-TZVP Geometry

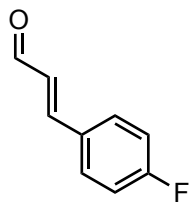
O	-4.30411	1.27771	1.19195
C	-4.93492	0.41900	0.64075
C	-4.49319	-0.30413	-0.60311
C	-3.08430	0.04331	-1.05797
C	-2.00612	-0.54674	-0.15518
C	-0.59793	-0.18014	-0.60513
C	0.48782	-0.77239	0.28440
C	1.89634	-0.40427	-0.16414
C	2.97849	-0.99488	0.73062
C	4.39853	-0.65462	0.26716
C	4.69266	0.81213	0.34010
C	5.03517	1.57419	-0.68753
H	-5.92711	0.11924	1.03394
H	-4.60543	-1.37853	-0.41733
H	-5.23948	-0.06607	-1.37028
H	-2.93813	-0.31573	-2.07971
H	-2.97916	1.13060	-1.08245
H	-2.16181	-0.19682	0.86856
H	-2.10776	-1.63773	-0.13693
H	-0.44521	-0.51703	-1.63640
H	-0.49790	0.91000	-0.62022
H	0.33499	-0.43206	1.31407
H	0.38523	-1.86292	0.30441
H	2.05323	-0.74910	-1.19252
H	1.99844	0.68462	-0.19068
H	2.83815	-0.63608	1.75574
H	2.86630	-2.08213	0.76622
H	5.11371	-1.19245	0.89682
H	4.54651	-1.00526	-0.75794
H	5.23146	2.63207	-0.57091
H	5.13344	1.16018	-1.68501
H	4.59805	1.26483	1.32517



Carbonyl 127

M06-2X/def2-TZVP Geometry

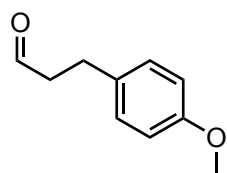
O	-3.69176	-0.90164	-0.91398
C	-4.06738	0.12844	-0.42708
C	-3.15968	1.22296	0.06687
C	-1.68193	0.86500	0.03155
C	-1.29827	-0.15061	1.10460
C	0.19593	-0.45554	1.14665
C	0.73248	-1.09457	-0.13949
C	2.16235	-1.52639	0.01551
C	3.23972	-0.80994	-0.28811
C	3.27064	0.58029	-0.84877
C	4.01634	1.54046	0.07968
H	-5.15216	0.33527	-0.33221
H	-3.38087	2.09970	-0.55325
H	-3.48812	1.49447	1.07662
H	-1.44792	0.46773	-0.95779
H	-1.08722	1.77311	0.16452
H	-1.61032	0.23360	2.08098
H	-1.85332	-1.07695	0.93537
H	0.75990	0.46304	1.34185
H	0.40432	-1.12533	1.98525
H	0.11248	-1.96047	-0.38833
H	0.63355	-0.39601	-0.97060
H	3.77174	0.56622	-1.82151
H	2.25916	0.95020	-1.02073
H	3.51731	1.60327	1.04774
H	5.03706	1.19626	0.25474
H	4.21545	-1.24749	-0.09051
H	2.31440	-2.50684	0.45777
H	4.06733	2.54279	-0.34651



Carbonyl 128

M06-2X/def2-TZVP Geometry

C	2.10299	1.22489	0.00001
C	0.71893	1.28530	0.00001
C	-0.06000	0.12638	0.00000
C	0.59018	-1.11225	-0.00001
C	1.96921	-1.19283	-0.00001
C	2.70281	-0.01818	0.00001
F	4.03811	-0.09437	-0.00000
C	-1.51441	0.25823	0.00002
C	-2.42275	-0.72144	-0.00004
C	-3.86436	-0.40118	0.00007
O	-4.31512	0.71609	-0.00008
H	2.71565	2.11562	0.00001
H	0.22767	2.25048	0.00001
H	0.01247	-2.02687	-0.00003
H	2.48612	-2.14249	-0.00003
H	-1.90206	1.27382	0.00013
H	-2.15333	-1.77051	-0.00012
H	-4.54429	-1.27289	0.00033

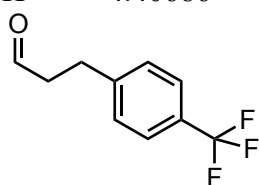


Carbonyl 129

M06-2X/def2-TZVP Geometry

H	4.75273	-0.09627	1.60414
C	4.19700	-0.11858	0.64535
C	2.70242	-0.01966	0.76380
C	1.97747	-0.05072	-0.57740
C	0.48598	0.05494	-0.40562
O	4.78865	-0.21659	-0.39362
C	-0.13220	1.29899	-0.26320
C	-1.49305	1.40692	-0.06061
C	-2.28251	0.25892	0.00635
C	-1.68907	-0.98949	-0.13432
C	-0.31445	-1.07475	-0.33777

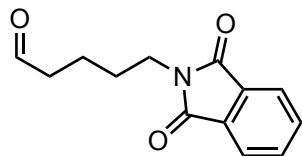
O	-3.61042	0.46014	0.20467
C	-4.44165	-0.67521	0.26886
H	2.36578	-0.83530	1.41407
H	2.47329	0.89805	1.31773
H	2.34876	0.76642	-1.19841
H	2.23598	-0.97336	-1.09904
H	0.46804	2.20056	-0.32054
H	-1.97467	2.37019	0.04306
H	-2.27642	-1.89521	-0.09392
H	0.13743	-2.05380	-0.45236
H	-5.45097	-0.30552	0.42832
H	-4.15855	-1.32733	1.09984
H	-4.40686	-1.24489	-0.66393



Carbonyl 130

M06-2X/def2-TZVP Geometry

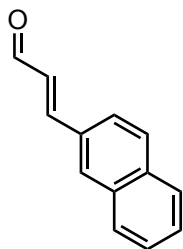
H	-4.30790	0.88809	1.87240
C	-3.83974	0.73351	0.88107
C	-3.60214	-0.70245	0.49597
C	-2.78475	-0.86725	-0.78425
C	-1.32153	-0.57605	-0.56674
O	-3.57861	1.67311	0.18273
C	-0.48968	-1.56011	-0.03104
C	0.85000	-1.30950	0.20147
C	1.37608	-0.05974	-0.10348
C	0.56654	0.92882	-0.63689
C	-0.77821	0.66822	-0.86520
C	2.83496	0.18286	0.15180
H	-4.59366	-1.15894	0.39417
H	-3.12913	-1.20869	1.34331
H	-2.89739	-1.89081	-1.14465
H	-3.18630	-0.20083	-1.54788
H	-0.89880	-2.53770	0.19812
H	1.49069	-2.07931	0.61305
H	0.98158	1.89911	-0.87213
H	-1.41863	1.44218	-1.26732
F	3.20693	1.43026	-0.14762
F	3.60794	-0.64365	-0.56858
F	3.15394	-0.02747	1.43763



Carbonyl 131

M06-2X/def2-TZVP Geometry

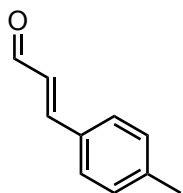
C	-5.78168	0.00027	0.72673
C	-4.31838	0.00010	1.07131
C	-3.40385	0.00011	-0.14043
C	-1.93229	0.00002	0.24868
O	-6.21251	-0.00034	-0.39240
C	-1.02942	0.00010	-0.97810
N	0.37499	0.00006	-0.62217
C	1.11829	1.15719	-0.39991
C	2.48776	0.69270	-0.02413
C	2.48771	-0.69274	-0.02414
C	1.11821	-1.15713	-0.39991
C	3.61818	1.41684	0.28754
C	4.76810	0.69609	0.60421
C	4.76805	-0.69628	0.60420
C	3.61809	-1.41695	0.28751
O	0.70143	-2.27897	-0.50008
O	0.70159	2.27906	-0.50006
H	-6.47368	-0.00052	1.59208
H	-4.13597	0.87065	1.71262
H	-4.13613	-0.87060	1.71246
H	-3.62944	-0.87243	-0.75837
H	-3.62935	0.87274	-0.75828
H	-1.70166	0.88153	0.85373
H	-1.70172	-0.88163	0.85356
H	-1.20962	-0.88739	-1.58577
H	-1.20958	0.88770	-1.58562
H	3.60492	2.49870	0.28383
H	5.67801	1.22531	0.85500
H	5.67793	-1.22556	0.85498
H	3.60475	-2.49881	0.28379



Carbonyl 132

M06-2X/def2-TZVP Geometry

C	-4.64302	-0.47775	-0.00001
C	-3.33177	0.17909	-0.00002
C	-2.21636	-0.55737	0.00002
O	-5.69512	0.10722	-0.00002
C	-0.83574	-0.08221	0.00002
C	-0.51270	1.30340	0.00002
C	0.78441	1.71487	0.00001
C	1.85098	0.77840	0.00000
C	1.54227	-0.60501	0.00000
C	0.18562	-1.00127	0.00001
C	3.20617	1.17907	-0.00001
C	4.20763	0.24782	-0.00001
C	3.90101	-1.13026	-0.00001
C	2.59945	-1.54634	-0.00001
H	-4.60988	-1.58596	0.00005
H	-3.33551	1.26203	-0.00006
H	-2.33200	-1.63947	0.00006
H	-1.30734	2.03711	0.00003
H	1.02222	2.77185	0.00001
H	-0.04603	-2.06102	0.00001
H	3.43775	2.23739	-0.00001
H	5.24250	0.56418	-0.00002
H	4.70362	-1.85598	-0.00002
H	2.35776	-2.60246	-0.00000

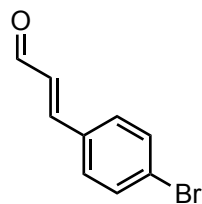


Carbonyl 133

M06-2X/def2-TZVP Geometry

C	3.86085	0.19364	-0.00011
C	2.47454	-0.28225	0.00009

C	1.46721	0.59613	-0.00022
O	4.82658	-0.52549	0.00015
C	0.03405	0.31267	-0.00011
C	-0.86714	1.37550	0.00007
C	-2.23607	1.15290	0.00025
C	-2.74697	-0.13904	0.00020
C	-1.84339	-1.20511	0.00007
C	-0.48079	-0.98853	-0.00009
C	-4.22637	-0.39901	-0.00015
H	3.97518	1.29643	-0.00050
H	2.33294	-1.35610	0.00051
H	1.72847	1.65277	-0.00058
H	-0.48777	2.39067	0.00012
H	-2.91645	1.99585	0.00045
H	0.19178	-1.83633	-0.00020
H	-4.79198	0.53121	0.00468
H	-2.22360	-2.22018	0.00013
H	-4.51786	-0.98028	0.87631
H	-4.51879	-0.97151	-0.88210

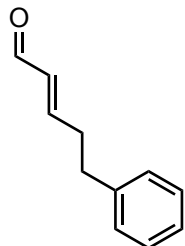


Carbonyl 134

M06-2X/def2-TZVP Geometry

C	-5.03199	0.09604	0.00053
C	-3.62364	-0.31764	0.00034
C	-2.65647	0.60326	0.00024
O	-5.96093	-0.66823	-0.00082
C	-1.21176	0.37818	0.00018
C	-0.35537	1.47979	0.00002
C	1.02143	1.32322	-0.00007
C	1.55003	0.04304	0.00001
C	0.72334	-1.07363	0.00018
C	-0.64779	-0.90080	0.00026
Br	3.42588	-0.19200	-0.00010
H	-5.19671	1.19251	-0.00093
H	-3.43682	-1.38472	0.00035
H	-2.96123	1.64792	0.00023
H	-0.77555	2.47848	-0.00005
H	1.67649	2.18297	-0.00020
H	-1.28498	-1.77525	0.00039

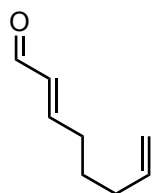
H	1.15393	-2.06509	0.00025
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Carbonyl 135

M06-2X/def2-TZVP Geometry

C	4.59931	-0.10743	0.08039
C	3.23505	0.24500	-0.33777
C	2.22090	-0.58662	-0.11177
O	5.56278	0.59262	-0.08825
C	0.79447	-0.33568	-0.46654
C	-0.10868	-0.32213	0.77910
H	4.69342	-1.09262	0.58028
H	3.10330	1.20133	-0.83233
H	2.43342	-1.52832	0.39379
H	0.23048	0.46605	1.45422
H	0.44182	-1.12486	-1.13804
H	0.69747	0.61085	-1.00147
H	0.00028	-1.27056	1.31090
C	-4.20601	0.31056	-0.36333
C	-3.39661	1.39078	-0.04083
C	-2.07936	1.18285	0.34313
C	-1.55150	-0.10314	0.41189
C	-2.37264	-1.17900	0.08572
C	-3.69027	-0.97658	-0.29865
H	-5.23435	0.47036	-0.65977
H	-3.79245	2.39728	-0.08436
H	-1.45162	2.02929	0.59859
H	-1.97544	-2.18674	0.13968
H	-4.31654	-1.82478	-0.54361

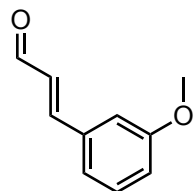


Carbonyl 136

M06-2X/def2-TZVP Geometry

C	3.56282	-0.06559	0.31891
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C	2.24634	-0.24634	-0.30709
C	1.13175	-0.10439	0.40688
O	4.61193	-0.17561	-0.25979
C	-0.25985	-0.24178	-0.10862
C	-1.05934	1.05346	0.05671
H	3.53395	0.18896	1.39776
H	2.23275	-0.49792	-1.36207
H	1.23004	0.15263	1.46141
H	-0.56406	1.85466	-0.49587
H	-0.76958	-1.04095	0.43903
H	-0.24172	-0.53483	-1.16103
H	-1.05740	1.35025	1.11018
C	-2.50514	0.91346	-0.42989
C	-3.29678	-0.05411	0.39475
C	-3.85095	-1.16730	-0.06114
H	-3.39809	0.19433	1.44925
H	-4.40912	-1.83100	0.58618
H	-2.51323	0.59657	-1.47609
H	-2.98276	1.89636	-0.38815
H	-3.76928	-1.44863	-1.10528

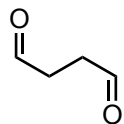


Carbonyl 137

M06-2X/def2-TZVP Geometry

C	3.86706	0.11215	0.00002
C	2.40904	0.26924	-0.00002
C	1.61958	-0.80847	0.00004
O	4.64757	1.02867	-0.00004
C	0.15701	-0.84808	0.00002
C	-0.47564	-2.08602	0.00000
C	-1.86463	-2.15987	-0.00002
C	-2.62425	-1.00951	-0.00003
C	-1.99599	0.24055	-0.00001
C	-0.61295	0.32266	0.00002
O	-2.82338	1.31168	-0.00001
H	4.22374	-0.93747	0.00008
H	2.03637	1.28630	-0.00009
H	2.10489	-1.78234	0.00010
H	0.11950	-2.99022	0.00001
H	-2.35467	-3.12457	-0.00004

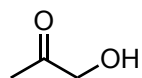
H	-0.12089	1.28356	0.00004
H	-3.70550	-1.04099	-0.00004
C	-2.24132	2.59650	0.00002
H	-1.62897	2.75243	-0.89210
H	-3.06639	3.30311	0.00001
H	-1.62899	2.75241	0.89216



Dialdehyde

M06-2X/def2-TZVP Geometry

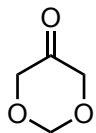
C	-0.36826	0.66100	0.00021
C	0.36826	-0.66100	0.00024
C	-1.86133	0.50143	0.00034
C	1.86133	-0.50143	0.00016
O	2.42707	0.55705	-0.00034
O	-2.42708	-0.55705	-0.00039
H	-0.09041	1.27029	-0.86556
H	-0.09030	1.27039	0.86587
H	0.09031	-1.27039	-0.86542
H	0.09041	-1.27029	0.86601
H	-2.43922	1.44555	-0.00056
H	2.43922	-1.44555	-0.00023



Ketone OH

M06-2X/def2-TZVP Geometry

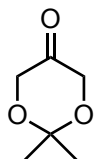
C	-1.83748	-0.46026	0.01846
C	-0.47067	0.16322	-0.01714
C	0.72115	-0.77081	-0.03638
O	1.92488	-0.07689	0.04071
O	-0.29239	1.35577	-0.01501
H	-2.06613	-0.72967	1.05221
H	-2.58048	0.25227	-0.33016
H	-1.87174	-1.37334	-0.57589
H	0.62081	-1.47565	0.79831
H	0.66194	-1.36229	-0.96007
H	1.69766	0.86472	0.02040



Dihydroxyacetone 1

M06-2X/def2-TZVP Geometry

C	-0.29936	1.28948	0.11673
C	-1.09329	0.00000	0.00209
C	-0.29936	-1.28948	0.11673
O	-2.29110	-0.00000	-0.07789
O	1.04339	1.15445	-0.29445
C	1.63372	0.00000	0.22175
O	1.04339	-1.15445	-0.29445
H	-0.77255	2.05810	-0.49060
H	-0.35096	1.60038	1.17130
H	-0.35096	-1.60038	1.17130
H	-0.77255	-2.05810	-0.49060
H	2.67324	0.00000	-0.09305
H	1.55819	0.00000	1.32216

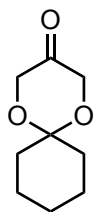


Dihydroxyacetone 2

M06-2X/def2-TZVP Geometry

C	0.88758	1.22470	0.25630
C	1.74747	0.00000	-0.00001
C	0.88758	-1.22470	-0.25629
O	2.94595	-0.00000	-0.00000
O	-0.32458	0.80204	0.84264
C	-1.13902	-0.00000	-0.00000
O	-0.32458	-0.80204	-0.84264
H	1.38513	1.88653	0.96197
H	0.73478	1.76625	-0.68462
H	1.38513	-1.88653	-0.96196
H	0.73478	-1.76624	0.68464
C	-1.98202	-0.85726	0.92405
H	-2.66199	-1.47160	0.33593
H	-1.34644	-1.50253	1.52946
H	-2.55733	-0.21965	1.59393
C	-1.98201	0.85727	-0.92406
H	-2.66198	1.47161	-0.33593
H	-1.34642	1.50253	-1.52946

H -2.55732 0.21965 -1.59393



Dihydroxyacetone 3

M06-2X/def2-TZVP Geometry

C	1.95424	1.06329	0.49410
C	2.56619	-0.14475	-0.19224
C	1.49580	-1.14800	-0.58376
O	3.73817	-0.28791	-0.39846
O	0.78187	0.64843	1.16231
C	-0.25577	0.19785	0.30814
O	0.29841	-0.44366	-0.83276
C	-1.08940	1.35960	-0.21535
C	-1.10173	-0.76841	1.12622
C	-2.29406	0.86675	-1.01460
C	-3.14609	-0.08525	-0.17854
C	-2.31020	-1.25691	0.33192
H	2.64237	1.45317	1.24115
H	1.76152	1.84618	-0.24856
H	1.78136	-1.65559	-1.50283
H	1.38774	-1.89495	0.21142
H	-1.42199	1.93385	0.65302
H	-0.45610	2.00651	-0.82512
H	-0.47511	-1.60088	1.45239
H	-1.42181	-0.23973	2.02772
H	-2.88741	1.71971	-1.34785
H	-1.94055	0.34949	-1.91002
H	-3.56400	0.45926	0.67526
H	-3.99000	-0.45189	-0.76550
H	-1.96177	-1.84775	-0.51951
H	-2.91585	-1.91728	0.95451

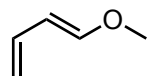


Cyclopentadiene

M06/def2-TZVP Geometry

C	-1.16941	0.28067	0.00000
C	-0.72913	-0.98349	-0.00000
C	0.72911	-0.98350	-0.00000

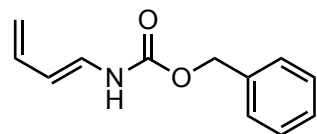
C	1.16942	0.28065	0.00000
C	0.00001	1.20527	0.00001
H	1.34407	-1.87389	-0.00001
H	2.19963	0.60781	0.00000
H	0.00002	1.86728	0.87460
H	-1.34410	-1.87387	-0.00001
H	-2.19962	0.60785	0.00000
H	0.00002	1.86729	-0.87458



Diene 1

M06/def2-TZVP Geometry

C	-2.66134	-0.38377	0.24549
C	-1.83466	0.58038	-0.14499
C	-0.38254	0.55698	-0.05782
C	0.32993	-0.56244	-0.20764
H	0.11893	1.50620	0.09787
O	1.65822	-0.71528	-0.12561
H	-2.26583	1.48581	-0.56761
H	-3.73148	-0.30095	0.10434
H	-2.30029	-1.28501	0.73010
H	-0.15321	-1.50612	-0.44399
C	2.41395	0.42187	0.20188
H	3.45380	0.10617	0.26063
H	2.31599	1.19893	-0.56458
H	2.10429	0.83907	1.16668

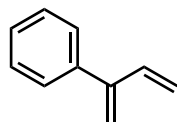


Diene 2

M06/def2-TZVP Geometry

C	-5.26230	1.74905	0.11469
C	-5.20909	0.56905	-0.49452
C	-4.00853	-0.19453	-0.78448
C	-2.89593	-0.14946	-0.05093
H	-4.03971	-0.86073	-1.64452
N	-1.74117	-0.84590	-0.34772
H	-6.14286	0.11773	-0.82296
H	-6.20775	2.23150	0.32678
H	-4.36479	2.27945	0.41553
H	-2.82254	0.43739	0.85819
C	-0.63945	-0.83685	0.46271

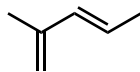
O	-0.54480	-0.23512	1.49695
O	0.31289	-1.61543	-0.07877
H	-1.68664	-1.38827	-1.19537
C	1.56601	-1.63996	0.61861
H	1.37934	-1.63498	1.69386
H	2.01392	-2.59467	0.33803
C	4.05144	1.62785	-0.57278
C	3.89815	0.52962	-1.40403
C	3.09905	-0.52702	-1.00833
C	2.44284	-0.49769	0.21626
C	2.59853	0.60769	1.04087
C	3.40210	1.66507	0.64913
H	4.68016	2.45589	-0.87901
H	4.40759	0.49595	-2.36003
H	2.97853	-1.39212	-1.65373
H	2.07235	0.63793	1.98862
H	3.51892	2.52367	1.29999



Diene 3

M06/def2-TZVP Geometry

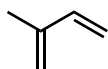
C	-1.77818	1.64665	-0.39091
C	-1.29149	0.47379	0.01845
C	-2.18437	-0.58852	0.50216
C	-3.35690	-0.89933	-0.03216
H	-1.82425	-1.15956	1.35620
H	-1.13779	2.41891	-0.79978
H	-2.83701	1.86572	-0.32819
H	-3.72678	-0.39263	-0.91742
H	-3.98346	-1.67646	0.38771
C	2.89250	-0.39012	-0.03669
C	1.96635	-1.39736	-0.24456
C	0.61260	-1.11420	-0.21344
C	0.15617	0.18232	0.01530
C	1.10106	1.18314	0.23398
C	2.45357	0.90169	0.20516
H	3.95323	-0.61136	-0.05521
H	2.29939	-2.41133	-0.43409
H	-0.10755	-1.90629	-0.39021
H	0.76505	2.19067	0.45302
H	3.17138	1.69396	0.38425



Diene 4

M06/def2-TZVP Geometry

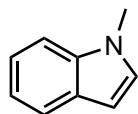
C	-1.44139	1.36871	-0.09029
C	-1.08639	0.08681	-0.05750
C	0.29938	-0.35677	-0.22963
C	1.38279	0.28036	0.20117
H	0.43071	-1.31861	-0.72836
H	-2.47081	1.67162	0.06341
H	-0.72074	2.15430	-0.28543
H	1.25138	1.21072	0.75160
C	-2.08699	-1.00681	0.13744
H	-1.84787	-1.60404	1.02227
H	-3.09856	-0.61531	0.24700
H	-2.07565	-1.69461	-0.71396
C	2.77725	-0.18727	0.00312
H	3.36348	0.54389	-0.56173
H	3.29304	-0.32361	0.95811
H	2.80722	-1.13446	-0.53876



Diene 5

M06/def2-TZVP Geometry

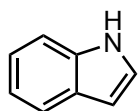
C	-0.58716	1.43260	-0.08943
C	-0.45258	0.10997	-0.05839
C	0.84389	-0.55027	-0.24446
C	2.01254	-0.09969	0.18967
H	0.81115	-1.51002	-0.75953
H	-1.55073	1.90437	0.06568
H	0.25550	2.08473	-0.28730
H	2.08955	0.82240	0.75629
H	2.93238	-0.64104	0.00692
C	-1.61581	-0.80656	0.14279
H	-1.47002	-1.43803	1.02405
H	-2.54853	-0.25525	0.26319
H	-1.72457	-1.48348	-0.71035



N-Me indole

M06/def2-TZVP Geometry

C	1.20383	1.05398	0.00000
C	0.00000	0.36010	0.00000
C	-0.05904	-1.04997	0.00000
C	1.13500	-1.77161	0.00000
C	2.33073	-1.08795	0.00000
C	2.36534	0.31119	0.00000
C	-1.44107	-1.40254	0.00000
C	-2.14355	-0.23833	0.00000
N	-1.28635	0.83561	0.00000
C	-1.65515	2.22257	0.00000
H	1.23167	2.13816	0.00000
H	1.12005	-2.85603	0.00000
H	3.26422	-1.63867	0.00000
H	3.32301	0.81865	0.00000
H	-1.85982	-2.39626	0.00000
H	-3.21081	-0.07126	0.00000
H	-2.74115	2.30422	0.00000
H	-1.26960	2.73359	0.88675
H	-1.26960	2.73359	-0.88675

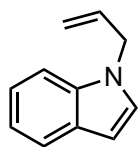


Indole

M06/def2-TZVP Geometry

C	1.35918	0.99681	0.00000
C	0.00000	0.70980	0.00000
C	-0.49042	-0.61234	0.00000
C	0.42294	-1.66827	0.00000
C	1.77065	-1.38796	0.00000
C	2.23469	-0.06687	0.00000
C	-1.91558	-0.52593	0.00000
C	-2.23455	0.79503	0.00000
N	-1.08551	1.54786	0.00000
H	1.71863	2.01998	0.00000
H	0.07268	-2.69459	0.00000
H	2.48869	-2.19971	0.00000
H	3.30202	0.12101	0.00000
H	-2.61593	-1.34594	0.00000
H	-3.20214	1.27234	0.00000

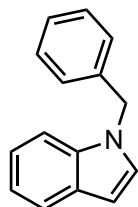
H -1.04685 2.55023 0.00000



N-allyl indole

M06/def2-TZVP Geometry

C	-0.73823	-1.39681	-0.49835
C	-0.30871	-0.08365	-0.35153
C	-1.16094	0.93861	0.11746
C	-2.48689	0.62476	0.41875
C	-2.91977	-0.67319	0.26187
C	-2.05247	-1.67507	-0.18893
C	-0.38103	2.13287	0.17106
C	0.86738	1.80732	-0.25610
N	0.92352	0.47503	-0.59405
H	-0.06508	-2.17857	-0.83241
H	-3.16419	1.39295	0.77524
H	-3.94663	-0.92883	0.49553
H	-2.42002	-2.68926	-0.29223
H	-0.71259	3.11285	0.47528
H	1.75092	2.42062	-0.35888
C	2.12123	-0.24451	-0.92917
C	2.82010	-0.85722	0.24266
H	1.87444	-1.01961	-1.66422
H	2.79879	0.44354	-1.44720
C	2.43424	-0.74774	1.50069
H	2.99111	-1.21535	2.30254
H	1.54560	-0.18968	1.77913
H	3.71340	-1.42616	-0.00485

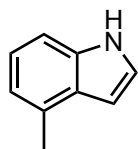


N-Bn indole

M06/def2-TZVP Geometry

C	1.30407	-1.24647	-0.88378
C	1.39413	0.06034	-0.42036
C	2.46238	0.50240	0.38795
C	3.47751	-0.39852	0.71286
C	3.39862	-1.69143	0.24533
C	2.32072	-2.11233	-0.54250
C	2.20861	1.87386	0.69149

C	1.04286	2.20446	0.07530
N	0.54496	1.12304	-0.61417
H	0.46227	-1.57695	-1.48240
H	4.31375	-0.08389	1.32739
H	4.17978	-2.40049	0.49336
H	2.28354	-3.13926	-0.88655
H	2.82422	2.53443	1.28102
H	0.50555	3.14163	0.05784
C	-0.73879	1.05563	-1.25485
H	-1.04409	2.08137	-1.48630
H	-0.63297	0.54612	-2.21941
C	-3.85366	-0.82615	1.01732
C	-2.69996	-0.40219	1.65288
C	-1.68183	0.19667	0.92914
C	-1.80881	0.37589	-0.44008
C	-2.96600	-0.05928	-1.07293
C	-3.98462	-0.65376	-0.35104
H	-4.64760	-1.29647	1.58540
H	-2.58732	-0.54083	2.72189
H	-0.77570	0.51928	1.43219
H	-3.06600	0.06879	-2.14719
H	-4.88151	-0.98969	-0.85852

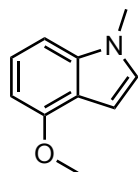


5-Me indole

M06/def2-TZVP Geometry

C	0.04025	1.95008	-0.00000
C	0.77007	0.76688	0.00000
C	0.15285	-0.49840	0.00000
C	-1.24606	-0.59139	-0.00000
C	-1.96147	0.58830	-0.00000
C	-1.33173	1.83921	-0.00000
C	1.19721	-1.47212	0.00000
C	2.37488	-0.79217	0.00000
N	2.12562	0.55821	0.00000
H	0.52909	2.91779	0.00000
C	-1.90997	-1.92680	-0.00000
H	-3.04601	0.54415	-0.00000
H	-1.93963	2.73648	-0.00000
H	1.08724	-2.54520	0.00000
H	3.38797	-1.16300	0.00000
H	2.82418	1.27824	0.00001

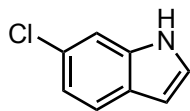
H	-2.99646	-1.83231	-0.00001
H	-1.62097	-2.51258	-0.87773
H	-1.62098	-2.51257	0.87774



N-Me 5-OMe indole

M06/def2-TZVP Geometry

C	0.80623	1.77533	-0.00000
C	1.00676	0.39569	-0.00000
C	-0.05336	-0.52616	0.00000
C	-1.36944	-0.04614	-0.00000
C	-1.58185	1.31960	-0.00000
C	-0.49804	2.20987	-0.00000
C	0.51666	-1.83050	0.00000
C	1.86610	-1.66145	0.00000
N	2.17502	-0.32065	-0.00000
H	1.63469	2.47368	-0.00000
O	-2.33981	-0.98577	0.00000
H	-2.58627	1.72161	-0.00000
H	-0.70504	3.27378	-0.00000
H	-0.01451	-2.76799	0.00000
H	2.65967	-2.39396	0.00000
C	3.49126	0.25028	0.00000
C	-3.67236	-0.55340	0.00000
H	-4.29343	-1.44772	0.00000
H	-3.90487	0.04177	0.89054
H	-3.90488	0.04177	-0.89054
H	4.22914	-0.55073	-0.00001
H	3.65354	0.86992	-0.88652
H	3.65355	0.86989	0.88654

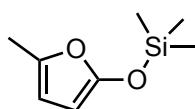


7-Cl indole

M06/def2-TZVP Geometry

C	-0.47334	-0.99055	-0.00000
C	0.86003	-0.60169	-0.00000
C	1.25556	0.75211	0.00000
C	0.26833	1.73818	0.00000

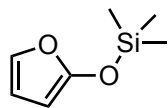
C	-1.05713	1.37015	0.00000
C	-1.40988	0.01717	0.00000
C	2.68265	0.76698	0.00000
C	3.09387	-0.52765	-0.00000
N	1.99982	-1.36049	-0.00000
H	-0.77601	-2.03058	-0.00000
H	-1.84226	2.11548	0.00001
Cl	-3.09927	-0.40192	0.00000
H	3.32276	1.63464	0.00000
H	4.09232	-0.93607	-0.00000
H	0.53955	2.78780	0.00001
H	2.03194	-2.36325	-0.00000



Furan 1

M06/def2-TZVP Geometry

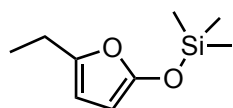
C	2.54107	-0.26808	-0.00001
C	2.89393	1.03316	0.00000
C	1.69061	1.80569	0.00001
C	0.68500	0.90225	-0.00000
O	1.17002	-0.36092	-0.00001
H	3.90661	1.40545	0.00001
H	1.58091	2.87664	0.00001
O	-0.62434	1.04784	-0.00000
H	3.06443	-2.14392	0.88136
C	3.28939	-1.53634	-0.00001
H	3.06443	-2.14391	-0.88140
H	4.35881	-1.32580	-0.00001
Si	-1.81801	-0.12968	0.00000
C	-1.67618	-1.16897	-1.53370
H	-2.50809	-1.87562	-1.58952
H	-1.70429	-0.54899	-2.43221
H	-0.74658	-1.74024	-1.54161
C	-1.67617	-1.16897	1.53371
H	-1.70427	-0.54899	2.43222
H	-2.50808	-1.87561	1.58954
H	-0.74657	-1.74023	1.54161
C	-3.38512	0.86305	0.00001
H	-3.44365	1.50192	0.88330
H	-3.44366	1.50192	-0.88329
H	-4.25850	0.20678	0.00001



Furan 2

M06/def2-TZVP Geometry

C	2.73474	-0.93634	0.00000
C	3.32491	0.27416	-0.00001
C	2.28057	1.24692	-0.00002
C	1.12615	0.53794	-0.00001
O	1.37374	-0.78884	-0.00000
H	4.38667	0.46123	-0.00001
H	2.36484	2.32012	-0.00002
O	-0.13230	0.92095	-0.00002
Si	-1.52522	-0.01610	0.00000
C	-1.57430	-1.06241	-1.53409
H	-2.52110	-1.60553	-1.59014
H	-1.48907	-0.44758	-2.43251
H	-0.76459	-1.79374	-1.54256
C	-1.57428	-1.06235	1.53414
H	-1.48905	-0.44749	2.43254
H	-2.52108	-1.60547	1.59022
H	-0.76458	-1.79368	1.54263
C	-2.88072	1.24984	-0.00001
H	-2.82067	1.88849	0.88331
H	-2.82068	1.88846	-0.88335
H	-3.86024	0.76611	0.00000
H	3.09873	-1.94900	0.00001

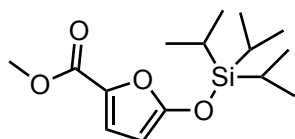


Furan 3

M06/def2-TZVP Geometry

C	-2.15300	0.04201	0.00000
C	-2.38051	1.37196	-0.00001
C	-1.10767	2.02482	-0.00001
C	-0.19341	1.02950	-0.00001
O	-0.79735	-0.18135	-0.00000
H	-3.34981	1.84517	-0.00001
H	-0.89622	3.08039	-0.00001
O	1.12374	1.04912	-0.00001
Si	2.20447	-0.23216	-0.00000
C	1.96954	-1.25468	1.53366

H	2.73541	-2.03252	1.58906
H	2.05314	-0.64009	2.43241
H	0.99315	-1.74153	1.54228
C	1.96954	-1.25470	-1.53365
H	0.99315	-1.74155	-1.54226
H	2.05315	-0.64012	-2.43241
H	2.73541	-2.03254	-1.58904
C	3.85635	0.61198	-0.00000
H	3.97398	1.24265	-0.88328
H	3.97398	1.24266	0.88327
H	4.66523	-0.12231	-0.00000
C	-3.01378	-1.15955	0.00001
H	-2.77412	-1.77955	0.87272
H	-2.77413	-1.77955	-0.87270
C	-4.48785	-0.81473	0.00001
H	-5.10059	-1.71642	0.00001
H	-4.75529	-0.22813	0.88171
H	-4.75529	-0.22813	-0.88170

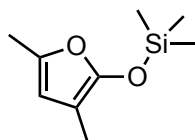


Furan 4

M06/def2-TZVP Geometry

C	-2.43267	-0.76327	-0.21027
C	-2.45707	-2.09121	-0.49870
C	-1.11728	-2.53736	-0.54117
C	-0.35969	-1.43351	-0.27070
O	-1.13077	-0.35685	-0.06988
H	-3.35066	-2.67231	-0.66126
H	-0.74389	-3.52714	-0.74027
O	0.93085	-1.26753	-0.17917
Si	1.74784	0.19526	0.12065
C	1.30440	0.84948	1.83718
H	2.27060	1.20430	2.22977
C	0.33598	2.02664	1.84686
C	0.79902	-0.24895	2.76927
C	3.54536	-0.35433	0.08904
C	3.85370	-1.34871	1.20293
C	3.97274	-0.92593	-1.25675
H	4.12557	0.56071	0.28006
C	1.31584	1.42214	-1.23762
C	2.35942	2.53441	-1.28802
C	1.11224	0.80149	-2.61348

H	0.36053	1.86462	-0.92721
C	-3.44236	0.25851	-0.03347
O	-3.22412	1.41303	0.22446
O	-4.67341	-0.25678	-0.19739
C	-5.73553	0.66845	-0.04272
H	-5.65836	1.47799	-0.77075
H	-6.65410	0.10853	-0.20312
H	-5.73244	1.10412	0.95805
H	0.17814	2.37822	2.87138
H	0.70143	2.87616	1.26520
H	-0.64169	1.74804	1.44399
H	0.70389	0.12966	3.79144
H	-0.19353	-0.59063	2.46250
H	1.45273	-1.12348	2.79770
H	2.04389	3.33639	-1.96205
H	2.54230	2.98561	-0.30738
H	3.31923	2.16183	-1.65925
H	2.02270	0.32351	-2.98448
H	0.32353	0.04598	-2.61576
H	0.83157	1.56906	-3.34175
H	3.34968	-1.78138	-1.53525
H	3.90686	-0.19225	-2.06279
H	5.00872	-1.27753	-1.21783
H	4.90773	-1.64254	1.17735
H	3.65098	-0.94245	2.19641
H	3.25991	-2.26077	1.08776

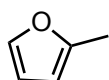


Furan 5

M06/def2-TZVP Geometry

C	2.34315	-0.85419	-0.00840
C	2.82222	0.40338	0.07366
C	1.71387	1.30578	-0.04535
C	0.63587	0.50267	-0.19562
O	0.98411	-0.80730	-0.17880
H	3.85977	0.67131	0.20775
C	1.72392	2.78871	-0.01755
O	-0.64255	0.78867	-0.37787
H	2.56841	-2.78431	0.88140
C	2.95753	-2.19154	0.04844
H	2.77936	-2.76091	-0.86824
H	4.03481	-2.09112	0.18005

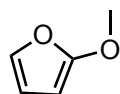
Si	-1.97162	-0.14624	0.02869
C	-2.12532	-1.57813	-1.14485
H	-3.04059	-2.13983	-0.94126
H	-2.16807	-1.23396	-2.18031
H	-1.27913	-2.26001	-1.04741
C	-1.78684	-0.73256	1.78328
H	-1.62454	0.10695	2.46274
H	-2.68921	-1.25650	2.10780
H	-0.94529	-1.42017	1.88496
C	-3.39989	1.02301	-0.16022
H	-3.30937	1.87066	0.52157
H	-3.45175	1.41269	-1.17881
H	-4.34383	0.51631	0.05362
H	2.13884	3.17532	0.91734
H	2.32308	3.20694	-0.83112
H	0.71072	3.18016	-0.11867



5-methyl furan

M06/def2-TZVP Geometry

O	1.03051	-0.23913	0.00000
C	0.49667	-1.48361	0.00000
C	-0.85029	-1.41815	0.00000
C	-1.17486	-0.02991	0.00000
C	-0.00000	0.64113	0.00000
C	0.34969	2.07314	0.00000
H	1.19821	-2.30158	0.00000
H	-1.53218	-2.25298	0.00000
H	-2.15712	0.41565	0.00000
H	-0.55806	2.67574	0.00000
H	0.93890	2.34032	0.88091
H	0.93890	2.34032	-0.88091

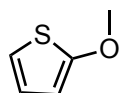


5-methoxy furan

M06/def2-TZVP Geometry

O	-0.17242	-0.92546	0.00005
C	-1.54226	-0.98369	0.00002
C	-2.05077	0.26360	-0.00007

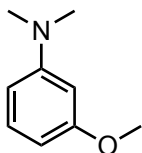
C	-0.94641	1.16657	-0.00009
C	0.15405	0.37572	-0.00001
O	1.43947	0.70250	0.00001
C	2.38086	-0.35068	0.00007
H	-1.96883	-1.97137	0.00006
H	-3.09773	0.52105	-0.00011
H	-0.95867	2.24283	-0.00015
H	3.36191	0.11923	0.00008
H	2.27702	-0.97860	0.88875
H	2.27706	-0.97866	-0.88858



5-methoxy thiophene

M06/def2-TZVP Geometry

C	-1.90786	-0.60265	0.00006
C	-1.98240	0.75186	0.00001
C	-0.72091	1.38917	-0.00009
C	0.30493	0.49425	-0.00007
O	1.60285	0.82146	-0.00019
C	2.53534	-0.22926	0.00003
H	-2.70731	-1.32637	0.00012
H	-2.92178	1.28912	0.00000
H	-0.55884	2.45801	-0.00017
H	3.52500	0.22310	-0.00016
H	2.42680	-0.85668	0.89234
H	2.42670	-0.85714	-0.89195
S	-0.27425	-1.14512	0.00011

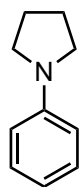


Aromatic amine 1

M06/def2-TZVP Geometry

C	0.74269	1.52603	-0.01319
C	-0.54106	2.02328	0.00296
C	-1.65509	1.19685	0.00551
C	-1.44528	-0.17545	-0.00618
C	-0.15959	-0.69920	-0.02177
C	0.95841	0.13624	-0.03155
N	2.23117	-0.38490	-0.06047
O	-2.43900	-1.09522	-0.00115

C	-3.76221	-0.63689	0.01828
C	3.36811	0.48982	0.03843
C	2.42302	-1.80738	0.01947
H	1.57671	2.21395	-0.01131
H	-0.68517	3.09808	0.01593
H	-2.64869	1.62207	0.01945
H	-0.06748	-1.77691	-0.02607
H	-4.39972	-1.51976	0.02017
H	-3.97464	-0.04415	0.91544
H	-3.99664	-0.03223	-0.86535
H	3.39579	1.21409	-0.78296
H	3.38592	1.05456	0.98010
H	4.28081	-0.10085	-0.01489
H	1.93481	-2.32854	-0.81140
H	3.48704	-2.03095	-0.03134
H	2.03116	-2.23310	0.95300

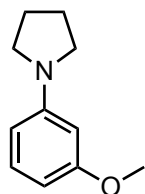


Aromatic amine 2

M06/def2-TZVP Geometry

C	1.25008	-1.19668	0.09842
C	2.63130	-1.18657	0.09685
C	3.33908	-0.00004	0.00040
C	2.63140	1.18651	-0.09648
C	1.25018	1.19665	-0.09888
C	0.52626	-0.00000	-0.00044
N	-0.84224	0.00003	-0.00092
C	-1.64640	1.20287	0.02679
C	-3.04257	0.68664	0.32617
C	-3.04283	-0.68664	-0.32533
C	-1.64644	-1.20279	-0.02697
H	0.72506	-2.13966	0.18836
H	3.16276	-2.12857	0.17694
H	4.42188	-0.00006	0.00073
H	0.72523	2.13963	-0.18922
H	-1.28739	1.90168	0.79031
H	-1.61263	1.73329	-0.93769
H	-3.17450	0.58568	1.40756
H	-3.82628	1.34727	-0.04518
H	-3.82624	-1.34727	0.04666
H	-3.17556	-0.58573	-1.40663

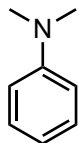
H	-1.28819	-1.90216	-0.79031
H	-1.61182	-1.73251	0.93789
H	3.16293	2.12849	-0.17626



Aromatic amine 3

M06/def2-TZVP Geometry

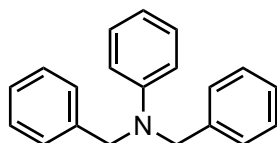
C	0.13336	1.71540	-0.08588
C	1.46974	2.04537	-0.09508
C	2.46914	1.08359	-0.04625
C	2.08788	-0.25076	0.01406
C	0.74632	-0.60698	0.02686
C	-0.25330	0.36508	-0.02357
N	-1.57417	0.01225	-0.01362
O	2.95843	-1.28653	0.06881
C	4.32859	-0.99806	0.06708
C	-2.03876	-1.35757	-0.05853
C	-3.52744	-1.21640	-0.32023
C	-3.86930	0.09409	0.36978
C	-2.66280	0.96355	0.06277
H	-0.61397	2.49611	-0.14030
H	1.75117	3.09147	-0.14677
H	3.50883	1.37891	-0.05687
H	0.50810	-1.66111	0.09007
H	4.84997	-1.95287	0.11684
H	4.63369	-0.47495	-0.84656
H	4.61822	-0.39062	0.93227
H	-1.52701	-1.92240	-0.84522
H	-1.84485	-1.87931	0.89160
H	-3.70646	-1.12881	-1.39603
H	-4.10350	-2.06666	0.04550
H	-4.80621	0.53625	0.03025
H	-3.94547	-0.06300	1.44987
H	-2.48055	1.71288	0.84044
H	-2.79077	1.50673	-0.88631



Aromatic amine 4

M06/def2-TZVP Geometry

C	-0.54640	1.19905	-0.01516
C	-1.92769	1.18895	0.00771
C	-2.63635	-0.00000	0.01809
C	-1.92769	-1.18895	0.00771
C	-0.54639	-1.19905	-0.01516
C	0.18120	0.00000	-0.03370
N	1.55793	0.00000	-0.07149
C	2.27621	1.24124	0.02830
C	2.27621	-1.24124	0.02830
H	-0.03068	2.15015	-0.01858
H	-2.45729	2.13525	0.02030
H	-3.71896	-0.00000	0.03754
H	-0.03068	-2.15015	-0.01858
H	2.02221	1.92309	-0.79064
H	2.08017	1.76875	0.97179
H	3.34505	1.04383	-0.02971
H	2.02221	-1.92309	-0.79064
H	3.34505	-1.04383	-0.02971
H	2.08017	-1.76875	0.97179
H	-2.45729	-2.13525	0.02030

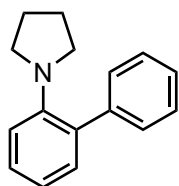


Aromatic amine 5

M06/def2-TZVP Geometry

C	-1.00482	2.26331	-0.65324
C	-0.99409	3.64510	-0.65256
C	0.00090	4.35239	0.00003
C	0.99556	3.64464	0.65263
C	1.00562	2.26284	0.65335
C	0.00022	1.53909	0.00008
N	-0.00009	0.15547	0.00008
C	0.81929	-0.60354	0.90606
C	-0.81964	-0.60320	-0.90603
H	-1.81938	1.74280	-1.14217
H	-1.79012	4.17509	-1.16367

H	0.00117	5.43519	0.00001
H	1.81994	1.74196	1.14228
H	0.92907	-0.05057	1.84601
H	0.27125	-1.51579	1.17564
H	-0.27182	-1.51554	-1.17576
H	-0.92929	-0.05005	-1.84589
H	1.79186	4.17426	1.16372
C	4.71145	-1.75714	-0.50035
C	3.91994	-0.92971	-1.27574
C	2.66205	-0.54958	-0.83364
C	2.18250	-0.99350	0.38848
C	2.98428	-1.82617	1.16088
C	4.23897	-2.20556	0.72361
H	5.69449	-2.05372	-0.84672
H	4.28246	-0.57327	-2.23312
H	2.04521	0.10481	-1.44092
H	2.61272	-2.18124	2.11848
H	4.85167	-2.85571	1.33757
C	-4.71202	-1.75627	0.50024
C	-3.92034	-0.92912	1.27575
C	-2.66238	-0.54917	0.83371
C	-2.18293	-0.99298	-0.38850
C	-2.98487	-1.82538	-1.16101
C	-4.23963	-2.20459	-0.72380
H	-5.69512	-2.05271	0.84657
H	-4.28277	-0.57278	2.23320
H	-2.04538	0.10497	1.44109
H	-2.61338	-2.18038	-2.11867
H	-4.85246	-2.85453	-1.33785

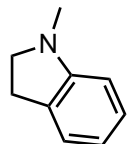


Aromatic amine 6

M06/def2-TZVP Geometry

C	-0.09647	1.22731	-0.04337
C	-0.16173	2.60873	-0.18359
C	0.96087	3.41281	-0.11769
C	2.18679	2.81605	0.11037
C	2.28927	1.44270	0.21558
C	1.16651	0.61241	0.10502
H	-1.14227	3.05947	-0.30047
H	0.87328	4.48790	-0.21320

H	3.26694	1.00388	0.36411
H	3.08285	3.42076	0.19387
N	1.31115	-0.76452	0.14108
C	2.59587	-1.36695	0.44585
C	2.34414	-2.84538	0.24984
C	1.44196	-2.83898	-0.97193
C	0.51570	-1.66478	-0.70056
H	3.38295	-1.03043	-0.24998
H	2.92130	-1.10444	1.45718
H	3.26353	-3.41572	0.11496
H	1.81202	-3.25461	1.11383
H	2.04167	-2.65034	-1.86768
H	0.89823	-3.77145	-1.12562
H	-0.39398	-1.99662	-0.18678
H	0.19657	-1.15765	-1.61673
C	-3.81726	-0.85293	0.26494
C	-3.51939	-0.12862	-0.87677
C	-2.31065	0.53823	-0.98145
C	-1.37434	0.48597	0.04603
C	-1.69067	-0.23717	1.19305
C	-2.89950	-0.90023	1.30220
H	-4.76282	-1.37575	0.34853
H	-4.23136	-0.08396	-1.69306
H	-2.07331	1.09829	-1.88051
H	-0.97117	-0.27761	2.00415
H	-3.12912	-1.45511	2.20481

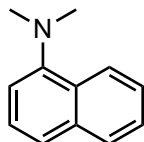


Aromatic amine 7

M06/def2-TZVP Geometry

C	-0.39275	0.93513	-0.03792
C	-1.74339	1.16211	0.07335
C	-2.61735	0.07764	0.09967
C	-2.12135	-1.21114	0.01379
C	-0.75747	-1.45547	-0.09998
C	0.09963	-0.36865	-0.13646
H	-2.12511	2.17507	0.15086
H	-3.68358	0.24247	0.19559
H	-0.38278	-2.47098	-0.15487
H	-2.80645	-2.05084	0.04595
N	1.48177	-0.35714	-0.27344
C	0.77086	1.87885	-0.12076

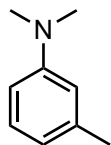
C	1.94480	0.95055	0.17653
H	2.14798	0.92300	1.26160
H	2.87147	1.23036	-0.33018
C	2.25468	-1.49474	0.13224
H	3.30600	-1.32386	-0.10686
H	2.17416	-1.69365	1.21372
H	1.93462	-2.38895	-0.40513
H	0.85503	2.29304	-1.13204
H	0.71035	2.71864	0.57267



Aromatic amine 8

M06/def2-TZVP Geometry

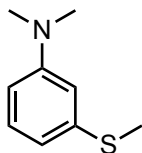
C	0.38980	-0.18396	-0.08160
C	1.42491	0.77583	0.06602
C	1.09899	2.14615	0.15472
C	-0.20097	2.54582	0.08927
C	-1.23572	1.60155	-0.02116
C	-0.96896	0.25611	-0.08306
C	2.76529	0.33704	0.08845
H	1.90150	2.86860	0.25839
H	-2.26152	1.94887	-0.03474
H	-0.45178	3.59907	0.14271
N	-1.99056	-0.71294	-0.16673
C	-2.18013	-1.48907	1.04523
H	-1.22527	-1.81229	1.45684
H	-2.70325	-0.90340	1.81951
C	-3.25673	-0.27339	-0.69586
H	-3.87391	-1.14919	-0.91009
H	-3.82435	0.36379	0.00391
H	-3.10947	0.27885	-1.62472
C	0.74838	-1.53556	-0.26615
H	-2.78011	-2.37627	0.82686
C	2.05744	-1.92665	-0.25327
C	3.07857	-0.98301	-0.05690
H	2.31128	-2.96896	-0.40797
H	-0.03521	-2.25986	-0.45145
H	4.11388	-1.30318	-0.04076
H	3.54699	1.07939	0.21432



Aromatic amine 9

M06/def2-TZVP Geometry

C	-0.50842	-0.78682	-0.02619
C	-1.83409	-0.38352	-0.01218
C	-2.13441	0.97287	-0.00007
C	-1.10605	1.89708	0.00589
C	0.21677	1.50009	-0.00404
C	0.54577	0.13756	-0.02618
H	-3.16938	1.29751	0.00501
H	0.99315	2.25315	0.00047
H	-1.33477	2.95720	0.01683
N	1.85793	-0.27893	-0.05277
C	2.91778	0.68827	0.03142
H	2.88376	1.40245	-0.79912
H	2.88807	1.26530	0.96543
C	2.16895	-1.68035	0.01481
H	3.24891	-1.81136	-0.02036
H	1.80227	-2.14878	0.93804
H	1.74122	-2.23412	-0.82877
H	3.87710	0.17617	-0.01508
H	-0.29814	-1.84968	-0.03958
C	-2.92868	-1.40239	0.02175
H	-3.80598	-1.06160	-0.53133
H	-2.60616	-2.35482	-0.40238
H	-3.25137	-1.59567	1.04897

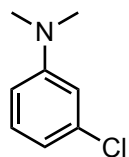


Aromatic amine 10

M06/def2-TZVP Geometry

C	0.11509	-0.59148	-0.01954
C	-1.13562	0.01535	-0.00831
C	-1.24328	1.39931	0.00056
C	-0.07924	2.15097	0.00017
C	1.16820	1.56552	-0.01166
C	1.29009	0.16588	-0.02732
H	-2.20505	1.89345	0.01038
H	2.04738	2.19488	-0.00842

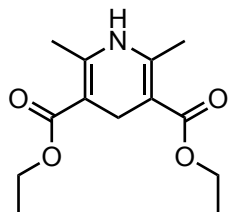
H	-0.14985	3.23324	0.01107
N	2.52454	-0.44008	-0.05119
C	3.71777	0.35786	0.03551
H	3.77467	0.93037	0.97076
H	4.58887	-0.29291	-0.01146
C	2.62246	-1.87277	0.01943
H	2.19749	-2.27795	0.94737
H	2.10873	-2.35659	-0.81882
H	3.67005	-2.16447	-0.02457
H	3.79229	1.06965	-0.79405
H	0.16115	-1.67375	-0.02198
S	-2.51030	-1.08867	-0.00464
C	-3.92269	0.02112	0.02460
H	-3.95510	0.65461	-0.86259
H	-4.80338	-0.61986	0.03048
H	-3.93075	0.63809	0.92392



Aromatic amine 11

M06/def2-TZVP Geometry

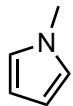
C	-0.28895	-0.60286	-0.00776
C	-1.51720	0.02516	-0.00111
C	-1.64897	1.40040	0.00361
C	-0.48581	2.15089	0.00254
C	0.76060	1.55817	-0.00418
C	0.88774	0.16035	-0.01214
H	-2.62795	1.86000	0.00943
H	1.64051	2.18670	-0.00310
H	-0.55259	3.23296	0.00802
N	2.11954	-0.44537	-0.02466
C	3.31436	0.35460	0.01249
H	3.37852	0.96541	0.92180
H	4.18451	-0.29828	-0.01212
C	2.21713	-1.88009	0.00813
H	1.77034	-2.30690	0.91491
H	1.72512	-2.34371	-0.85480
H	3.26569	-2.16977	-0.01465
H	3.38144	1.03074	-0.84771
H	-0.25897	-1.68327	-0.00940
Cl	-2.95158	-0.96212	0.00299



HE

M06/def2-TZVP Geometry

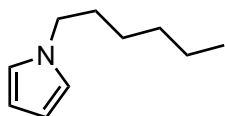
C	0.00003	0.10426	0.01095
C	-1.25800	-0.72479	0.00295
C	-1.21880	-2.07311	0.00599
N	0.00006	-2.71383	0.01228
C	1.21891	-2.07308	0.00594
C	1.25808	-0.72477	0.00299
C	-2.38939	-2.99666	0.00159
C	2.38951	-2.99663	0.00152
C	2.54834	-0.03742	-0.00601
C	-2.54828	-0.03751	-0.00626
O	2.38252	1.30036	0.00315
O	-2.38257	1.30028	0.00331
O	-3.64439	-0.54625	-0.02065
O	3.64447	-0.54612	-0.01988
C	3.57713	2.07634	-0.00477
C	3.18026	3.52379	0.00595
C	-3.57725	2.07613	-0.00477
C	-3.18055	3.52362	0.00673
H	0.00001	0.77414	0.87918
H	0.00005	0.78896	-0.84520
H	0.00007	-3.71924	0.01311
H	-3.04395	-2.81004	0.85194
H	-3.00477	-2.84952	-0.88559
H	-2.05856	-4.03710	0.03156
H	3.00558	-2.84860	-0.88502
H	2.05867	-4.03710	0.03017
H	3.04338	-2.81091	0.85262
H	4.16738	1.81979	-0.88957
H	4.18434	1.81153	0.86602
H	2.59525	3.76115	0.89599
H	2.57875	3.76973	-0.87066
H	4.06809	4.15786	0.00073
H	-4.18480	1.81088	0.86564
H	-4.16710	1.81990	-0.88994
H	-2.59605	3.76070	0.89719
H	-2.57858	3.76997	-0.86945
H	-4.06844	4.15759	0.00128



N-Me pyrrole

M06/def2-TZVP Geometry

N	-0.62070	0.00000	-0.03413
C	0.17340	-1.11101	-0.01253
C	1.48085	-0.70654	0.01382
C	1.48086	0.70654	0.01382
C	0.17341	1.11101	-0.01253
C	-2.05788	-0.00000	0.02328
H	-0.26405	-2.09772	-0.02197
H	2.34272	-1.35492	0.01986
H	2.34272	1.35492	0.01987
H	-0.26404	2.09773	-0.02196
H	-2.44653	0.88411	-0.48280
H	-2.44656	-0.88389	-0.48318
H	-2.42316	-0.00021	1.05388

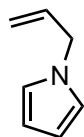


N-hexyl pyrrole

M06/def2-TZVP Geometry

N	1.97243	0.48389	-0.13958
C	2.23115	-0.46146	-1.09077
C	2.82913	-1.53417	-0.48557
C	2.93000	-1.23160	0.89152
C	2.38919	0.01340	1.07354
C	1.20535	1.69264	-0.34134
H	1.95990	-0.28722	-2.12106
H	3.16727	-2.43137	-0.97913
H	3.36512	-1.84994	1.66071
H	2.27157	0.61135	1.96476
H	1.74493	2.53619	0.10010
H	1.15819	1.86934	-1.41986
C	-0.19479	1.59667	0.23519
H	-0.13221	1.51914	1.32740
H	-0.71939	2.53647	0.02641
C	-0.98927	0.42659	-0.30710
H	-0.47357	-0.51018	-0.06012
H	-1.01037	0.47501	-1.40499
C	-2.40639	0.37871	0.22527
H	-2.38143	0.34005	1.32268

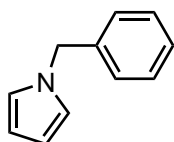
H	-2.92720	1.31271	-0.02614
C	-3.20432	-0.79806	-0.29956
H	-3.22437	-0.75823	-1.39525
H	-2.68107	-1.72729	-0.04565
C	-4.61723	-0.83430	0.24233
H	-5.16331	0.07448	-0.02541
H	-5.18199	-1.68531	-0.14211
H	-4.61612	-0.90293	1.33361



N-allyl pyrrole

M06/def2-TZVP Geometry

N	-0.15069	-0.58649	0.00022
C	-0.85561	-0.21912	-1.11209
C	-2.02439	0.36581	-0.70759
C	-2.02438	0.36637	0.70732
C	-0.85558	-0.21824	1.11227
C	1.20707	-1.06362	0.00040
H	-0.45635	-0.40516	-2.09767
H	-2.80209	0.73798	-1.35545
H	-2.80206	0.73905	1.35490
H	-0.45630	-0.40348	2.09798
H	1.34804	-1.70897	0.87470
H	1.34804	-1.70962	-0.87342
C	2.23342	0.02373	-0.00001
C	1.96918	1.31749	-0.00051
H	2.76337	2.05312	-0.00079
H	0.94929	1.69022	-0.00066
H	3.26458	-0.32215	0.00014

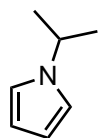


N-Bn pyrrole

M06/def2-TZVP Geometry

N	-1.54062	-0.66211	-0.00001
C	-2.15296	-0.15499	-1.11225
C	-3.17220	0.66336	-0.70719
C	-3.17218	0.66331	0.70728
C	-2.15294	-0.15506	1.11227
C	-0.30918	-1.40476	-0.00005

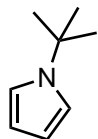
H	-1.80265	-0.42122	-2.09807
H	-3.85448	1.19086	-1.35475
H	-3.85446	1.19077	1.35489
H	-1.80262	-0.42136	2.09807
H	-0.30505	-2.06245	0.87560
H	-0.30506	-2.06239	-0.87574
C	3.27660	0.95112	0.00001
C	2.04467	1.57956	0.00003
C	0.87611	0.83356	0.00002
C	0.93247	-0.55139	-0.00003
C	2.17366	-1.17674	-0.00005
C	3.33885	-0.43367	-0.00003
H	4.18819	1.53712	0.00002
H	1.98805	2.66201	0.00007
H	-0.08723	1.33339	0.00004
H	2.22253	-2.26242	-0.00008
H	4.29967	-0.93545	-0.00005



N-iPr pyrrole

M06/def2-TZVP Geometry

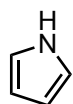
N	-0.12810	-0.10024	-0.15829
C	-1.09131	-0.98095	-0.56169
C	-2.31666	-0.47484	-0.22004
C	-2.08909	0.76045	0.42582
C	-0.73455	0.96157	0.45340
C	1.30643	-0.33185	-0.25636
H	-0.81785	-1.89520	-1.06645
H	-3.27015	-0.93685	-0.42121
H	-2.83400	1.43341	0.82043
H	-0.15672	1.77632	0.86118
H	1.41328	-1.17493	-0.94754
C	1.88084	-0.72746	1.09005
H	2.94130	-0.97227	1.00012
H	1.78294	0.09533	1.80309
H	1.35684	-1.59338	1.49785
C	2.02019	0.86767	-0.84339
H	1.57746	1.16408	-1.79514
H	1.97445	1.72293	-0.16467
H	3.07411	0.63474	-1.00641



N-tBu pyrrole

M06/def2-TZVP Geometry

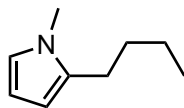
N	0.31949	0.02488	-0.00000
C	1.10851	-1.09503	0.00004
C	2.42127	-0.71055	0.00002
C	2.44060	0.70023	-0.00005
C	1.13876	1.12302	-0.00006
C	-1.15337	-0.00070	0.00001
H	0.67677	-2.08337	0.00009
H	3.27189	-1.37387	0.00004
H	3.30874	1.34025	-0.00008
H	0.74183	2.12380	-0.00010
C	-1.63549	-0.72178	1.25098
H	-2.72774	-0.73402	1.28012
H	-1.28662	-1.75552	1.27794
H	-1.26990	-0.21604	2.14736
C	-1.63550	-0.72190	-1.25089
H	-1.26993	-0.21625	-2.14733
H	-1.28664	-1.75564	-1.27775
H	-2.72775	-0.73414	-1.28001
C	-1.70111	1.41430	-0.00006
H	-1.38865	1.96750	-0.88830
H	-2.79174	1.37011	-0.00005
H	-1.38864	1.96759	0.88813



Pyrrole

M06/def2-TZVP Geometry

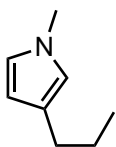
N	-1.11554	0.00000	-0.00000
C	-0.32884	1.11598	-0.00000
C	0.97627	0.70759	-0.00000
C	0.97627	-0.70759	0.00000
C	-0.32885	-1.11598	0.00000
H	-0.75966	2.10408	-0.00001
H	1.83894	1.35460	-0.00000
H	1.83893	-1.35461	0.00000
H	-0.75967	-2.10408	0.00000
H	-2.11888	0.00000	0.00000



N-Me 2-butyl pyrrole

M06/def2-TZVP Geometry

N	1.94693	0.52061	0.00000
C	2.95762	-0.40385	-0.00000
C	2.39978	-1.65005	-0.00001
C	0.99601	-1.47759	-0.00001
C	0.73793	-0.12955	-0.00000
H	3.98894	-0.08604	-0.00000
H	2.93831	-2.58431	-0.00002
H	0.25170	-2.25882	-0.00001
C	2.12603	1.94641	0.00001
H	1.67869	2.40549	-0.88567
H	1.67869	2.40548	0.88570
H	3.19178	2.16996	0.00002
C	-0.54236	0.62389	0.00000
H	-0.58575	1.29201	0.87274
H	-0.58575	1.29201	-0.87272
C	-1.77216	-0.26054	-0.00000
H	-1.74850	-0.92104	-0.87538
H	-1.74850	-0.92104	0.87537
C	-3.06364	0.53240	0.00000
H	-3.08121	1.19395	0.87455
H	-3.08121	1.19396	-0.87454
C	-4.28982	-0.35507	-0.00000
H	-5.21472	0.22406	0.00000
H	-4.30365	-1.00309	-0.88053
H	-4.30365	-1.00310	0.88051

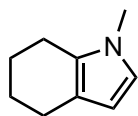


N-Me 3-Pr pyrrole

M06/def2-TZVP Geometry

N	-1.86763	-0.14075	0.01662
C	-1.58729	1.05332	-0.58014
C	-0.28745	1.38039	-0.30242
C	0.25459	0.34191	0.49693
C	-0.74520	-0.57977	0.66498
H	-2.34423	1.57367	-1.14721
H	0.22215	2.27793	-0.62045

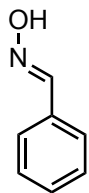
C	-3.09935	-0.87134	-0.10423
H	-3.05822	-1.60892	-0.91075
H	-3.31775	-1.39126	0.82961
H	-3.91604	-0.17914	-0.30963
H	-0.74715	-1.51607	1.20438
C	1.64459	0.25702	1.02655
H	1.85372	1.12236	1.66549
H	1.72921	-0.62694	1.67024
C	2.70453	0.17916	-0.06700
H	2.63720	1.07506	-0.69474
H	3.69630	0.20646	0.39614
C	2.56998	-1.05922	-0.92745
H	3.36393	-1.12212	-1.67386
H	2.61520	-1.96506	-0.31495
H	1.61270	-1.06944	-1.45395



N-Me dihydroindole

M06/def2-TZVP Geometry

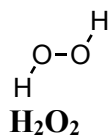
N	-1.61912	-0.20190	0.02344
C	-1.98550	1.11710	-0.01418
C	-0.85240	1.88191	-0.06039
C	0.25233	0.99576	-0.05072
C	-0.25161	-0.27850	-0.00355
H	-3.02847	1.39448	-0.00228
H	-0.81849	2.96047	-0.08975
C	-2.51522	-1.32357	0.06560
H	-3.53757	-0.96013	0.16025
H	-2.44762	-1.92686	-0.84430
H	-2.29933	-1.96912	0.92087
C	1.71842	1.26730	-0.06910
H	2.04371	1.54965	-1.07941
H	1.96393	2.11887	0.57315
C	2.48500	0.02830	0.37770
H	3.55555	0.16060	0.19993
H	2.35911	-0.10472	1.45957
C	1.98460	-1.22034	-0.33386
H	2.62230	-2.07728	-0.10255
H	2.05108	-1.06034	-1.41687
C	0.53794	-1.53441	0.03390
H	0.50033	-1.98720	1.03560
H	0.12802	-2.28635	-0.65067



OH imine

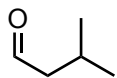
M06/def2-TZVP Geometry

N	2.28360	-0.47405	-0.00000
C	1.43326	0.46803	-0.00000
C	0.00000	0.20872	0.00000
O	3.57447	0.00788	-0.00000
C	-0.52136	-1.08494	0.00000
C	-1.88607	-1.28413	0.00000
C	-2.75418	-0.20065	0.00000
C	-2.24680	1.08605	0.00000
C	-0.87782	1.28800	0.00000
H	1.76794	1.50904	-0.00000
H	4.11001	-0.79087	-0.00000
H	0.16138	-1.92623	-0.00000
H	-2.28200	-2.29313	0.00000
H	-3.82565	-0.36306	0.00000
H	-2.91828	1.93661	0.00000
H	-0.47645	2.29653	0.00000



M06/def2-TZVP Geometry

O	0.00000	0.71060	-0.05745
H	-0.79283	0.89892	0.45962
O	-0.00000	-0.71060	-0.05745
H	0.79283	-0.89892	0.45962

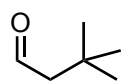


Carbonyl 15

M06/def2-TZVP Geometry

C	-0.30471	-0.82361	0.40585
C	0.72902	0.04273	-0.29014
C	-1.73486	-0.43176	0.20325
O	-2.12264	0.42724	-0.53475

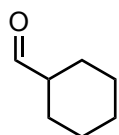
C	2.08232	-0.64302	-0.27115
H	-0.11627	-0.86358	1.48879
H	-0.23152	-1.87085	0.07776
H	0.40849	0.17247	-1.33053
C	0.81637	1.41318	0.35772
H	-2.45925	-1.03754	0.79904
H	2.05275	-1.61529	-0.76926
H	2.41479	-0.80710	0.75962
H	2.84088	-0.03363	-0.76729
H	1.55230	2.03980	-0.15085
H	-0.14149	1.93414	0.33468
H	1.13151	1.31848	1.40289



Carbonyl 16

M06/def2-TZVP Geometry

C	0.41069	1.03128	0.00007
C	-0.70050	-0.01581	0.00009
C	1.83998	0.58466	-0.00022
O	2.24517	-0.54180	-0.00030
C	-0.62125	-0.88309	-1.24999
H	0.30333	1.70015	0.86748
H	0.30308	1.70038	-0.86713
C	-0.62130	-0.88307	1.25019
C	-2.03043	0.72784	0.00006
H	2.55870	1.44055	0.00006
H	0.30361	-1.45970	-1.28075
H	-0.67546	-0.26922	-2.15463
H	-1.46053	-1.58371	-1.27551
H	-2.86444	0.02090	0.00004
H	-2.13009	1.36334	0.88519
H	-2.13005	1.36335	-0.88507
H	-1.46062	-1.58364	1.27572
H	0.30353	-1.45973	1.28097
H	-0.67548	-0.26918	2.15481

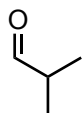


Carbonyl 64

M06/def2-TZVP Geometry

C	-0.11006	-1.01537	0.97068
C	-0.67187	0.38574	0.78754

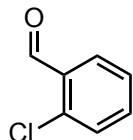
C	0.42653	1.41241	0.52119
C	1.30868	0.99060	-0.64160
C	1.89915	-0.38835	-0.40158
C	0.80399	-1.41696	-0.17664
C	-1.73411	0.46572	-0.27631
O	-2.27622	-0.46230	-0.80132
H	0.45769	-1.03800	1.90861
H	-0.92911	-1.73096	1.07319
H	-1.20234	0.69244	1.70286
H	-0.01827	2.39625	0.33562
H	1.03924	1.51303	1.42416
H	0.71340	0.97227	-1.56518
H	2.09915	1.72890	-0.80072
H	2.53415	-0.68380	-1.24109
H	2.54975	-0.34857	0.48266
H	1.23815	-2.40009	0.02362
H	0.21077	-1.52232	-1.09174
H	-2.01666	1.51651	-0.54101



Carbonyl 65

M06/def2-TZVP Geometry

C	1.10665	-1.25156	0.04386
C	0.34011	-0.00006	-0.35429
C	1.10519	1.25234	0.04384
C	-0.98806	-0.00088	0.34687
O	-2.06123	-0.00031	-0.17819
H	2.09710	-1.25563	-0.41550
H	1.24677	-1.28671	1.12912
H	0.14169	-0.00019	-1.43037
H	1.24525	1.28768	1.12910
H	-0.89152	0.00055	1.46531
H	0.58707	-2.16233	-0.25915
H	0.58454	2.16250	-0.25919
H	2.09564	1.25758	-0.41550

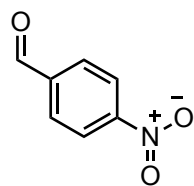


Carbonyl 66

M06/def2-TZVP Geometry

C	1.54750	1.24040	0.00054
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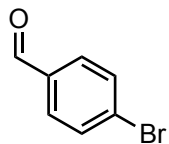
O	1.73107	2.42707	-0.00060
H	2.39622	0.52725	-0.00069
C	-2.37555	-0.42333	-0.00019
C	-1.28929	-1.27793	-0.00016
C	-0.00914	-0.75273	0.00006
C	0.20321	0.62360	0.00026
C	-0.90973	1.46176	0.00022
C	-2.18917	0.95127	0.00000
H	-3.37695	-0.83788	-0.00036
H	-1.42281	-2.35247	-0.00031
Cl	1.32096	-1.87291	0.00008
H	-0.72528	2.53034	0.00038
H	-3.04318	1.61742	-0.00002



Carbonyl 67

M06/def2-TZVP Geometry

C	-3.16536	0.33114	-0.00000
O	-3.92187	-0.59730	0.00001
H	-3.53400	1.38314	0.00001
C	1.03544	0.01039	-0.00002
C	0.46596	1.26806	-0.00002
C	-0.91251	1.35926	-0.00001
C	-1.69145	0.21020	-0.00001
C	-1.09123	-1.04488	-0.00001
C	0.28269	-1.15148	-0.00002
H	1.10182	2.14267	-0.00002
H	-1.39561	2.33114	-0.00001
H	-1.72350	-1.92500	-0.00001
H	0.78414	-2.10967	-0.00002
N	2.51085	-0.09927	-0.00003
O	2.98427	-1.21115	0.00004
O	3.14384	0.93051	0.00005

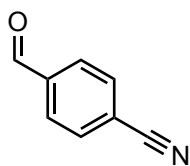


Carbonyl 69

M06/def2-TZVP Geometry

C	-3.56875	0.30545	0.00000
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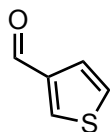
O	-4.32231	-0.62798	0.00000
H	-3.94747	1.35499	-0.00001
C	0.64952	0.03599	-0.00000
C	0.05010	1.28343	-0.00001
C	-1.33000	1.35770	-0.00001
C	-2.10011	0.20301	0.00000
C	-1.47809	-1.04170	0.00001
C	-0.10282	-1.13078	0.00001
H	0.65896	2.17865	-0.00002
H	-1.82193	2.32585	-0.00002
H	-2.09646	-1.93229	0.00002
H	0.39410	-2.09297	0.00002
Br	2.53349	-0.08254	-0.00000



Carbonyl 70

M06/def2-TZVP Geometry

C	-2.77911	0.32910	0.00001
O	-3.54164	-0.59500	0.00000
H	-3.14211	1.38335	0.00005
C	1.44778	-0.01420	-0.00000
C	0.85510	1.24537	0.00002
C	-0.52127	1.34524	0.00002
C	-1.30745	0.20144	0.00001
C	-0.71160	-1.05577	-0.00001
C	0.66019	-1.16697	-0.00002
H	1.47984	2.12978	0.00003
H	-0.99903	2.31991	0.00003
H	-1.34805	-1.93303	-0.00002
H	1.14036	-2.13774	-0.00003
N	4.01690	-0.22003	-0.00001
C	2.87034	-0.12790	-0.00001

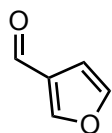


Carbonyl 71

M06/def2-TZVP Geometry

C	2.02630	-0.51987	0.00009
O	2.92921	0.27243	-0.00007
H	2.21901	-1.61847	0.00001

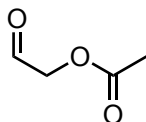
S	-1.92923	-0.37494	0.00019
C	-0.39095	-1.09880	-0.00006
C	0.60861	-0.16459	0.00001
C	0.10762	1.16436	-0.00009
C	-1.24570	1.20395	-0.00026
H	-0.28026	-2.17380	-0.00005
H	0.75200	2.03316	-0.00014
H	-1.89208	2.06841	-0.00042



Carbonyl 72

M06/def2-TZVP Geometry

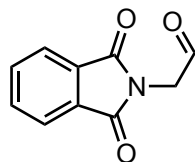
C	1.72281	0.44733	-0.00002
O	2.57832	-0.39652	-0.00002
H	1.97937	1.53238	-0.00002
O	-1.89639	0.51780	0.00000
C	-0.69556	1.10509	0.00003
C	0.29507	0.17372	-0.00000
C	-0.36129	-1.09613	0.00002
C	-1.67927	-0.82719	-0.00001
H	-0.67933	2.18400	0.00004
H	0.11767	-2.06138	0.00002
H	-2.56365	-1.44218	-0.00002



Carbonyl 73

M06/def2-TZVP Geometry

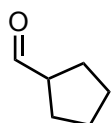
C	1.94333	-0.15149	0.04984
O	1.65356	-1.28063	-0.19965
C	1.02800	1.02507	-0.13809
O	-0.21528	0.65684	-0.67272
C	-1.07402	0.08372	0.20262
C	-2.27750	-0.42993	-0.51032
O	-0.86185	0.01690	1.37676
H	2.94664	0.13056	0.44626
H	1.49284	1.72466	-0.83906
H	0.92267	1.53660	0.82579
H	-2.66713	0.31846	-1.20009
H	-1.98738	-1.30003	-1.10218
H	-3.03805	-0.71938	0.20991



Carbonyl 74

M06/def2-TZVP Geometry

C	3.20682	0.00003	0.64936
O	2.61142	0.00020	1.68255
C	2.54452	-0.00011	-0.70621
N	1.12010	-0.00008	-0.61261
C	0.37117	-1.16182	-0.40214
C	-1.00889	-0.69257	-0.13024
C	-1.00886	0.69256	-0.13029
C	0.37120	1.16172	-0.40239
C	-2.15762	-1.41256	0.10527
C	-3.32296	-0.69465	0.34357
C	-3.32292	0.69478	0.34355
C	-2.15754	1.41262	0.10522
O	0.80536	2.27800	-0.45005
O	0.80523	-2.27813	-0.44993
H	4.31958	-0.00002	0.60835
H	2.87798	0.88364	-1.25900
H	2.87795	-0.88399	-1.25880
H	-2.14233	-2.49605	0.10604
H	-4.24866	-1.22412	0.53555
H	-4.24859	1.22431	0.53550
H	-2.14220	2.49611	0.10590

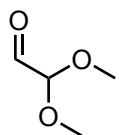


Carbonyl 75

M06/def2-TZVP Geometry

C	1.68305	0.31776	0.06944
O	2.14190	-0.44477	-0.72955
C	0.38143	0.16064	0.80784
C	-0.57306	1.27027	0.32173
C	-1.35277	0.58678	-0.78895
C	-1.64322	-0.78129	-0.19281
C	-0.33951	-1.16170	0.51572
H	2.20891	1.27444	0.30922
H	0.61502	0.30197	1.86876
H	-1.24986	1.55666	1.13179

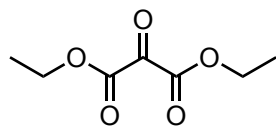
H	-0.04630	2.17549	0.00594
H	-0.71747	0.47994	-1.67587
H	-2.24764	1.13510	-1.08808
H	-2.45782	-0.69084	0.53368
H	-1.95319	-1.52059	-0.93287
H	0.29230	-1.76847	-0.13727
H	-0.51471	-1.74022	1.42326



Carbonyl 76

M06/def2-TZVP Geometry

C	-1.21754	-1.03618	-0.14192
O	-2.31830	-0.59898	-0.01073
C	0.03775	-0.37575	0.41845
O	-0.09567	0.96705	0.70301
O	1.05645	-0.67629	-0.47783
C	2.33853	-0.36575	0.00846
C	-0.35293	1.79471	-0.41224
H	-1.00799	-1.99938	-0.66102
H	0.23856	-0.85317	1.39693
H	3.06143	-0.71520	-0.72722
H	2.46757	0.71122	0.15631
H	2.52652	-0.87100	0.96473
H	-1.30218	1.54355	-0.89326
H	-0.40989	2.81473	-0.03618
H	0.45133	1.73278	-1.15238

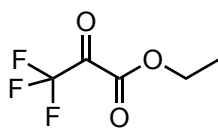


Carbonyl 77

M06/def2-TZVP Geometry

O	-0.00001	1.83834	-0.00000
C	-0.00000	0.64659	0.00000
C	-1.21558	-0.19373	-0.38528
C	1.21558	-0.19372	0.38530
O	2.33606	0.28836	-0.11189
O	-2.33606	0.28836	0.11189
O	-1.09799	-1.13372	-1.11757
O	1.09800	-1.13370	1.11758
C	3.53924	-0.40333	0.26314

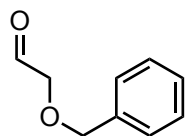
C	4.68322	0.26286	-0.43895
C	-3.53924	-0.40334	-0.26315
C	-4.68322	0.26287	0.43893
H	3.63657	-0.36102	1.35123
H	3.43510	-1.45605	-0.01282
H	4.56044	0.21007	-1.52148
H	4.75736	1.31302	-0.15381
H	5.61939	-0.23116	-0.17610
H	-3.63655	-0.36103	-1.35123
H	-3.43511	-1.45605	0.01283
H	-4.75735	1.31302	0.15377
H	-5.61939	-0.23115	0.17606
H	-4.56046	0.21009	1.52145



Carbonyl 78

M06/def2-TZVP Geometry

O	-0.45341	1.81723	-0.00019
C	-0.56921	0.63618	0.00003
C	-1.96891	-0.03200	-0.00000
C	0.61888	-0.33975	0.00004
O	1.75664	0.32315	0.00010
O	0.48196	-1.52760	-0.00012
C	2.94935	-0.48026	0.00004
C	4.12360	0.45012	0.00011
F	-2.12102	-0.78512	-1.07968
F	-2.12094	-0.78532	1.07956
F	-2.90744	0.89215	0.00012
H	2.92923	-1.12885	0.87999
H	2.92923	-1.12871	-0.88001
H	5.05098	-0.12374	0.00007
H	4.11572	1.08902	-0.88372
H	4.11572	1.08889	0.88404

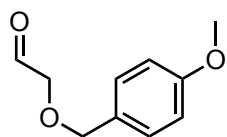


Carbonyl 79

M06/def2-TZVP Geometry

C	0.88878	0.70699	0.07198
C	-0.30230	1.61586	0.16319

O	-1.47487	0.95678	0.57935
C	1.29616	-0.01266	1.18975
C	2.38503	-0.86080	1.11962
C	3.08366	-0.99756	-0.07073
C	2.68394	-0.28790	-1.18850
C	1.58731	0.55675	-1.11579
C	-1.93787	0.01540	-0.33993
C	-3.24849	-0.53552	0.14505
O	-3.89946	-1.32356	-0.47260
H	-0.13014	2.40075	0.90499
H	-0.46929	2.10671	-0.80828
H	0.74342	0.09631	2.11767
H	2.69538	-1.41636	1.99700
H	3.93878	-1.66102	-0.12509
H	3.22265	-0.39578	-2.12267
H	1.26646	1.10847	-1.99453
H	-1.23662	-0.82361	-0.47295
H	-2.09043	0.45848	-1.33812
H	-3.56293	-0.14311	1.14008

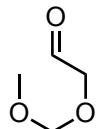


Carbonyl 80

M06/def2-TZVP Geometry

C	0.10201	-1.05472	-0.23641
C	1.45192	-1.64875	-0.49786
O	2.49915	-0.96435	0.15479
C	-0.65848	-0.50574	-1.25134
C	-1.90225	0.06053	-1.00509
C	-2.39355	0.08593	0.29214
C	-1.63221	-0.45620	1.32753
C	-0.40573	-1.01698	1.06156
C	2.68185	0.33864	-0.30498
C	3.88703	0.92909	0.36929
O	4.31972	2.01273	0.11357
O	-3.58464	0.60891	0.64987
C	-4.39119	1.16862	-0.35153
H	1.50456	-2.67543	-0.12529
H	1.64135	-1.67672	-1.58238
H	-0.27437	-0.51628	-2.26746
H	-2.46970	0.47906	-1.82568
H	-2.03590	-0.42520	2.33264
H	0.18450	-1.43428	1.87166
H	2.83765	0.37147	-1.39638

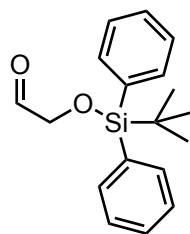
H	1.81543	0.98542	-0.09335
H	4.34570	0.26415	1.13766
H	-4.66790	0.42764	-1.11003
H	-5.29474	1.52667	0.13845
H	-3.89674	2.01259	-0.84555



Carbonyl 111

M06/def2-TZVP Geometry

C	-1.52603	-0.49962	-0.25558
C	-1.12016	0.94664	-0.11020
O	-2.46868	-0.97190	0.30490
O	0.18408	1.22060	-0.53984
C	1.15416	0.90707	0.41124
O	1.27247	-0.45358	0.64697
C	1.94369	-1.14413	-0.37875
H	-0.89786	-1.08528	-0.96683
H	-1.28554	1.25343	0.93210
H	-1.80019	1.53593	-0.73559
H	0.90093	1.36239	1.37816
H	2.09390	1.32867	0.03081
H	1.44043	-1.03050	-1.34553
H	2.97583	-0.78601	-0.47979
H	1.95953	-2.19928	-0.10976

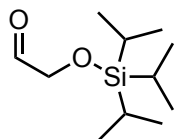


Carbonyl 112

M06/def2-TZVP Geometry

C	2.25736	-1.67184	-2.40840
C	0.83204	-1.23939	-2.21881
O	2.95605	-2.14400	-1.56359
O	0.33331	-1.52898	-0.96616
Si	-0.10693	-0.42442	0.18508
C	1.14691	0.96988	0.18176
C	-1.81099	0.22138	-0.25322
C	-0.15552	-1.40930	1.79298
C	-0.57801	-0.50850	2.94829

C	1.21613	-2.00444	2.09522
C	-1.16888	-2.54006	1.63499
C	-2.51778	-0.35380	-1.30899
C	-3.79541	0.06934	-1.63791
C	-4.39827	1.07952	-0.90936
C	-3.72092	1.65999	0.15049
C	-2.44436	1.23331	0.47235
C	2.50969	0.67012	0.28109
C	3.46705	1.66947	0.27069
C	3.08386	2.99623	0.16130
C	1.74238	3.31606	0.04943
C	0.78779	2.31203	0.05514
H	2.62316	-1.50658	-3.45074
H	0.79447	-0.16422	-2.47146
H	0.23985	-1.74010	-3.00178
H	-1.59603	-0.12946	2.82104
H	-0.55746	-1.07493	3.88709
H	0.09394	0.34813	3.06743
H	1.59359	-2.60741	1.26483
H	1.95457	-1.22866	2.31572
H	1.14931	-2.65022	2.97932
H	-0.88692	-3.22404	0.83031
H	-1.22288	-3.12165	2.56335
H	-2.17367	-2.16241	1.42297
H	-2.06334	-1.15878	-1.87908
H	-4.32334	-0.39385	-2.46389
H	-5.39783	1.41281	-1.16390
H	-4.19042	2.44731	0.72930
H	-1.93332	1.69951	1.31062
H	2.83067	-0.36502	0.34660
H	4.51710	1.41077	0.34600
H	3.83277	3.78007	0.15535
H	1.43671	4.35157	-0.04916
H	-0.25722	2.58279	-0.05541

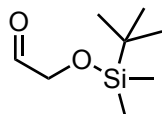


Carbonyl 113

M06/def2-TZVP Geometry

C	-3.40009	-0.10068	0.71329
C	-2.22937	-0.48239	-0.15720
O	-4.53617	-0.13918	0.34890
O	-1.04686	-0.41993	0.56928

Si	0.43724	0.04565	-0.01369
C	0.23991	1.73579	-0.82848
C	1.54187	0.14751	1.51106
C	1.05938	-1.22402	-1.26286
C	1.57481	2.29400	-1.30659
C	-0.45676	2.72676	0.09460
C	3.01815	-0.03600	1.17353
C	1.12728	-0.80885	2.62279
C	0.32197	-1.15994	-2.59518
C	0.98949	-2.63417	-0.68754
H	-3.10279	0.22886	1.73813
H	-2.41709	-1.49353	-0.54722
H	-2.24070	0.19121	-1.02901
H	-0.39783	1.58669	-1.71135
H	1.40967	1.17216	1.88796
H	2.11469	-0.97956	-1.44844
H	1.44035	3.24421	-1.83292
H	2.24107	2.49097	-0.46028
H	2.09646	1.61309	-1.98529
H	-0.61352	3.68827	-0.40449
H	-1.43166	2.36782	0.43486
H	0.14415	2.92516	0.98774
H	3.64232	0.13999	2.05511
H	3.22253	-1.05726	0.83754
H	3.36304	0.64077	0.38722
H	0.09570	-0.64939	2.93814
H	1.21072	-1.85216	2.30376
H	1.77427	-0.68599	3.49743
H	0.72010	-1.89939	-3.29747
H	-0.74305	-1.38362	-2.47428
H	0.40005	-0.18018	-3.07256
H	1.34724	-3.37342	-1.41146
H	1.58789	-2.74660	0.21990
H	-0.04053	-2.90247	-0.43133

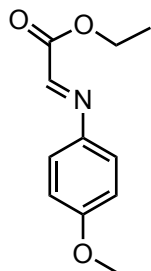


Carbonyl 114

M06/def2-TZVP Geometry

C	3.12797	-0.44569	-0.14452
C	2.26668	0.55611	-0.86107
O	2.73202	-1.42820	0.40551
O	0.93749	0.21150	-0.93110

Si	-0.22490	0.62070	0.18299
C	-1.64212	-0.57539	-0.13708
C	-0.72353	2.39553	-0.11491
C	0.44847	0.48118	1.91602
C	-1.19375	-1.99439	0.19673
C	-2.05480	-0.51040	-1.60363
C	-2.83302	-0.19869	0.73793
H	4.21373	-0.18221	-0.17048
H	2.44839	1.53189	-0.37181
H	2.68598	0.66733	-1.87290
H	0.14647	3.05496	-0.04883
H	-1.17071	2.53374	-1.10140
H	-1.44294	2.73272	0.63540
H	0.80877	-0.52568	2.13173
H	1.27872	1.17578	2.07350
H	-0.32472	0.73842	2.64472
H	-0.94457	-2.10461	1.25608
H	-1.99959	-2.70454	-0.02635
H	-0.31503	-2.28830	-0.38323
H	-2.39605	0.48916	-1.89006
H	-2.88422	-1.20382	-1.78990
H	-1.23228	-0.78909	-2.26668
H	-3.65533	-0.90676	0.57860
H	-2.58538	-0.22482	1.80387
H	-3.21411	0.80010	0.50380

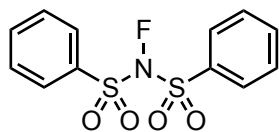


Imine

M06/def2-TZVP Geometry

C	-1.43108	-0.96840	-0.18958
N	-0.69491	0.03341	0.02705
C	0.69598	-0.07140	0.05522
C	-2.91657	-0.88763	-0.18475
O	-3.38415	0.33578	0.03199
O	-3.59939	-1.86167	-0.36406
C	-4.80752	0.46300	0.04424
C	-5.13177	1.90565	0.29574
C	1.42240	1.08566	-0.19284

C	2.80542	1.08120	-0.20636
C	3.48802	-0.09735	0.07030
C	2.76944	-1.25791	0.35850
C	1.39638	-1.24676	0.34625
O	4.82963	-0.21457	0.10127
C	5.60414	0.92515	-0.16435
H	-1.06890	-1.98072	-0.40969
H	-5.20455	0.11128	-0.91256
H	-5.21655	-0.19299	0.81828
H	-4.72513	2.23471	1.25305
H	-4.71389	2.54054	-0.48685
H	-6.21298	2.04952	0.31395
H	0.87183	1.99779	-0.39134
H	3.33872	1.99801	-0.41944
H	3.32343	-2.15740	0.59963
H	0.85574	-2.15269	0.59593
H	6.64580	0.61835	-0.09184
H	5.41726	1.31523	-1.17097
H	5.41580	1.72085	0.56480

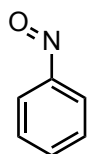


NFSI

M06/def2-TZVP Geometry

N	-0.22231	0.87037	-0.41966
F	-0.29094	0.38686	-1.71937
S	1.35637	1.60324	-0.19093
S	-0.74828	-0.44568	0.59378
O	1.23782	2.26867	1.05461
O	1.57421	2.28522	-1.41554
O	-0.19006	-1.66126	0.10928
O	-0.51323	0.02193	1.91493
C	-2.46066	-0.40194	0.22077
C	2.45975	0.24966	-0.06155
C	2.80698	-0.22213	1.19521
C	3.63057	-1.32851	1.28323
C	4.08637	-1.94812	0.13109
C	3.73388	-1.46304	-1.11829
C	2.91623	-0.35444	-1.22383
C	-3.25201	0.55224	0.84242
C	-4.60283	0.58217	0.55685
C	-5.14224	-0.32840	-0.33936
C	-4.33857	-1.27269	-0.95597

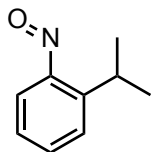
C	-2.98385	-1.31455	-0.67957
H	2.42757	0.27204	2.08077
H	3.91469	-1.71050	2.25599
H	4.72692	-2.81893	0.20739
H	4.09924	-1.94957	-2.01428
H	2.63213	0.04669	-2.18869
H	-2.80611	1.25181	1.53933
H	-5.23832	1.31763	1.03459
H	-6.20297	-0.30010	-0.55954
H	-4.76735	-1.97984	-1.65535
H	-2.33208	-2.04253	-1.14621



PhNO

M06/def2-TZVP Geometry

O	-1.33252	2.38174	0.00000
N	-0.19009	2.01603	0.00000
C	-0.00000	0.59011	0.00000
C	-1.04771	-0.32210	0.00000
C	-0.75869	-1.66913	0.00000
C	0.56490	-2.09702	0.00000
C	1.60468	-1.18236	0.00000
C	1.32036	0.17083	0.00000
H	-2.06557	0.05030	0.00000
H	-1.56019	-2.39874	0.00000
H	0.78364	-3.15888	0.00000
H	2.63204	-1.52606	0.00000
H	2.09960	0.92526	0.00000

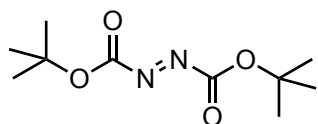


PhNO 2-ipr

M06/def2-TZVP Geometry

C	-0.29445	1.61160	-0.00002
C	-0.36207	0.21998	-0.00002
C	0.85213	-0.47396	-0.00000
C	2.07732	0.19020	0.00001
C	2.11374	1.56264	0.00000
C	0.91690	2.27283	-0.00001

N	0.78685	-1.90837	0.00001
O	1.84559	-2.47642	0.00003
C	-1.70003	-0.47602	-0.00002
C	-2.49358	-0.13686	-1.25412
C	-2.49352	-0.13696	1.25414
H	-1.21285	2.18892	-0.00003
H	2.98047	-0.40871	0.00002
H	3.06059	2.08927	0.00001
H	0.93415	3.35693	-0.00001
H	-1.51160	-1.55111	-0.00007
H	-1.93707	-0.38760	-2.15937
H	-3.43364	-0.69301	-1.26885
H	-2.74044	0.92780	-1.29674
H	-1.93697	-0.38780	2.15934
H	-2.74036	0.92770	1.29687
H	-3.43359	-0.69310	1.26885

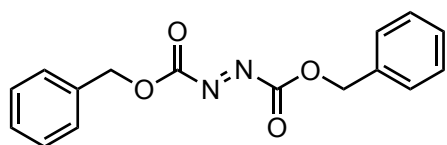


tBu diimide

M06/def2-TZVP Geometry

N	-0.30330	-0.24072	0.47594
N	0.30326	0.23997	-0.47554
C	1.63674	0.67314	-0.12770
O	2.45165	-0.35140	-0.19563
O	1.86210	1.82194	0.09658
C	-1.63692	-0.67358	0.12821
O	-2.45158	0.35118	0.19603
O	-1.86243	-1.82222	-0.09665
C	3.89858	-0.18906	0.01031
C	-3.89849	0.18929	-0.01045
C	-4.46454	-0.73086	1.04847
C	-4.15765	-0.31065	-1.41456
C	-4.41931	1.59741	0.16481
C	4.15801	0.31165	1.41409
C	4.46410	0.73071	-1.04923
C	4.41971	-1.59713	-0.16440
H	-4.19987	-0.37244	2.04560
H	-5.55385	-0.73469	0.96843
H	-4.10706	-1.75265	0.93086
H	-3.67080	0.33916	-2.14483
H	-3.80100	-1.33018	-1.55289
H	-5.23289	-0.29024	-1.60560
H	-4.18829	1.97191	1.16357

H	-3.96927	2.26789	-0.56931
H	-5.50253	1.60912	0.03013
H	3.67154	-0.33791	2.14483
H	5.23331	0.29163	1.60484
H	3.80111	1.33116	1.55201
H	4.19923	0.37174	-2.04610
H	4.10641	1.75247	-0.93202
H	5.55344	0.73484	-0.96952
H	3.97005	-2.26736	0.57018
H	4.18849	-1.97219	-1.16291
H	5.50297	-1.60851	-0.03003

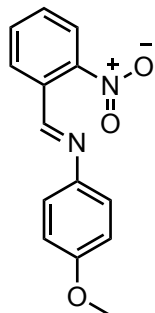


Bn diimide

M06/def2-TZVP Geometry

N	0.20206	-0.49840	-0.50606
N	-0.17673	0.38211	0.26025
C	-1.24777	1.17484	-0.28714
O	-2.39827	0.56409	-0.09484
O	-1.05299	2.25023	-0.75765
C	1.27491	-1.28982	0.04151
O	2.41372	-0.63662	-0.06065
O	1.09235	-2.39554	0.44135
C	-3.56461	1.29700	-0.51940
C	3.58105	-1.35737	0.37944
H	-3.47381	1.47609	-1.59522
H	-3.57301	2.27028	-0.02302
C	-7.06093	-0.97776	0.38949
C	-6.04579	-1.53690	-0.37182
C	-4.91284	-0.80184	-0.66253
C	-4.77721	0.49730	-0.18734
C	-5.79303	1.04728	0.57883
C	-6.93436	0.31545	0.86297
H	-7.95053	-1.55416	0.61474
H	-6.14086	-2.55084	-0.74218
H	-4.11584	-1.23773	-1.25579
H	-5.68791	2.05870	0.95821
H	-7.72264	0.75576	1.46209
H	3.67268	-2.27649	-0.20454
H	3.42392	-1.64505	1.42356
C	7.02095	1.13748	-0.03353
C	5.91286	1.59051	0.66605

C	4.79783	0.78509	0.79490
C	4.77385	-0.47886	0.21733
C	5.88234	-0.92236	-0.48686
C	7.00532	-0.12026	-0.60829
H	7.89607	1.76901	-0.13191
H	5.92063	2.57672	1.11508
H	3.92857	1.13857	1.33930
H	5.86488	-1.90543	-0.94649
H	7.86654	-0.47755	-1.16045

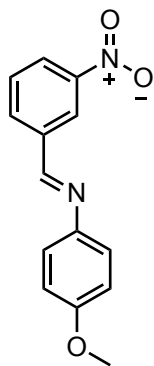


Imine a

M06/def2-TZVP Geometry

C	-0.77086	-0.11542	0.14427
N	0.16524	-0.87564	-0.24376
C	1.49266	-0.44950	-0.16376
C	2.47741	-1.41168	0.01304
C	3.81333	-1.06564	0.11380
C	4.18744	0.26777	-0.00214
C	3.21133	1.23742	-0.22251
C	1.88449	0.88613	-0.29902
C	-2.17170	-0.54072	0.03780
C	-2.46165	-1.90275	-0.02016
C	-3.76146	-2.36251	-0.05483
C	-4.82233	-1.47000	-0.01378
C	-4.56965	-0.11566	0.05245
C	-3.26098	0.33144	0.06225
O	5.45923	0.71491	0.06353
C	6.48287	-0.22224	0.26167
H	-0.57919	0.85961	0.60035
H	2.17343	-2.44957	0.08604
H	4.55224	-1.84061	0.26912
H	3.52762	2.26673	-0.34385
H	1.13942	1.64781	-0.50408
H	-1.62404	-2.58938	-0.02801
H	-3.95193	-3.42808	-0.10453
H	-5.84408	-1.82802	-0.03653
H	-5.37052	0.61085	0.08024

H	7.41730	0.33553	0.28553
H	6.36462	-0.75755	1.21065
H	6.52643	-0.95353	-0.55341
N	-3.07013	1.79278	0.04586
O	-3.93391	2.47246	0.54994
O	-2.07312	2.22593	-0.49231

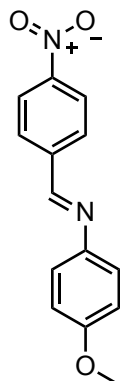


Imine b

M06/def2-TZVP Geometry

C	-0.31809	-0.03020	0.01169
N	0.65589	0.77278	0.11298
C	1.97557	0.32053	0.11406
C	2.95466	1.18688	-0.35395
C	4.28641	0.81525	-0.40074
C	4.66550	-0.43902	0.06209
C	3.69740	-1.30347	0.56970
C	2.37432	-0.93148	0.59232
C	-1.70712	0.42125	0.05457
C	-2.03079	1.76696	0.23126
C	-3.34844	2.17585	0.26528
C	-4.37291	1.25298	0.12685
C	-4.04055	-0.07578	-0.04532
C	-2.72978	-0.50678	-0.08422
O	5.93371	-0.89821	0.07887
C	6.94994	-0.05935	-0.40121
H	-0.18186	-1.11308	-0.13081
H	2.64650	2.16693	-0.69946
H	5.01883	1.51170	-0.78688
H	4.01799	-2.26438	0.95456
H	1.64027	-1.60607	1.01879
H	-1.22030	2.47802	0.33974
H	-3.58739	3.22338	0.40222
H	-5.41426	1.54371	0.15091
H	7.88336	-0.61020	-0.30132
H	6.79960	0.19652	-1.45607

H	7.01954	0.86652	0.18079
H	-2.51692	-1.55986	-0.22256
N	-5.12042	-1.06956	-0.19279
O	-4.79769	-2.22661	-0.33773
O	-6.25983	-0.66486	-0.15934

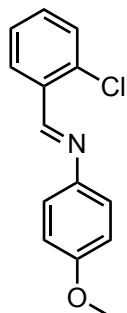


Imine c

M06/def2-TZVP Geometry

C	-0.11360	0.56271	0.10182
N	0.72163	-0.36882	-0.09914
C	2.09477	-0.13016	-0.10214
C	2.93132	-1.18583	0.23736
C	4.30564	-1.03532	0.27727
C	4.87202	0.18728	-0.06355
C	4.04556	1.24359	-0.44406
C	2.68027	1.08891	-0.45956
C	-1.55557	0.33705	0.06683
C	-2.08618	-0.92250	-0.21386
C	-3.44876	-1.11531	-0.23769
C	-4.28115	-0.03800	0.01907
C	-3.78707	1.22088	0.29844
C	-2.41874	1.39997	0.32049
O	6.19589	0.44129	-0.07533
C	7.07481	-0.59344	0.27849
H	0.19418	1.59396	0.33264
H	2.47600	-2.13694	0.48802
H	4.92390	-1.87616	0.56228
H	4.50930	2.17809	-0.73713
H	2.05662	1.91315	-0.78729
H	-1.40313	-1.73972	-0.41060
H	-3.88396	-2.08201	-0.45195
H	8.08161	-0.18649	0.20599
H	6.90326	-0.93700	1.30469
H	6.98709	-1.44872	-0.40069
H	-2.00561	2.37921	0.53861
H	-4.47439	2.03274	0.49299

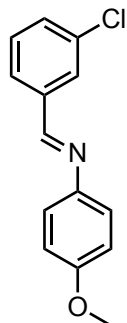
N	-5.73945	-0.24037	-0.00694
O	-6.14459	-1.35398	-0.25280
O	-6.44130	0.71959	0.21958



Imine d

M06/def2-TZVP Geometry

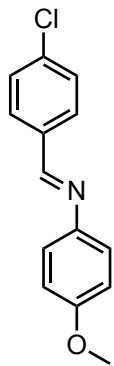
C	-0.93143	0.05129	-0.00227
N	-0.00161	-0.80595	0.09779
C	1.33673	-0.41348	0.11804
C	2.27999	-1.30622	-0.37391
C	3.62755	-0.99311	-0.40182
C	4.05941	0.22667	0.10433
C	3.12776	1.11570	0.63568
C	1.78880	0.80263	0.63985
C	-2.33960	-0.33907	0.02484
C	-3.37840	0.58211	-0.10976
C	-4.70514	0.18835	-0.08203
C	-5.01820	-1.14683	0.08128
C	-4.00515	-2.08514	0.21755
C	-2.68920	-1.68082	0.19029
O	5.34844	0.62797	0.14252
C	6.32728	-0.24014	-0.36023
H	-0.72908	1.12113	-0.12978
H	1.93089	-2.25960	-0.75352
H	4.33023	-1.70880	-0.80773
H	3.48815	2.04835	1.05367
H	1.08191	1.49460	1.08396
Cl	-3.05317	2.28077	-0.32033
H	-5.48102	0.93581	-0.18990
H	6.35124	-1.18724	0.19077
H	7.28478	0.26320	-0.23850
H	6.17187	-0.45481	-1.42370
H	-1.87928	-2.39312	0.29574
H	-4.24733	-3.13311	0.34652
H	-6.05724	-1.45346	0.10257



Imine e

M06/def2-TZVP Geometry

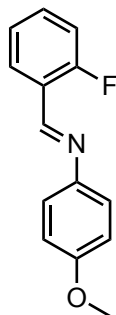
C	-0.56635	0.88819	-0.12817
N	0.17130	-0.13029	0.02237
C	1.56091	-0.01510	0.06832
C	2.31636	-1.08578	-0.39122
C	3.69950	-1.04706	-0.39184
C	4.35573	0.07036	0.10968
C	3.60970	1.13511	0.60960
C	2.23520	1.09455	0.58645
C	-2.02464	0.81250	-0.13365
C	-2.68070	-0.40227	0.05409
C	-4.05707	-0.43428	0.03932
C	-4.80724	0.71646	-0.15645
C	-4.15268	1.92002	-0.34102
C	-2.77014	1.96982	-0.33010
O	5.69773	0.20788	0.17215
C	6.49390	-0.84647	-0.29640
H	-0.15178	1.89701	-0.28179
H	1.79205	-1.95687	-0.76691
H	4.25373	-1.89477	-0.77269
H	4.14027	1.98339	1.02596
H	1.67108	1.91915	1.00807
H	-2.10014	-1.30345	0.20825
Cl	-4.87974	-1.94664	0.27278
H	6.31991	-1.04469	-1.36016
H	6.31791	-1.76936	0.26787
H	7.52980	-0.54135	-0.15943
H	-2.25547	2.91392	-0.47563
H	-4.72915	2.82439	-0.49468
H	-5.88840	0.65819	-0.16160



Imine f

M06/def2-TZVP Geometry

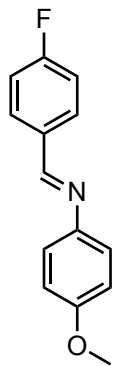
C	-0.41219	0.49760	0.13267
N	0.42473	-0.41604	-0.13350
C	1.79629	-0.16063	-0.12165
C	2.64901	-1.20115	0.22270
C	4.02087	-1.02620	0.27060
C	4.56886	0.20558	-0.06579
C	3.72714	1.24633	-0.45061
C	2.36358	1.06724	-0.47527
C	-1.85402	0.28623	0.08536
C	-2.71183	1.32870	0.42039
C	-4.08342	1.16208	0.38968
C	-4.59865	-0.06601	0.01828
C	-3.76499	-1.12203	-0.32121
C	-2.39977	-0.94158	-0.28727
O	5.89112	0.48210	-0.06885
C	6.78181	-0.53875	0.29018
H	-0.09813	1.50936	0.43507
H	2.21003	-2.16078	0.47035
H	4.65150	-1.85674	0.55922
H	4.17553	2.18947	-0.74025
H	1.72582	1.87912	-0.80704
H	-2.29408	2.28750	0.71121
H	-4.75347	1.97154	0.65024
H	6.60888	-0.88660	1.31505
H	7.78352	-0.11761	0.22527
H	6.71224	-1.39570	-0.38951
H	-1.72659	-1.74969	-0.54823
H	-4.19668	-2.07257	-0.60908
Cl	-6.31745	-0.29214	-0.02561



Imine g

M06/def2-TZVP Geometry

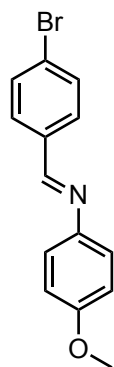
C	1.12085	0.25072	0.04840
N	0.23171	-0.63859	-0.12018
C	-1.12215	-0.30112	-0.12598
C	-2.03071	-1.25367	0.31635
C	-3.38961	-0.99475	0.35425
C	-3.86797	0.23116	-0.09161
C	-2.97089	1.18096	-0.57431
C	-1.62048	0.92061	-0.58851
C	2.54375	-0.06867	0.00732
C	3.50435	0.91269	0.22221
C	4.85739	0.64885	0.19196
C	5.27857	-0.64308	-0.06113
C	4.34817	-1.65024	-0.28050
C	3.00076	-1.36240	-0.24706
O	-5.17195	0.58373	-0.11400
C	-6.11645	-0.34473	0.34410
H	0.86808	1.29930	0.24872
H	-1.64572	-2.21072	0.64918
H	-4.06478	-1.75666	0.72098
H	-3.36636	2.11870	-0.94676
H	-0.93996	1.66056	-0.99499
F	3.11189	2.16368	0.46783
H	5.55588	1.45752	0.36715
H	-5.95186	-0.60612	1.39571
H	-6.10535	-1.26357	-0.25331
H	-7.09254	0.12732	0.24687
H	2.25600	-2.13111	-0.41653
H	4.68097	-2.66160	-0.47937
H	6.33884	-0.86455	-0.08779



Imine h

M06/def2-TZVP Geometry

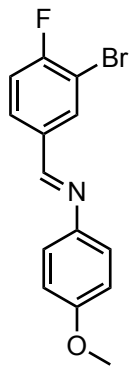
C	0.86943	0.45661	0.13184
N	0.02265	-0.44621	-0.13990
C	-1.34596	-0.17393	-0.12509
C	-2.21157	-1.20114	0.22671
C	-3.58106	-1.00791	0.27638
C	-4.11371	0.22911	-0.06511
C	-3.25934	1.25649	-0.45693
C	-1.89807	1.05916	-0.48391
C	2.30910	0.23361	0.08218
C	3.17575	1.26700	0.42405
C	4.54629	1.09000	0.39142
C	5.03879	-0.14038	0.01077
C	4.20691	-1.19028	-0.33605
C	2.84336	-0.99712	-0.29952
O	-5.43279	0.52293	-0.06667
C	-6.33531	-0.48458	0.29943
H	0.56462	1.46926	0.44150
H	-1.78496	-2.16527	0.47852
H	-4.22189	-1.82866	0.57058
H	-3.69579	2.20410	-0.75028
H	-1.25012	1.86064	-0.82128
H	2.76445	2.22643	0.72150
H	5.23428	1.88353	0.65440
H	-6.27828	-1.34591	-0.37599
H	-6.16456	-0.82966	1.32567
H	-7.33186	-0.05126	0.23470
H	2.16104	-1.79596	-0.56492
H	4.64285	-2.13746	-0.62887
F	6.35514	-0.32550	-0.02554



Imine i

M06/def2-TZVP Geometry

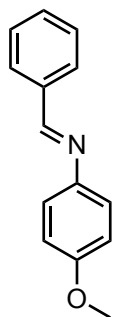
C	-0.41012	0.53609	0.14140
N	-1.23604	-0.38795	-0.12295
C	-2.61055	-0.14925	-0.11516
C	-3.45130	-1.20123	0.22386
C	-4.82541	-1.04387	0.26677
C	-5.38770	0.18157	-0.06930
C	-4.55774	1.23388	-0.44848
C	-3.19202	1.07218	-0.46822
C	1.03426	0.34034	0.09607
C	1.88001	1.39499	0.42294
C	3.25388	1.24379	0.39108
C	3.78340	0.01942	0.02767
C	2.96116	-1.04848	-0.30218
C	1.59342	-0.88377	-0.26798
O	-6.71321	0.44115	-0.07731
C	-7.59243	-0.59216	0.27458
H	-0.73562	1.54544	0.43951
H	-3.00106	-2.15575	0.47100
H	-5.44652	-1.88301	0.55109
H	-5.01699	2.17186	-0.73786
H	-2.56355	1.89293	-0.79587
H	1.45162	2.35106	0.70744
H	3.91032	2.06644	0.64534
H	-7.50846	-1.44613	-0.40722
H	-7.41991	-0.94067	1.29927
H	-8.59914	-0.18376	0.20600
H	0.92948	-1.70161	-0.52243
H	3.39815	-1.99851	-0.58401
Br	5.65962	-0.20436	-0.02375



Imine j

M06/def2-TZVP Geometry

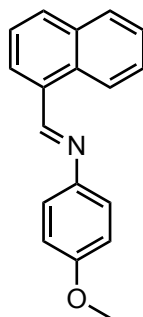
C	0.40830	1.08965	-0.10429
N	1.08178	0.02195	-0.00248
C	2.47551	0.05318	0.05824
C	3.17477	-1.02427	-0.46913
C	4.55795	-1.06242	-0.45912
C	5.27038	-0.02023	0.12169
C	4.57954	1.04784	0.68896
C	3.20505	1.08558	0.65491
C	-1.05048	1.10475	-0.12117
C	-1.78416	-0.07204	0.01310
C	-3.16092	-0.04097	-0.00853
C	-3.81549	1.17498	-0.16394
C	-3.10623	2.35007	-0.29690
C	-1.72578	2.31058	-0.27476
O	6.61731	0.03736	0.20149
C	7.35874	-1.02439	-0.33512
H	0.88515	2.07763	-0.20417
H	2.60732	-1.83732	-0.90707
H	5.06783	-1.91161	-0.89454
H	5.15191	1.83495	1.16569
H	2.68288	1.90937	1.12897
H	-1.25584	-1.01030	0.13396
Br	-4.16138	-1.62565	0.17249
H	7.12559	-1.97349	0.16081
H	7.18571	-1.13698	-1.41149
H	8.40842	-0.78841	-0.16961
H	-1.15799	3.22913	-0.37923
H	-3.65244	3.27755	-0.41591
F	-5.13712	1.21564	-0.18476



Imine k

M06/def2-TZVP Geometry

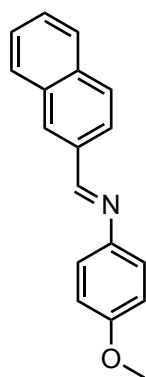
C	1.32949	0.41246	0.12913
N	0.47070	-0.47826	-0.14491
C	-0.89392	-0.18767	-0.12746
C	-1.77264	-1.20421	0.22304
C	-3.13940	-0.99306	0.27506
C	-3.65604	0.25160	-0.06311
C	-2.78880	1.26852	-0.45377
C	-1.43024	1.05345	-0.48274
C	2.76763	0.17220	0.07789
C	3.64272	1.19838	0.41966
C	5.01128	1.00008	0.38320
C	5.51786	-0.23066	0.00376
C	4.65228	-1.26106	-0.33936
C	3.28783	-1.06348	-0.30444
O	-4.97139	0.56268	-0.06242
C	-5.88623	-0.43371	0.30298
H	1.03723	1.42777	0.44235
H	-1.35824	-2.17441	0.47187
H	-3.79071	-1.80590	0.56827
H	-3.21315	2.22245	-0.74442
H	-0.77196	1.84701	-0.81874
H	3.23802	2.16097	0.71732
H	-5.84129	-1.29450	-0.37411
H	-5.71858	-0.78307	1.32831
H	-6.87727	0.01247	0.24049
H	2.59696	-1.85528	-0.56937
H	5.05099	-2.22410	-0.63670
H	5.68373	1.80636	0.65149
H	6.58946	-0.39038	-0.02618



Imine I

M06/def2-TZVP Geometry

C	-0.32983	0.81766	0.16700
N	0.33396	-0.26252	0.10770
C	1.72945	-0.22631	0.09381
C	2.42206	-1.24798	0.74713
C	3.79559	-1.27038	0.76902
C	4.52590	-0.28660	0.10526
C	3.85316	0.71503	-0.58069
C	2.46678	0.74051	-0.57881
C	-1.78250	0.95631	0.13478
C	-2.25081	2.24521	0.27429
C	-3.61572	2.55105	0.27076
C	-4.52656	1.54795	0.12337
O	5.87135	-0.40287	0.16981
C	6.64957	0.56208	-0.48230
H	0.19017	1.78436	0.27279
H	1.84841	-2.01746	1.25084
H	4.33794	-2.05233	1.28731
H	4.39466	1.47295	-1.13171
H	1.95122	1.50812	-1.14546
H	-1.52867	3.04682	0.39311
H	7.69072	0.29956	-0.30252
H	6.46743	0.56866	-1.56328
H	6.46381	1.56795	-0.08804
H	-3.93890	3.57859	0.38549
H	-5.59065	1.76116	0.11834
C	-4.11004	0.20882	-0.02792
C	-2.72326	-0.11071	-0.02601
C	-2.35721	-1.46394	-0.18695
C	-3.30686	-2.43682	-0.33665
C	-4.67252	-2.11856	-0.33417
C	-5.06124	-0.81991	-0.18330
H	-1.30666	-1.71564	-0.18763
H	-2.99822	-3.46869	-0.45965
H	-5.41259	-2.90131	-0.45307
H	-6.11304	-0.55259	-0.18069

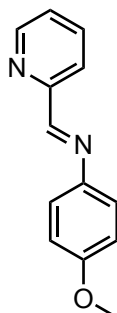


Imine m

M06/def2-TZVP Geometry

C	0.00387	-0.22606	0.02937
N	-0.91062	0.63893	-0.12419
C	-2.25503	0.26569	-0.12026
C	-3.18444	1.17801	0.36177
C	-4.53481	0.87869	0.40864
C	-4.98445	-0.34668	-0.06765
C	-4.06741	-1.25531	-0.58942
C	-2.72493	-0.95552	-0.61245
C	1.42124	0.10398	-0.01704
C	1.85739	1.42872	-0.26013
C	3.18455	1.71934	-0.29972
O	-6.27874	-0.73573	-0.08436
C	-7.24258	0.15274	0.41060
H	-0.22155	-1.28656	0.22528
H	-2.82285	2.13571	0.71818
H	-5.22620	1.60987	0.80642
H	-4.44089	-2.19255	-0.98521
H	-2.02853	-1.66228	-1.05008
H	1.10544	2.19381	-0.41135
H	-7.26302	1.08867	-0.15948
H	-8.20673	-0.34264	0.30981
H	-7.07349	0.38800	1.46773
H	3.51962	2.73485	-0.48578
C	2.35144	-0.88562	0.17738
H	2.02198	-1.90461	0.36438
C	4.16114	0.71509	-0.10243
C	3.73252	-0.61562	0.14117
C	4.70166	-1.62054	0.33870
C	6.03385	-1.32445	0.29717
C	6.45798	-0.00642	0.05550
C	5.54159	0.98839	-0.13942

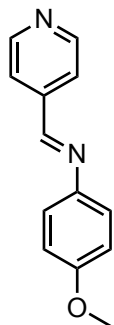
H	4.36678	-2.63594	0.52492
H	6.76968	-2.10505	0.45050
H	7.51776	0.21805	0.02445
H	5.86472	2.00742	-0.32629



Imine n

M06/def2-TZVP Geometry

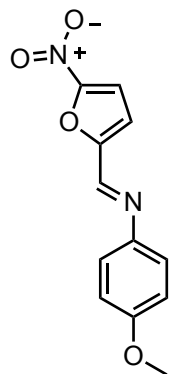
C	1.34786	-0.43552	0.12781
N	0.48690	0.45615	-0.13337
C	-0.87861	0.16811	-0.11564
C	-1.75389	1.20544	0.17708
C	-3.12222	1.00508	0.22862
C	-3.64217	-0.25236	-0.05196
C	-2.77709	-1.29296	-0.38390
C	-1.41803	-1.08741	-0.41203
C	2.78796	-0.17057	0.07337
N	3.57345	-1.20433	0.37949
C	4.88399	-1.01925	0.34726
O	-4.95782	-0.55660	-0.04707
C	-5.87174	0.46019	0.26198
H	1.09579	-1.46199	0.42835
H	-1.33503	2.18418	0.38094
H	-3.77148	1.83452	0.47607
H	-3.20483	-2.25823	-0.62822
H	-0.76200	-1.90194	-0.69788
H	-5.81714	1.28664	-0.45577
H	-6.86392	0.01510	0.21265
H	-5.71076	0.85773	1.27056
H	5.50049	-1.87868	0.60041
C	3.28984	1.08026	-0.27493
H	2.59667	1.87718	-0.51378
C	5.47687	0.18737	0.01491
C	4.65642	1.25740	-0.30203
H	6.55564	0.28248	0.00512
H	5.08164	2.21844	-0.56792



Imine o

M06/def2-TZVP Geometry

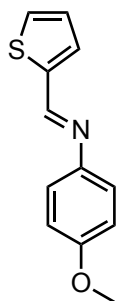
C	-1.33785	0.44440	0.12778
N	-0.47669	-0.44679	-0.13266
C	0.88886	-0.16314	-0.11755
C	1.76017	-1.20031	0.18847
C	3.12849	-1.00307	0.24077
C	3.65309	0.24963	-0.05375
C	2.79197	1.28886	-0.40086
C	1.43246	1.08706	-0.42876
C	-2.77435	0.18118	0.07507
C	-5.03410	0.91360	0.33392
O	4.96854	0.54964	-0.04990
C	5.88021	-0.46651	0.27082
H	-1.05924	1.46691	0.42645
H	1.33777	-2.17524	0.40260
H	3.77484	-1.83141	0.49904
H	3.22357	2.24889	-0.65848
H	0.78040	1.89924	-0.73031
H	5.82387	-1.29995	-0.43840
H	6.87322	-0.02403	0.21740
H	5.71730	-0.85241	1.28345
H	-5.75586	1.69010	0.57655
C	-3.28813	-1.06089	-0.28257
H	-2.61358	-1.86961	-0.53524
N	-5.52796	-0.26822	-0.00493
C	-4.65774	-1.22902	-0.30483
H	-5.08162	-2.19165	-0.58052
C	-3.67812	1.18719	0.38911
H	-3.32609	2.17326	0.67395



Imine p

M06/def2-TZVP Geometry

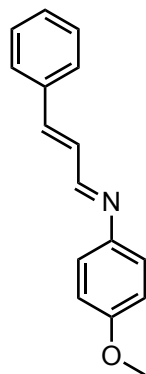
C	-1.34611	0.57888	0.18469
N	-0.51629	-0.34056	-0.09541
C	0.85633	-0.09540	-0.09221
C	1.70432	-1.14978	0.22112
C	3.07818	-0.98756	0.25634
C	3.63318	0.24646	-0.05917
C	2.79627	1.30225	-0.41152
C	1.43098	1.13477	-0.42606
C	-2.76963	0.37624	0.14300
C	-5.04626	0.77337	0.30571
O	4.95836	0.51200	-0.07092
C	5.84312	-0.52461	0.25487
H	-1.03489	1.58885	0.49458
H	1.25931	-2.11050	0.45321
H	3.70465	-1.82964	0.51968
H	3.24944	2.24793	-0.68519
H	0.79729	1.95928	-0.73385
H	5.75764	-1.36571	-0.44271
H	6.84814	-0.11162	0.18770
H	5.67872	-0.89392	1.27370
S	-3.45816	-1.13613	-0.32036
C	-5.04066	-0.52706	-0.10142
C	-3.74399	1.29032	0.44514
H	-3.51493	2.30183	0.75776
H	-5.89279	-1.16429	-0.28495
H	-5.94936	1.33662	0.49811



Imine q

M06/def2-TZVP Geometry

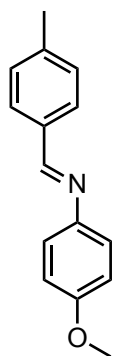
C	0.54558	-0.08507	-0.00370
N	-0.42318	0.72620	-0.12928
C	-1.74674	0.29650	-0.11254
C	-2.71694	1.24308	0.19374
C	-4.05828	0.91239	0.25326
C	-4.45560	-0.38911	-0.02945
C	-3.49525	-1.34147	-0.37243
C	-2.16462	-1.00594	-0.41069
C	1.90142	0.39140	-0.06423
C	3.84533	1.45940	-0.20902
O	-5.73127	-0.81990	-0.01613
C	-6.74205	0.09934	0.30559
H	0.43605	-1.16372	0.16925
H	-2.39079	2.25563	0.40117
H	-4.78298	1.67371	0.50936
H	-3.83045	-2.34243	-0.61705
H	-1.43968	-1.75619	-0.70591
H	-6.77578	0.92910	-0.40894
H	-7.68372	-0.44432	0.26105
H	-6.61261	0.50514	1.31494
O	2.87619	-0.53244	0.10078
C	4.03248	0.13088	0.00997
C	2.45030	1.63002	-0.25870
H	4.62526	2.19427	-0.31731
N	5.23830	-0.62018	0.14803
O	5.14617	-1.81159	0.33833
O	6.26947	0.01655	0.06048
H	1.89070	2.53727	-0.41623



Imine r

M06/def2-TZVP Geometry

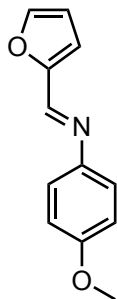
C	0.21423	0.04719	0.00875
N	-0.73186	-0.77902	-0.19685
C	-2.06245	-0.36626	-0.15740
C	-3.01934	-1.30018	0.22038
C	-4.36184	-0.97340	0.29429
C	-4.77719	0.30747	-0.04853
C	-3.83381	1.24328	-0.46548
C	-2.49954	0.91327	-0.51623
C	1.59464	-0.34733	-0.07529
O	-6.06101	0.72946	-0.02797
C	-7.05025	-0.18203	0.36443
H	0.02904	1.10000	0.27701
H	-2.68324	-2.29953	0.47189
H	-5.07405	-1.72519	0.60809
H	-4.18114	2.22713	-0.75880
H	-1.78440	1.64625	-0.87282
H	-6.89414	-0.53417	1.39063
H	-8.00096	0.34593	0.31375
H	-7.09034	-1.05030	-0.30333
C	2.59891	0.51118	0.14098
H	2.33386	1.53862	0.38969
H	1.77100	-1.38904	-0.32767
C	6.78675	-0.18619	0.00841
C	5.90955	-1.22571	-0.26661
C	4.54676	-1.01703	-0.22924
C	4.02419	0.23988	0.08542
C	4.92049	1.27365	0.35789
C	6.28655	1.06565	0.32086
H	7.85672	-0.35453	-0.02209
H	6.29553	-2.20808	-0.51286
H	3.87573	-1.83982	-0.44777
H	4.52842	2.25558	0.60335
H	6.96335	1.88404	0.53678



Imine s

M06/def2-TZVP Geometry

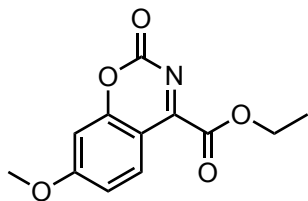
N	-0.00542	-0.45084	-0.14362
C	0.83941	0.45252	0.13497
C	-1.37385	-0.17884	-0.12736
C	2.27958	0.23792	0.08550
C	-2.23981	-1.20403	0.22984
C	-3.60931	-1.01018	0.27967
C	-4.14205	0.22524	-0.06703
C	-3.28789	1.25042	-0.46402
C	-1.92644	1.05259	-0.49118
O	-5.46189	0.51930	-0.06887
C	2.82719	-0.98563	-0.30222
C	4.19210	-1.15608	-0.33489
C	5.06052	-0.12059	0.01333
C	4.51188	1.09452	0.39627
C	3.14026	1.27201	0.43241
C	6.53836	-0.33179	-0.02764
C	-6.36331	-0.48663	0.30269
H	0.52934	1.46170	0.45160
H	-1.81326	-2.16717	0.48557
H	-4.25002	-1.82952	0.57821
H	-3.72421	2.19699	-0.76105
H	-1.27810	1.85223	-0.83217
H	2.15420	-1.79060	-0.57379
H	4.60936	-2.11199	-0.63784
H	5.17033	1.91264	0.66996
H	2.72417	2.22838	0.73475
H	7.08175	0.57667	0.23430
H	6.84327	-1.11791	0.66817
H	6.86493	-0.64582	-1.02226
H	-7.36030	-0.05428	0.23700
H	-6.30671	-1.35134	-0.36859
H	-6.19157	-0.82717	1.33037



Imine t

M06/def2-TZVP Geometry

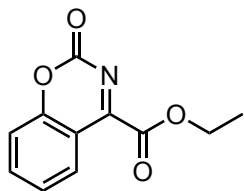
N	-0.78235	0.53225	-0.17574
C	-1.66131	-0.33126	0.13263
C	0.57433	0.21448	-0.13699
C	-3.06474	-0.03821	0.04703
C	1.47371	1.24225	0.11679
C	2.83669	1.01216	0.18316
C	3.32918	-0.26757	-0.04028
C	2.44164	-1.30035	-0.33243
C	1.08749	-1.06400	-0.37817
O	4.63851	-0.60141	-0.01533
C	-3.77326	1.05400	-0.35124
C	-5.13964	0.72060	-0.19654
C	-5.16448	-0.54791	0.28192
O	-3.91745	-1.02416	0.43611
C	5.57306	0.40774	0.25242
H	-1.41902	-1.34087	0.49532
H	1.07714	2.23820	0.27715
H	3.50387	1.83643	0.39842
H	2.84746	-2.28470	-0.53470
H	0.41535	-1.87437	-0.63807
H	-5.96654	-1.21642	0.54909
H	5.41847	0.85231	1.24231
H	6.55577	-0.05991	0.22573
H	5.53810	1.20366	-0.50035
H	-5.99634	1.33800	-0.41218
H	-3.34247	1.97501	-0.70854



Imine u

M06/def2-TZVP Geometry

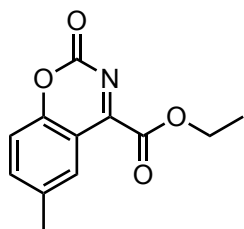
C	0.36577	-0.22397	-0.15932
C	-0.97119	0.27191	-0.25284
N	-1.28473	1.52117	-0.23333
C	-0.30287	2.48469	-0.13467
O	1.01775	2.05452	-0.00130
C	1.34829	0.75590	-0.01220
O	-0.49027	3.65654	-0.14663
C	-2.11873	-0.69602	-0.43198
O	-3.17311	-0.33832	0.27530
O	-2.05390	-1.65613	-1.14969
C	-4.33994	-1.16001	0.12841
C	-5.41347	-0.57999	0.99892
C	2.69029	0.44056	0.12807
C	3.05775	-0.89469	0.11947
C	2.08713	-1.90013	-0.02704
C	0.77014	-1.56977	-0.16360
O	4.31685	-1.32519	0.24391
C	5.34520	-0.37411	0.39183
H	-4.62348	-1.17463	-0.92732
H	-4.08508	-2.18616	0.40826
H	-6.32500	-1.17249	0.91102
H	-5.10740	-0.57502	2.04590
H	-5.63947	0.44557	0.70496
H	3.40025	1.24837	0.23760
H	2.41717	-2.93115	-0.03181
H	0.02513	-2.34339	-0.29262
H	6.27428	-0.93373	0.47314
H	5.40109	0.29105	-0.47546
H	5.20677	0.22580	1.29668



Imine v

M06/def2-TZVP Geometry

C	2.42246	-2.41307	-0.20515
C	1.17515	-1.87910	0.01253
C	1.00580	-0.49066	0.05624
C	2.11916	0.33014	-0.12314
C	3.37944	-0.20311	-0.34374
C	3.52027	-1.57262	-0.38228
C	-0.23769	0.21070	0.23194
N	-0.34516	1.48919	0.25454
C	0.77787	2.29221	0.12794
O	1.99750	1.66791	-0.08716
C	-1.51389	-0.56869	0.45508
O	-1.57019	-1.52150	1.18242
O	-2.52186	-0.05728	-0.22334
C	-3.79736	-0.68816	-0.03175
C	-4.79256	0.03547	-0.88739
O	0.76744	3.47700	0.18260
H	2.55370	-3.48726	-0.23556
H	0.31827	-2.52098	0.16784
H	4.21795	0.46831	-0.47843
H	4.50140	-2.00056	-0.55193
H	-3.70926	-1.74546	-0.29697
H	-4.05029	-0.64140	1.03073
H	-5.78105	-0.40889	-0.76506
H	-4.85139	1.08817	-0.60885
H	-4.51823	-0.02402	-1.94145

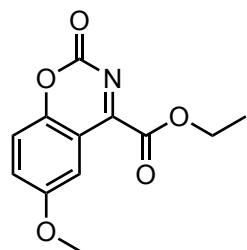


Imine w

M06/def2-TZVP Geometry

C	-2.65777	-1.63752	-0.13598
C	-1.32503	-1.35581	0.06535
C	-0.86155	-0.03440	0.08144

C	-1.77040	1.00283	-0.10994
C	-3.11645	0.74102	-0.31558
C	-3.54081	-0.56673	-0.32551
C	0.50429	0.38661	0.23856
N	0.88411	1.61278	0.23639
C	-0.04052	2.63626	0.09901
O	-1.36612	2.28511	-0.10129
C	1.58635	-0.64315	0.47061
O	1.44728	-1.57099	1.21889
O	2.67279	-0.37339	-0.22645
C	3.78657	-1.25692	-0.02827
C	4.90660	-0.77432	-0.89948
O	0.22540	3.79224	0.13253
C	-3.16975	-3.04138	-0.15035
H	-0.62047	-2.16165	0.23195
H	-3.79826	1.56930	-0.46170
H	-4.59368	-0.78029	-0.48364
H	4.05118	-1.24808	1.03236
H	3.47493	-2.27574	-0.27524
H	5.77939	-1.41614	-0.77346
H	4.61830	-0.79041	-1.95138
H	5.18905	0.24619	-0.63867
H	-3.65198	-3.27722	-1.10225
H	-2.36545	-3.76027	0.00607
H	-3.91577	-3.19792	0.63270

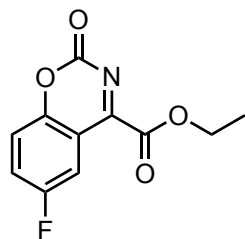


Imine x

M06/def2-TZVP Geometry

C	2.75342	-0.86187	-0.14707
C	1.39169	-0.87656	0.05953
C	0.68168	0.33395	0.07671
C	1.35993	1.53195	-0.11376
C	2.73257	1.54595	-0.32715
C	3.41604	0.35826	-0.34223
C	-0.74170	0.47450	0.23338
N	-1.35600	1.60168	0.24371
C	-0.65411	2.79086	0.12039
O	0.70923	2.71001	-0.09802
C	-1.60230	-0.75163	0.44115

O	-1.26937	-1.66952	1.14019
O	-2.74077	-0.66492	-0.21782
C	-3.65975	-1.75260	-0.03893
C	-4.87434	-1.45896	-0.86652
O	-1.14492	3.87040	0.17778
O	3.53963	-1.95641	-0.17641
C	2.93353	-3.20697	0.02724
H	0.85409	-1.79709	0.23394
H	3.23352	2.49436	-0.47435
H	4.48759	0.33425	-0.50197
H	-3.16642	-2.68208	-0.33713
H	-3.89271	-1.83795	1.02578
H	-4.61697	-1.37779	-1.92341
H	-5.60525	-2.26044	-0.75235
H	-5.33871	-0.52249	-0.55576
H	2.19172	-3.42593	-0.74890
H	3.72720	-3.94971	-0.02126
H	2.44769	-3.26463	1.00724

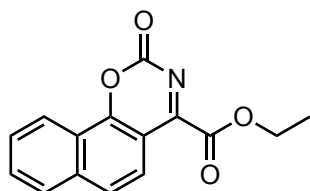


Imine y

M06/def2-TZVP Geometry

C	2.63025	-1.68060	-0.13461
C	1.30026	-1.42125	0.06147
C	0.87227	-0.08938	0.07787
C	1.80640	0.92915	-0.10315
C	3.14978	0.64683	-0.30130
C	3.56146	-0.66602	-0.31609
C	-0.48849	0.36157	0.22490
N	-0.83606	1.59546	0.22748
C	0.11292	2.60036	0.10583
O	1.42975	2.22027	-0.09133
C	-1.59498	-0.64769	0.43646
O	-1.46037	-1.61532	1.13376
O	-2.69058	-0.31321	-0.21355
C	-3.82375	-1.17661	-0.02928
C	-4.95235	-0.62048	-0.84336
O	-0.12854	3.76060	0.14976
F	3.05490	-2.93995	-0.15109
H	0.60318	-2.23281	0.21961

H	3.84523	1.46479	-0.43871
H	4.60182	-0.92763	-0.46527
H	-3.54606	-2.18886	-0.33604
H	-4.05897	-1.21490	1.03755
H	-5.83880	-1.24474	-0.72502
H	-5.19949	0.39245	-0.52384
H	-4.69306	-0.59088	-1.90243

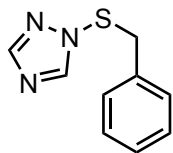


Imine z

M06/def2-TZVP Geometry

C	-1.57374	-2.17981	-0.05659
C	-0.29883	-1.74006	-0.18798
C	-0.02045	-0.34833	-0.19334
C	-1.06348	0.54927	-0.06439
C	-2.40612	0.12323	0.07382
C	-2.65486	-1.27060	0.07631
C	1.27795	0.25099	-0.28030
N	1.49747	1.51960	-0.27047
C	0.44511	2.40545	-0.19362
O	-0.83704	1.86623	-0.06451
C	2.49772	-0.62563	-0.44716
O	2.52677	-1.55556	-1.20492
O	3.49559	-0.22315	0.31549
C	4.72501	-0.95197	0.18325
C	5.71862	-0.33663	1.12160
O	0.53482	3.58802	-0.21960
C	-3.47445	1.02928	0.20502
C	-4.75346	0.56564	0.33492
C	-5.00842	-0.81411	0.33780
C	-3.98335	-1.71049	0.21132
H	-1.79049	-3.24217	-0.05532
H	0.51922	-2.43754	-0.30709
H	4.53497	-2.00516	0.40862
H	5.04906	-0.89827	-0.85942
H	6.67359	-0.85824	1.04698
H	5.88065	0.71455	0.88071
H	5.37288	-0.40081	2.15418
H	-3.26546	2.09149	0.20018
H	-5.57511	1.26434	0.43529
H	-6.02697	-1.16973	0.44077

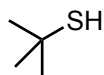
H	-4.17923	-2.77735	0.21274
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sulfur

M06/def2-TZVP Geometry

N	2.43714	-0.36285	0.68780
N	1.67552	0.17350	-0.29809
C	1.28526	-0.80811	-1.14537
N	1.77632	-1.95685	-0.77196
C	2.46570	-1.62969	0.35321
S	1.24111	1.81238	-0.32836
C	-0.11783	1.75656	0.89486
C	-1.15140	0.74763	0.53725
C	-2.07935	1.00219	-0.46708
C	-2.98912	0.03318	-0.84426
C	-2.97765	-1.20875	-0.22637
C	-2.05709	-1.47166	0.77202
C	-1.14939	-0.49679	1.15227
H	0.64941	-0.60457	-1.99606
H	3.00887	-2.35630	0.94056
H	0.32301	1.56396	1.87452
H	-0.50737	2.77842	0.88308
H	-2.07503	1.96930	-0.96144
H	-3.71087	0.24444	-1.62466
H	-3.68742	-1.97061	-0.52616
H	-2.03920	-2.44178	1.25418
H	-0.41682	-0.70485	1.92633

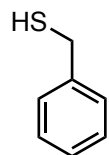


SHtBu

M06/def2-TZVP Geometry

H	1.70841	-1.23556	0.00000
S	1.49382	0.09389	0.00000
C	-0.34875	-0.00932	0.00000
C	-0.82793	1.43115	0.00000
C	-0.82793	-0.72642	1.24707
C	-0.82793	-0.72642	-1.24707
H	-0.47712	1.96539	-0.88619
H	-1.92167	1.45374	0.00000
H	-0.47712	1.96539	0.88619

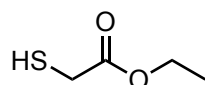
H	-0.46709	-1.75778	1.27305
H	-0.47893	-0.22161	2.14978
H	-1.92319	-0.75318	1.26626
H	-0.46709	-1.75778	-1.27305
H	-1.92319	-0.75318	-1.26626
H	-0.47893	-0.22161	-2.14978



SHBn

M06/def2-TZVP Geometry

H	-2.04571	0.60052	-1.43415
S	-2.62105	-0.16001	-0.48483
C	-1.44970	0.30215	0.84245
H	-1.65191	1.32542	1.16254
H	-1.71103	-0.36201	1.66910
C	2.63471	-0.16105	-0.34232
C	2.07695	1.10085	-0.24577
C	0.75597	1.24692	0.14631
C	-0.02190	0.13666	0.44430
C	0.54716	-1.12777	0.33868
C	1.86503	-1.27662	-0.04757
H	3.66831	-0.27810	-0.64604
H	2.67219	1.97770	-0.47303
H	0.31998	2.23819	0.22783
H	-0.06162	-2.00045	0.55519
H	2.29713	-2.26796	-0.12066

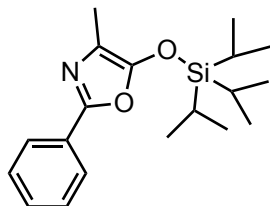


SHCH₂COOEt

M06/def2-TZVP Geometry

H	2.37089	-0.19113	-1.11760
S	1.86272	-1.11737	-0.28326
C	1.12594	0.09351	0.86176
H	0.60352	-0.49174	1.61759
H	1.90796	0.67825	1.34186
C	0.23878	1.03949	0.09392
O	0.65888	2.07564	-0.33009
O	-1.02946	0.68700	-0.14757
C	-1.58371	-0.54019	0.31901
H	-0.96449	-1.37830	-0.01837
H	-1.60193	-0.54497	1.41510

C	-2.97538	-0.64138	-0.23445
H	-3.44957	-1.56383	0.10325
H	-3.58370	0.20185	0.09491
H	-2.95533	-0.64192	-1.32478

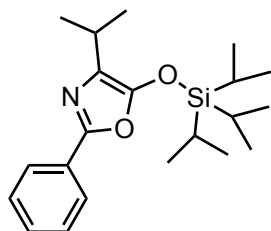


Silanyloxy oxazole 1

M06/def2-TZVP Geometry

N	-1.97611	2.11071	-0.30447
C	-0.62668	2.30429	-0.53214
C	-0.05411	1.08835	-0.68900
O	-1.01651	0.13499	-0.57668
C	-2.15700	0.83398	-0.33349
C	-3.38188	0.08439	-0.13626
C	0.01335	3.63591	-0.57745
O	1.17809	0.69635	-0.93174
Si	2.07934	-0.38650	-0.00188
C	1.94782	0.11704	1.80813
C	1.39113	-2.11380	-0.28098
C	-4.57327	0.77138	0.08815
C	-5.74916	0.07585	0.28375
C	-5.75481	-1.31077	0.25877
C	-4.57358	-1.99824	0.03632
C	-3.39182	-1.30817	-0.16043
C	0.57826	-0.15500	2.42309
C	2.34205	1.57452	2.02398
C	2.23177	-3.17288	0.42201
C	1.24269	-2.43755	-1.76147
C	3.82139	-0.20861	-0.69615
C	4.88854	-0.60967	0.31821
C	4.10990	1.17985	-1.25556
H	-0.42501	4.26022	-1.35934
H	-0.10967	4.16857	0.36903
H	1.08197	3.53616	-0.77978
H	2.68143	-0.51615	2.32878
H	0.38876	-2.11121	0.16782
H	-4.55371	1.85462	0.10545
H	-6.67126	0.61833	0.45710
H	-6.67970	-1.85414	0.41240
H	-4.57195	-3.08184	0.01566
H	-2.46802	-1.84752	-0.33667

H	0.58876	0.06570	3.49498
H	-0.19297	0.48014	1.97624
H	0.25919	-1.19344	2.30433
H	2.27757	1.84220	3.08335
H	3.36127	1.78819	1.69347
H	1.67091	2.24748	1.48078
H	1.78381	-4.16536	0.31237
H	3.23571	-3.22857	-0.01197
H	2.34447	-2.98075	1.49311
H	0.80232	-3.43003	-1.90087
H	0.60821	-1.71565	-2.27955
H	2.21420	-2.44781	-2.26631
H	3.86911	-0.92216	-1.53130
H	4.92921	0.09916	1.15069
H	4.72101	-1.60282	0.74326
H	5.87992	-0.61392	-0.14492
H	5.12685	1.22858	-1.65775
H	3.41733	1.45376	-2.05226
H	4.03215	1.94832	-0.47997

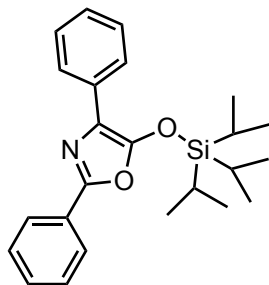


Silanyloxy oxazole 2

M06/def2-TZVP Geometry

N	-2.08607	1.63356	-0.10175
C	-0.75281	1.86839	-0.38032
C	-0.18480	0.69010	-0.72447
O	-1.13750	-0.28162	-0.67621
C	-2.26382	0.36878	-0.28521
C	-3.47895	-0.40632	-0.12531
C	-0.12924	3.21492	-0.26069
O	1.02969	0.33402	-1.08347
Si	2.14037	-0.50488	-0.12100
C	3.70397	-0.27556	-1.13576
C	2.16600	0.35018	1.55901
C	-3.49933	-1.78094	-0.34767
C	-4.67211	-2.49422	-0.18214
C	-5.83380	-1.84811	0.20564
C	-5.81786	-0.47932	0.42788
C	-4.65090	0.23905	0.26431
C	4.86404	-1.19034	-0.76618

C	4.13938	1.18531	-1.14936
C	3.44557	0.09209	2.34804
C	0.94386	0.01773	2.41047
C	1.53786	-2.28362	-0.02574
C	2.30998	-3.16149	0.95172
C	1.48742	-2.91538	-1.41165
C	-0.17509	3.70240	1.18061
H	0.92052	3.10691	-0.56464
C	-0.80873	4.21309	-1.18598
H	3.37673	-0.53522	-2.15332
H	2.12745	1.42366	1.31543
H	-2.59088	-2.28786	-0.65180
H	-4.67877	-3.56368	-0.35762
H	-6.75152	-2.40979	0.33457
H	-6.72460	0.03110	0.73111
H	-4.62377	1.30875	0.43450
H	4.61388	-2.24712	-0.88451
H	5.73148	-0.98811	-1.40261
H	5.18669	-1.04360	0.26900
H	4.96491	1.33909	-1.85123
H	4.49370	1.50494	-0.16441
H	3.32654	1.85368	-1.44298
H	3.41187	0.60409	3.31500
H	3.58464	-0.97352	2.55617
H	4.33806	0.44147	1.82432
H	0.95375	0.59837	3.33878
H	-0.00063	0.23398	1.90370
H	0.93288	-1.03848	2.69573
H	0.50440	-2.19851	0.34016
H	3.36685	-3.24171	0.68089
H	2.26315	-2.78524	1.97645
H	1.90476	-4.17844	0.95978
H	1.02450	-3.90649	-1.37253
H	0.91520	-2.30851	-2.11778
H	2.49210	-3.04835	-1.82576
H	0.28040	4.69104	1.27446
H	-1.21258	3.77185	1.51774
H	0.34917	3.01793	1.85271
H	-0.75709	3.89191	-2.22805
H	-0.34428	5.19867	-1.10560
H	-1.86363	4.31102	-0.91724

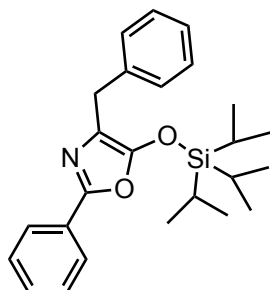


Silanyloxy oxazole 3

M06/def2-TZVP Geometry

N	1.92887	1.58578	-0.18131
C	0.55858	1.67973	-0.36003
C	0.08424	0.41610	-0.54608
O	1.12671	-0.44962	-0.49986
C	2.21478	0.33434	-0.26580
C	3.50277	-0.31872	-0.14230
O	-1.10962	-0.08339	-0.75646
Si	-1.86318	-1.31476	0.13324
C	-1.79514	-0.85842	1.95728
C	-3.62281	-1.20957	-0.51465
C	4.64185	0.45389	0.07395
C	5.87633	-0.15050	0.19815
C	5.99232	-1.52961	0.10903
C	4.86324	-2.30182	-0.10587
C	3.62337	-1.70331	-0.23156
C	-2.41272	0.51268	2.21220
C	-0.39987	-0.93369	2.56806
C	-4.64089	-1.92239	0.36679
C	-3.75684	-1.65801	-1.96413
C	-0.94675	-2.92694	-0.18244
C	-0.61999	-3.20204	-1.64423
C	-1.67888	-4.10778	0.44565
H	-2.42145	-1.61409	2.45524
H	-3.83347	-0.13003	-0.47669
H	4.53642	1.53014	0.14104
H	6.75752	0.45779	0.36542
H	6.96308	-2.00114	0.20652
H	4.94845	-3.37983	-0.17701
H	2.74041	-2.30859	-0.40344
H	-2.43375	0.73608	3.28319
H	-1.83066	1.30531	1.73157
H	-3.43794	0.58988	1.84120
H	-0.43887	-0.72711	3.64197
H	0.06571	-1.91403	2.43924
H	0.26901	-0.18716	2.12754
H	-5.65423	-1.78154	-0.02210

H	-4.45885	-3.00086	0.39694
H	-4.63270	-1.55925	1.39722
H	-3.02084	-1.18322	-2.61754
H	-4.75144	-1.42048	-2.35414
H	-3.63054	-2.74149	-2.05160
H	0.00651	-2.79884	0.34928
H	0.02101	-4.08511	-1.73429
H	-1.52252	-3.40223	-2.22750
H	-0.09946	-2.36597	-2.11590
H	-1.08175	-5.02200	0.37319
H	-1.90568	-3.94755	1.50405
H	-2.62495	-4.30373	-0.06906
C	-1.48863	5.39806	-0.19456
C	-0.13139	5.32599	0.07346
C	0.52979	4.11406	0.01521
C	-0.15556	2.94565	-0.31372
C	-1.52227	3.02835	-0.58728
C	-2.17847	4.24351	-0.52597
H	-2.00582	6.34922	-0.14839
H	0.41845	6.22409	0.33116
H	1.59102	4.05204	0.22351
H	-2.06983	2.13308	-0.85966
H	-3.23951	4.28954	-0.74362



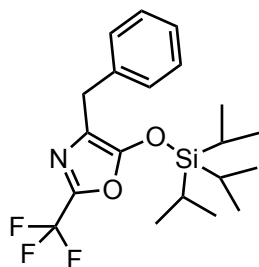
Silanyloxy oxazole 4

M06/def2-TZVP Geometry

N	1.86133	-1.67187	-1.09122
C	0.55181	-1.35625	-1.39431
C	0.36954	-0.03817	-1.14509
O	1.54499	0.48436	-0.70673
C	2.40260	-0.56954	-0.69129
C	3.75840	-0.33429	-0.23688
C	-0.45616	-2.35410	-1.84349
O	-0.66387	0.76542	-1.24915
Si	-1.42707	1.53152	0.05755
C	-0.32896	2.95025	0.62734
C	-3.07246	2.05868	-0.67653

C	4.67625	-1.38266	-0.25382
C	5.96974	-1.17950	0.18236
C	6.36602	0.06815	0.64025
C	5.45761	1.11315	0.65930
C	4.16011	0.91722	0.22416
C	-1.09277	3.87046	1.57409
C	0.32696	3.74133	-0.49653
C	-3.81814	0.84765	-1.22819
C	-2.93705	3.12772	-1.75363
C	-1.65735	0.23641	1.40852
C	-2.84201	0.52041	2.32554
C	-0.40164	-0.00935	2.23710
C	-1.38761	-2.78265	-0.73976
C	-2.76264	-2.65469	-0.87246
C	-3.61365	-3.00406	0.16527
C	-3.09564	-3.49352	1.35106
C	-1.72279	-3.63788	1.48960
C	-0.87788	-3.28429	0.45390
H	-1.04581	-1.94183	-2.66846
H	0.08416	-3.21999	-2.23800
H	0.47385	2.46484	1.20020
H	-3.65517	2.47647	0.15690
H	4.35328	-2.35195	-0.61473
H	6.67732	-2.00027	0.16502
H	7.38249	0.22479	0.98163
H	5.76176	2.09004	1.01665
H	3.44931	1.73592	0.24002
H	-0.43844	4.64968	1.97727
H	-1.91399	4.37763	1.05715
H	-1.52346	3.33384	2.42448
H	1.01138	4.49195	-0.08752
H	0.90001	3.10067	-1.16949
H	-0.41044	4.27696	-1.09976
H	-3.95580	0.05758	-0.48479
H	-3.26995	0.40940	-2.06809
H	-4.80722	1.13579	-1.59769
H	-3.90812	3.34040	-2.21227
H	-2.54815	4.06898	-1.35959
H	-2.26565	2.79973	-2.55351
H	-1.87803	-0.68793	0.85518
H	-2.95445	-0.28396	3.05998
H	-2.70711	1.45010	2.88828
H	-3.78635	0.59825	1.78185
H	-0.56126	-0.83911	2.93321
H	-0.14167	0.86948	2.83646
H	0.47067	-0.26150	1.62740

H	-3.17213	-2.26279	-1.79860
H	-4.68518	-2.88885	0.04526
H	-3.75765	-3.76577	2.16475
H	-1.30914	-4.02609	2.41356
H	0.19784	-3.38180	0.56817

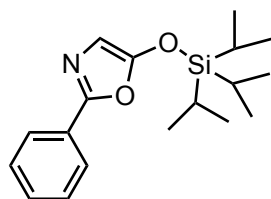


Silanyloxy oxazole 5

M06/def2-TZVP Geometry

N	-1.76237	-2.36353	-0.71927
C	-0.47951	-1.88503	-0.91100
C	-0.48682	-0.55417	-0.63310
O	-1.75037	-0.19023	-0.28514
C	-2.44868	-1.34720	-0.35764
C	0.65142	-2.74630	-1.35142
O	0.44216	0.35677	-0.63565
Si	0.45464	1.85628	0.16141
C	-0.03496	1.63381	1.97592
C	2.26022	2.34878	0.03175
C	0.18507	0.21174	2.48787
C	-1.44105	2.10267	2.32925
C	2.74701	2.44523	-1.40897
C	3.14949	1.39116	0.81709
C	-0.71661	3.01579	-0.74418
C	-0.78512	2.79107	-2.24867
C	-0.37179	4.46639	-0.42022
C	1.93391	-2.51377	-0.60017
C	1.97815	-2.66994	0.78101
C	3.15895	-2.48689	1.47747
C	4.31996	-2.14332	0.80171
C	4.28648	-1.97852	-0.57150
C	3.09974	-2.16057	-1.26433
H	0.32870	-3.78416	-1.22217
H	0.83511	-2.61795	-2.42380
H	0.67673	2.28946	2.50193
H	2.32705	3.34462	0.49430
H	0.06861	0.17460	3.57513
H	-0.55796	-0.47544	2.06831
H	1.17252	-0.18685	2.24254

H	-1.61353	2.01167	3.40614
H	-1.61978	3.14540	2.05741
H	-2.20097	1.49490	1.83059
H	3.81238	2.69442	-1.44084
H	2.62256	1.48813	-1.92564
H	2.21547	3.20686	-1.98385
H	4.19990	1.69038	0.74266
H	2.89563	1.35021	1.87916
H	3.07526	0.37510	0.41723
H	-1.71067	2.80260	-0.33033
H	-1.10188	1.77677	-2.49966
H	0.18194	2.95956	-2.72976
H	-1.49890	3.48210	-2.70816
H	-0.29466	4.65166	0.65617
H	0.58407	4.75373	-0.86895
H	-1.13067	5.14808	-0.81554
H	1.07008	-2.94096	1.31246
H	3.17561	-2.61763	2.55367
H	5.24607	-2.00140	1.34624
H	5.18737	-1.70462	-1.10852
H	3.07690	-2.02999	-2.34192
C	-3.88748	-1.26771	0.02544
F	-4.54892	-0.40760	-0.74938
F	-4.46443	-2.44722	-0.06980
F	-4.01953	-0.83142	1.28127

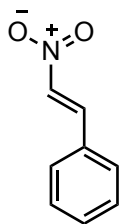


Silanyloxy oxazole 6

M06/def2-TZVP Geometry

C	-2.15880	-1.10570	-0.36478
N	-2.06728	-2.38227	-0.50698
C	-0.72340	-2.64073	-0.66964
C	-0.04897	-1.46837	-0.61781
O	-0.95046	-0.47255	-0.43032
O	1.21543	-1.14734	-0.71576
C	-3.33684	-0.29130	-0.14513
C	-3.24323	1.08533	0.04461
C	-4.38445	1.83723	0.25462
C	-5.62745	1.22781	0.27855
C	-5.72469	-0.14308	0.09172
C	-4.59014	-0.89995	-0.11879

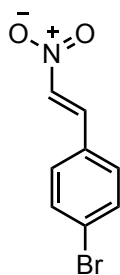
Si	2.07251	0.15473	-0.05932
C	2.02499	1.55400	-1.32314
C	3.17667	2.54277	-1.17402
C	0.69540	2.29676	-1.35662
C	1.28404	0.64121	1.58036
C	2.18140	1.61498	2.33842
C	0.88681	-0.52762	2.47458
C	3.81545	-0.53465	0.07289
C	4.31377	-0.98880	-1.29634
C	3.93096	-1.67676	1.07468
H	-0.32703	-3.63251	-0.80876
H	-2.27041	1.56425	0.02948
H	-4.30199	2.90787	0.40126
H	-6.52030	1.81945	0.44294
H	-6.69537	-0.62480	0.10997
H	-4.65123	-1.97164	-0.26659
H	2.14693	1.03574	-2.28543
H	3.14195	3.29519	-1.96811
H	3.12033	3.08387	-0.22456
H	4.15718	2.06389	-1.22009
H	0.68744	3.03984	-2.16010
H	-0.15374	1.62843	-1.51244
H	0.52383	2.83826	-0.41991
H	0.36434	1.17464	1.30370
H	1.70277	1.94131	3.26698
H	3.13244	1.14902	2.61571
H	2.41228	2.51243	1.75842
H	0.35049	-0.16563	3.35732
H	0.23663	-1.24802	1.97168
H	1.76188	-1.07400	2.83431
H	4.44991	0.29458	0.41648
H	5.34239	-1.35651	-1.23085
H	3.69934	-1.80878	-1.67876
H	4.29777	-0.19032	-2.04210
H	4.93293	-2.11666	1.04590
H	3.74645	-1.35303	2.10084
H	3.21965	-2.47676	0.84580



Nitrostyrene 1

M06/def2-TZVP Geometry

C	-0.60922	0.44132	0.00003
C	-1.58865	-0.45464	-0.00018
C	0.81606	0.17450	0.00005
C	1.69580	1.25638	-0.00009
C	3.06380	1.05927	-0.00012
C	3.57452	-0.22658	0.00002
C	2.71175	-1.31385	0.00018
C	1.34741	-1.11718	0.00020
H	-0.91523	1.48461	0.00020
H	-1.49996	-1.53103	-0.00039
H	1.29077	2.26288	-0.00018
H	3.73271	1.91147	-0.00023
H	4.64634	-0.38579	0.00000
H	3.11041	-2.32132	0.00030
H	0.68539	-1.97554	0.00035
N	-2.97772	-0.02973	-0.00011
O	-3.23508	1.15433	0.00021
O	-3.79933	-0.92339	-0.00019

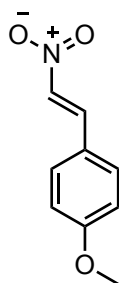


Nitrostyrene 2

M06/def2-TZVP Geometry

C	-2.29405	0.46416	0.00002
C	-3.22232	-0.48455	-0.00024
C	-0.85713	0.27789	0.00006
C	-0.03815	1.40613	-0.00009
C	1.33825	1.29453	-0.00011
C	1.90998	0.03536	0.00006
C	1.12095	-1.10590	0.00024

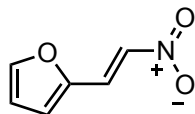
C	-0.25065	-0.98032	0.00024
H	-2.65752	1.48875	0.00020
H	-3.07518	-1.55464	-0.00048
H	-0.49505	2.39001	-0.00021
H	1.96559	2.17693	-0.00023
Br	3.78796	-0.13567	0.00006
H	1.58558	-2.08401	0.00040
H	-0.85882	-1.87756	0.00042
N	-4.63287	-0.13453	-0.00019
O	-4.95186	1.03421	0.00011
O	-5.40494	-1.07083	-0.00034



Nitrostyrene 3

M06/def2-TZVP Geometry

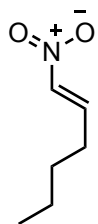
C	-1.53547	-0.44177	-0.00000
C	-2.53141	0.43999	-0.00000
C	-0.11989	-0.15857	-0.00000
C	0.78102	-1.21928	0.00002
C	2.14883	-1.01753	0.00002
C	2.64531	0.28035	0.00001
C	1.75651	1.35920	-0.00001
C	0.40431	1.14146	-0.00002
H	-1.82787	-1.48906	-0.00000
H	-2.45773	1.51743	-0.00000
H	0.39569	-2.23364	0.00003
H	2.81418	-1.87033	0.00004
O	3.94911	0.59798	0.00001
H	2.16773	2.36141	-0.00003
H	-0.26486	1.99432	-0.00003
N	-3.90940	-0.00525	-0.00001
O	-4.15074	-1.19416	-0.00002
O	-4.74774	0.87439	-0.00002
C	4.89403	-0.44289	0.00003
H	5.87480	0.02799	0.00003
H	4.79974	-1.07138	0.89179
H	4.79975	-1.07140	-0.89172



Nitrostyrene 4

M06/def2-TZVP Geometry

C	-0.28318	0.52469	0.00002
C	-1.22591	-0.41496	0.00002
H	-0.60184	1.56228	0.00002
H	-1.07160	-1.48352	0.00001
N	-2.62480	-0.04420	-0.00006
O	-2.92376	1.13184	-0.00005
O	-3.41581	-0.96537	-0.00007
C	1.11793	0.28791	0.00003
C	2.17608	1.14912	0.00011
C	3.34464	0.35327	-0.00016
C	2.91520	-0.93219	0.00012
O	1.57299	-0.99276	0.00006
H	2.10883	2.22552	0.00014
H	4.36931	0.68611	-0.00033
H	3.43302	-1.87762	0.00016

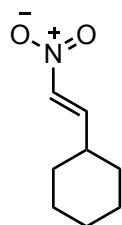


Nitrostyrene 5

M06/def2-TZVP Geometry

C	0.62590	-0.95483	-0.00005
C	1.22778	0.22140	-0.00005
H	1.26943	-1.83084	-0.00007
H	0.76470	1.19731	-0.00003
N	2.68434	0.31361	-0.00007
O	3.34081	-0.70350	0.00007
O	3.13746	1.43849	0.00006
C	-0.83879	-1.17822	-0.00004
H	-1.08279	-1.80875	0.86594
H	-1.08282	-1.80871	-0.86604
C	-1.71532	0.05545	-0.00000
H	-1.48620	0.67459	0.87631
H	-1.48623	0.67462	-0.87631
C	-3.19241	-0.28578	0.00001
H	-3.41826	-0.90761	0.87443

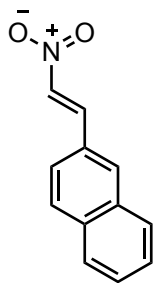
H	-3.41828	-0.90758	-0.87442
C	-4.07138	0.94586	0.00005
H	-5.13171	0.68953	0.00006
H	-3.87950	1.56442	0.88078
H	-3.87953	1.56445	-0.88067



Nitrostyrene 6

M06/def2-TZVP Geometry

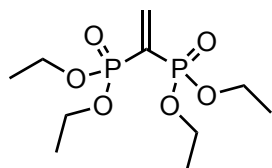
C	-0.77589	0.00002	0.21643
C	-1.84483	0.00002	-0.55874
H	-0.93005	0.00003	1.29472
H	-1.85622	0.00000	-1.64008
N	-3.19025	0.00002	0.00536
O	-3.32384	0.00000	1.20842
O	-4.09708	-0.00003	-0.79992
C	2.80721	-1.25120	-0.23858
C	1.35578	-1.25347	0.20587
C	0.62343	0.00001	-0.27473
C	1.35580	1.25347	0.20586
C	2.80723	1.25118	-0.23859
C	3.52602	-0.00001	0.23421
H	2.84780	-1.29914	-1.33452
H	3.31200	-2.14844	0.12894
H	1.30682	-1.28515	1.30319
H	0.83760	-2.14658	-0.15509
H	0.62124	0.00000	-1.37421
H	0.83762	2.14659	-0.15510
H	1.30683	1.28517	1.30318
H	2.84782	1.29912	-1.33453
H	3.31203	2.14842	0.12892
H	3.56452	-0.00001	1.33142
H	4.56261	-0.00002	-0.11278



Nitrostyrene 7

M06/def2-TZVP Geometry

C	1.86983	-0.37285	0.00001
C	2.93971	0.41502	0.00001
H	2.06210	-1.44278	0.00001
H	2.96516	1.49459	0.00001
N	4.27431	-0.15551	0.00000
O	4.40361	-1.36077	-0.00001
O	5.18786	0.64442	-0.00001
C	-1.21558	1.75788	0.00001
C	0.09749	1.40908	0.00001
C	0.48493	0.04457	0.00001
C	-0.49453	-0.92109	0.00001
H	-1.50440	2.80376	0.00001
H	0.85688	2.18205	0.00001
H	-0.21083	-1.96969	0.00001
C	-2.23437	0.77742	0.00000
C	-1.86163	-0.59141	0.00000
C	-2.87084	-1.57630	-0.00000
C	-4.18902	-1.22191	-0.00001
C	-4.55729	0.13454	-0.00001
C	-3.60133	1.11099	-0.00000
H	-2.57839	-2.62117	-0.00000
H	-4.95750	-1.98564	-0.00001
H	-5.60699	0.40359	-0.00001
H	-3.88207	2.15907	-0.00000

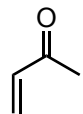


Phosphonate

M06/def2-TZVP Geometry

C	0.37109	-1.57212	-2.19391
C	0.06299	-0.85792	-1.11785
P	1.29685	-0.22503	0.01596

P	-1.67423	-0.64504	-0.71527
O	1.36943	-0.94998	1.28659
O	2.60063	-0.24432	-0.87551
O	1.00781	1.32259	0.16899
C	0.41891	1.86731	1.35543
C	3.84272	0.13468	-0.27236
C	4.93829	-0.07792	-1.27443
C	1.48873	2.30551	2.31522
O	-2.57213	-1.52444	-1.45855
O	-1.75780	-0.75992	0.86427
O	-1.86365	0.90989	-0.90845
C	-1.68506	-2.05488	1.47986
C	-1.45571	-1.85735	2.94790
C	-3.11770	1.51965	-0.58601
C	-3.13754	2.89464	-1.18547
H	-0.41363	-2.00427	-2.80751
H	1.39952	-1.74588	-2.49060
H	-0.19204	2.70869	1.01930
H	-0.24839	1.12904	1.81021
H	3.77804	1.18613	0.03123
H	3.99701	-0.46635	0.62958
H	5.89997	0.20981	-0.84709
H	4.99414	-1.12705	-1.56855
H	4.76603	0.52134	-2.16964
H	2.16127	3.02391	1.84165
H	2.07258	1.44546	2.64952
H	1.04381	2.78028	3.19180
H	-0.85713	-2.61831	1.03473
H	-2.61533	-2.58943	1.26724
H	-1.43129	-2.82145	3.45819
H	-0.49947	-1.35682	3.10854
H	-2.25471	-1.25685	3.38707
H	-3.93086	0.89887	-0.97669
H	-3.21435	1.55581	0.50485
H	-4.07261	3.40055	-0.94030
H	-3.04642	2.84356	-2.27115
H	-2.30996	3.49402	-0.80170

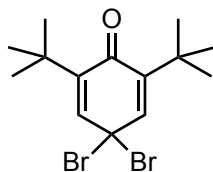


MVK

M06/def2-TZVP Geometry

C	0.83573	1.28797	0.00016
C	0.54534	-0.18685	-0.00104

C	-0.86567	-0.63592	-0.00011
O	1.43312	-1.00547	0.00038
C	-1.92260	0.16296	0.00014
H	0.40216	1.76952	0.87960
H	1.91306	1.43820	0.00090
H	0.40320	1.77059	-0.87919
H	-0.97848	-1.71624	0.00029
H	-2.93179	-0.23085	0.00066
H	-1.82981	1.24354	-0.00025

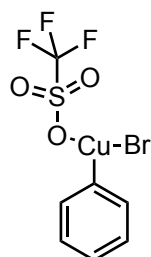


Bromide

M06/def2-TZVP Geometry

C	-1.14725	-0.00000	0.00001
C	-0.37605	1.24894	-0.00004
C	0.95830	1.28700	-0.00007
C	1.71797	0.00000	-0.00001
C	0.95831	-1.28700	0.00006
C	-0.37605	-1.24894	0.00005
O	2.93118	0.00000	-0.00002
C	1.72855	-2.59972	0.00010
C	1.72855	2.59972	-0.00012
C	2.59814	2.69768	1.25575
C	0.78763	3.79847	0.00031
C	2.59740	2.69803	-1.25647
C	2.59815	-2.69766	-1.25576
C	0.78763	-3.79847	-0.00036
C	2.59739	-2.69805	1.25646
Br	-2.30819	0.00006	1.59416
Br	-2.30821	-0.00006	-1.59414
H	-0.97562	2.15098	-0.00008
H	-0.97562	-2.15098	0.00009
H	3.35023	1.91231	1.29283
H	3.10983	3.66387	1.26754
H	1.98151	2.63579	2.15697
H	0.14977	3.82155	-0.88750
H	0.15036	3.82138	0.88856
H	1.38149	4.71492	0.00021
H	1.98026	2.63634	-2.15735
H	3.10903	3.66426	-1.26833
H	3.34951	1.91271	-1.29419
H	3.35024	-1.91229	-1.29283

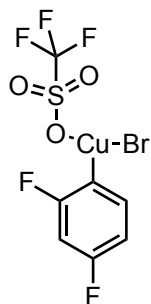
H	3.10984	-3.66385	-1.26756
H	1.98154	-2.63576	-2.15699
H	0.14976	-3.82156	0.88745
H	0.15038	-3.82136	-0.88862
H	1.38150	-4.71492	-0.00026
H	1.98024	-2.63637	2.15733
H	3.10901	-3.66428	1.26831
H	3.34951	-1.91274	1.29420



Copper 1

M06/def2-TZVP Geometry

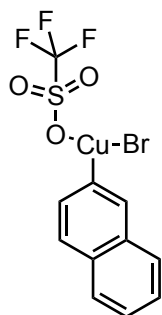
Br	-1.48892	-2.28641	-0.42261
C	-1.87279	0.58656	0.03717
O	0.81646	0.95924	0.88885
S	2.05700	0.13587	0.87529
O	2.99229	0.36832	1.90993
O	1.60898	-1.23486	0.60987
C	2.87242	0.66000	-0.69066
F	3.22755	1.92447	-0.60823
F	3.93398	-0.08301	-0.91180
F	2.02392	0.51612	-1.69986
C	-1.78459	1.42004	-1.04909
C	-2.67360	2.48752	-1.08248
C	-3.61255	2.64846	-0.07770
C	-3.68279	1.75029	0.97253
C	-2.81009	0.66931	1.03338
H	-1.04671	1.28036	-1.83018
H	-2.62350	3.18875	-1.90722
H	-4.30661	3.47907	-0.12077
H	-4.42780	1.87014	1.75037
H	-2.86956	-0.05790	1.83284
Cu	-0.35009	-0.52424	0.27284



Copper 2

M06/def2-TZVP Geometry

Br	-0.69110	2.63443	-0.44575
C	-1.62621	-0.09694	-0.11714
O	0.91600	-1.02652	0.79558
S	2.28828	-0.44783	0.81276
O	3.13628	-0.82686	1.87716
O	2.09526	0.98150	0.52580
C	3.04399	-1.12260	-0.72615
F	2.27252	-0.82951	-1.76185
F	4.23088	-0.58747	-0.90553
F	3.15655	-2.42918	-0.62870
C	-2.03161	-0.52830	-1.35720
C	-3.14129	-1.35520	-1.44425
C	-3.82708	-1.66713	-0.28674
C	-3.45307	-1.19109	0.95558
C	-2.34432	-0.37370	1.02771
H	-1.49240	-0.24007	-2.25137
H	-3.48360	-1.74209	-2.39510
F	-1.95680	0.10963	2.19351
H	-4.00804	-1.44927	1.84857
F	-4.89367	-2.44713	-0.36489
Cu	0.08179	0.65619	0.16217

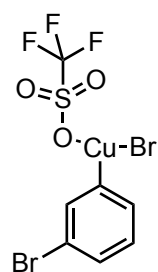


Copper 3

M06/def2-TZVP Geometry

Br	-0.31243	2.88186	0.62575
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C	1.16804	0.57492	-0.36103
O	-1.20256	-0.83550	-1.10641
S	-2.64554	-0.71023	-0.76563
O	-3.57456	-1.14078	-1.74129
O	-2.79237	0.62709	-0.18108
C	-2.82878	-1.85460	0.66584
F	-1.95269	-1.53222	1.60650
F	-4.04436	-1.75872	1.15891
F	-2.60628	-3.09280	0.27940
C	1.68425	0.66228	-1.65270
C	2.91508	0.10197	-1.85738
C	1.81153	0.07635	0.71774
H	1.12632	1.11308	-2.46349
H	3.35004	0.11280	-2.85152
H	1.39453	0.11077	1.71781
C	3.63513	-0.50054	-0.80378
C	3.07876	-0.52017	0.50181
C	3.80764	-1.10783	1.55457
C	5.03563	-1.65649	1.32260
C	5.58932	-1.64153	0.03069
C	4.90557	-1.07629	-1.00660
H	3.37432	-1.11722	2.54873
H	5.58859	-2.10903	2.13711
H	6.56432	-2.08250	-0.13866
H	5.32942	-1.06143	-2.00503
Cu	-0.69969	0.87692	-0.22206

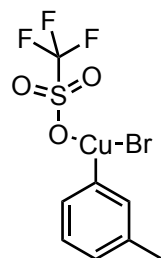


Copper 4

M06/def2-TZVP Geometry

Br	-0.51886	-2.78854	1.05034
C	1.04641	-0.92028	-0.54497
O	-1.22582	0.65688	-1.22639
S	-2.65238	0.69689	-0.79907
O	-3.60272	1.08547	-1.77066
O	-2.86211	-0.54913	-0.05169
C	-2.65743	2.01030	0.49249

F	-3.84115	2.06788	1.06086
F	-1.74617	1.72808	1.41230
F	-2.37123	3.17227	-0.05330
C	1.51263	-1.59865	-1.64167
C	2.77845	-1.24539	-2.09345
C	3.52717	-0.29165	-1.42864
C	3.01440	0.32376	-0.29909
C	1.75164	0.00385	0.18451
H	0.93005	-2.36266	-2.13971
H	3.18451	-1.73630	-2.97010
Br	4.04356	1.61124	0.61659
H	1.35624	0.48023	1.07326
H	4.51802	-0.02979	-1.77732
Cu	-0.81389	-0.97406	-0.17749

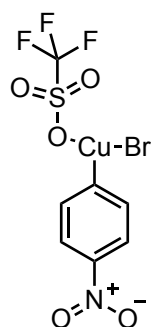


Copper 5

M06/def2-TZVP Geometry

Br	-0.97413	-2.56920	0.27343
C	-1.71200	0.25026	0.27547
O	0.83081	1.08898	-0.71529
S	2.15125	0.43591	-0.92575
O	1.89525	-1.00396	-0.81753
O	2.94102	0.91661	-1.99612
C	3.06381	0.85294	0.61868
F	4.22241	0.23115	0.63290
F	3.25999	2.15279	0.68493
F	2.35346	0.47056	1.67065
C	-1.69936	0.82591	1.51992
C	-2.69525	1.76505	1.75748
C	-3.64748	2.04256	0.79302
C	-3.64760	1.40169	-0.43949
C	-2.65651	0.45106	-0.69397
H	-0.95559	0.58530	2.26922
H	-2.72345	2.27163	2.71528
H	-2.64268	-0.09038	-1.63315
H	-4.42573	2.76770	1.00612
C	-4.66734	1.71625	-1.48430
H	-4.93874	0.82852	-2.05741

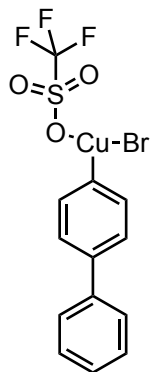
H	-5.57367	2.12968	-1.04050
H	-4.28134	2.45437	-2.19234
Cu	-0.09219	-0.60473	-0.22659



Copper 6

M06/def2-TZVP Geometry

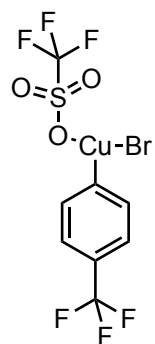
Br	0.24213	2.84525	0.50370
C	-1.26603	0.42120	-0.06306
O	1.02669	-1.00425	-0.92552
S	2.49826	-0.76132	-0.88999
O	3.26621	-1.31747	-1.93684
O	2.63475	0.66800	-0.57987
C	3.01488	-1.61634	0.65825
F	2.82964	-2.91167	0.53319
F	4.28182	-1.36903	0.89897
F	2.28297	-1.16966	1.66974
C	-1.55936	-0.40176	0.99932
C	-2.81576	-0.98552	1.01656
C	-3.70299	-0.69041	-0.00063
C	-3.39432	0.16910	-1.03642
C	-2.14218	0.76383	-1.06417
H	-0.84076	-0.61118	1.78262
H	-3.11094	-1.66070	1.80883
H	-1.87594	1.46157	-1.84752
H	-4.13205	0.37693	-1.80012
N	-5.04463	-1.31015	0.02871
O	-5.29067	-2.05240	0.94968
O	-5.80221	-1.03112	-0.87006
Cu	0.57903	0.79974	-0.26239



Copper 7

M06/def2-TZVP Geometry

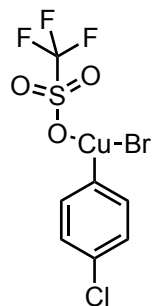
Br	1.36616	2.88099	-0.54866
C	-0.52890	0.75087	0.05038
O	1.52080	-1.03927	0.94721
S	3.00801	-1.03389	0.90760
O	3.68235	-1.69945	1.95739
O	3.38270	0.34585	0.57952
C	3.37602	-1.98092	-0.62848
F	2.72461	-1.43873	-1.64885
F	4.66677	-1.94737	-0.87570
F	2.98571	-3.23010	-0.48851
C	-0.94544	-0.05329	-0.98098
C	-2.27661	-0.44062	-0.96996
C	-1.34713	1.27513	1.01731
H	-0.27243	-0.39476	-1.75865
H	-2.64041	-1.08309	-1.76426
H	-0.98183	1.95614	1.77510
C	-3.15511	0.00739	0.01520
C	-2.67231	0.86524	1.00082
H	-3.33747	1.21542	1.78229
C	-7.24701	-1.19666	-0.02481
C	-6.90585	0.09788	0.32897
C	-5.57972	0.48794	0.34386
C	-4.56897	-0.40743	0.00199
C	-4.92623	-1.70594	-0.35335
C	-6.25221	-2.09743	-0.36495
H	-8.28624	-1.50294	-0.03492
H	-7.67869	0.81190	0.58829
H	-5.32426	1.51107	0.59765
H	-4.15198	-2.42594	-0.59528
H	-6.50929	-3.11519	-0.63392
Cu	1.35639	0.82106	0.25357



Copper 8

M06/def2-TZVP Geometry

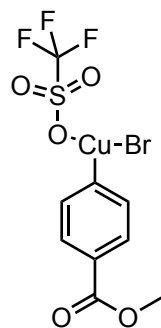
Br	-0.68755	2.89655	0.45906
C	0.97391	0.56683	-0.08348
O	-1.23677	-1.02171	-0.90650
S	-2.71916	-0.86999	-0.86883
O	-3.45511	-1.49315	-1.90161
O	-2.94787	0.55165	-0.58249
C	-3.17594	-1.72993	0.69507
F	-4.45640	-1.56293	0.93617
F	-2.90689	-3.01308	0.59237
F	-2.47362	-1.22011	1.69783
C	1.31884	-0.24355	0.97268
C	2.60885	-0.74636	0.97628
C	3.49608	-0.40209	-0.03400
C	3.11275	0.44739	-1.05496
C	1.82477	0.96969	-1.07877
H	0.61714	-0.50439	1.75588
H	2.92507	-1.40921	1.77427
H	3.81536	0.72201	-1.83149
H	1.51829	1.65770	-1.85596
C	4.88658	-0.96843	0.02726
F	5.64023	-0.56848	-0.98968
F	5.50202	-0.60493	1.15277
F	4.86167	-2.30089	0.01178
Cu	-0.89535	0.82251	-0.27639



Copper 9

M06/def2-TZVP Geometry

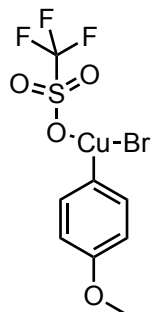
Br	0.11200	2.80456	0.44713
C	1.47299	0.28160	-0.06416
O	-0.92584	-1.02917	-0.89645
S	-2.37371	-0.68217	-0.87373
O	-3.17955	-1.21489	-1.90557
O	-2.41727	0.76013	-0.60418
C	-2.95284	-1.45518	0.69465
F	-4.20176	-1.11689	0.92354
F	-2.85706	-2.76438	0.60852
F	-2.19677	-1.03265	1.69907
C	1.70384	-0.56329	0.99431
C	2.91780	-1.23363	1.01586
C	3.84614	-0.99900	0.01496
C	3.59562	-0.10264	-1.00954
C	2.38754	0.57968	-1.04280
H	0.96715	-0.73365	1.77064
H	3.14098	-1.93484	1.81033
H	4.34494	0.07457	-1.77096
H	2.18425	1.30564	-1.81950
Cl	5.36053	-1.83350	0.05706
Cu	-0.34662	0.76773	-0.27865



Copper 10

M06/def2-TZVP Geometry

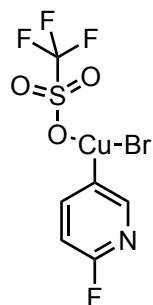
Br	0.85968	2.87015	0.60947
C	-0.92261	0.67932	-0.10476
O	1.21113	-0.99139	-0.97488
S	2.69726	-0.94076	-0.88337
O	3.42616	-1.55064	-1.92955
O	3.01081	0.44113	-0.50248
C	3.04342	-1.92210	0.63658
F	4.32290	-1.85435	0.92839
F	2.34013	-1.43059	1.64792
F	2.69848	-3.17714	0.44568
C	-1.34269	-0.14705	0.90818
C	-2.65749	-0.58458	0.84915
C	-3.49373	-0.15928	-0.17585
C	-3.02223	0.71136	-1.14929
C	-1.71358	1.16769	-1.11389
H	-0.68184	-0.47029	1.70360
H	-3.03197	-1.25843	1.60907
H	-3.69833	1.03953	-1.93011
H	-1.34199	1.86620	-1.85230
C	-4.91252	-0.59332	-0.27345
O	-5.25476	-1.42467	0.71447
O	-5.66419	-0.23936	-1.13847
C	-6.59959	-1.88408	0.68412
H	-6.71622	-2.54195	1.54162
H	-7.29501	-1.04655	0.75271
H	-6.80026	-2.42813	-0.23973
Cu	0.96414	0.83128	-0.23786



Copper 11

M06/def2-TZVP Geometry

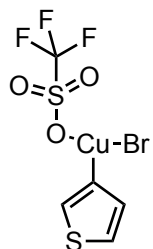
Br	-0.13578	2.84586	-0.39504
C	-1.46717	0.32082	0.17898
O	0.99065	-0.98299	0.92710
S	2.43236	-0.65144	0.77967
O	3.30236	-1.09747	1.80216
O	2.46806	0.75996	0.38011
C	2.91546	-1.56607	-0.74381
F	2.80445	-2.86209	-0.54080
F	2.12033	-1.21642	-1.74382
F	4.15877	-1.27545	-1.06050
C	-2.04990	-0.01787	-1.01288
C	-3.25383	-0.71201	-0.96705
C	-2.05632	0.14160	1.41180
H	-1.59135	0.22264	-1.96362
H	-3.71190	-1.02481	-1.89582
H	-1.59024	0.47936	2.32924
C	-3.85514	-0.97408	0.25901
C	-3.25497	-0.53998	1.44221
H	-3.74930	-0.75106	2.38292
O	-5.02010	-1.62552	0.40651
C	-5.68864	-2.07592	-0.74523
H	-5.07918	-2.78922	-1.31022
H	-6.59279	-2.57520	-0.40369
H	-5.96664	-1.24376	-1.40057
Cu	0.36894	0.78603	0.22945



Copper 12

M06/def2-TZVP Geometry

Br	-0.87770	2.64348	0.21232
C	-1.73471	-0.12419	-0.09794
O	0.88877	-1.00538	-0.81569
S	2.25402	-0.40545	-0.77342
O	2.02891	1.01610	-0.48083
O	3.14045	-0.76345	-1.81423
C	2.96516	-1.09022	0.78198
F	3.08788	-2.39510	0.67430
F	4.14358	-0.55019	0.99867
F	2.16253	-0.81016	1.79505
C	-2.19285	-0.71597	-1.25682
C	-3.28334	-1.55387	-1.14612
C	-2.36897	-0.28506	1.11140
H	-1.70792	-0.56178	-2.21351
H	-2.04419	0.22257	2.01293
N	-3.41447	-1.10272	1.20124
C	-3.83474	-1.69701	0.11999
H	-3.70000	-2.07776	-1.99637
F	-4.88109	-2.48547	0.25583
Cu	-0.01297	0.65826	-0.24041

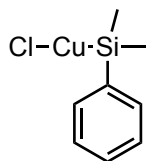


Copper 13

M06/def2-TZVP Geometry

Br	1.38664	-2.38026	0.11270
C	1.87176	0.48747	0.03901
O	-0.85689	1.05971	-0.70786
S	-2.10731	0.25411	-0.78814

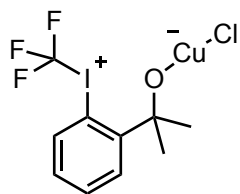
O	-1.67057	-1.13758	-0.61841
O	-3.00769	0.57073	-1.83116
C	-2.97104	0.65875	0.78749
F	-4.05561	-0.07687	0.89520
F	-2.16980	0.40656	1.80915
F	-3.29828	1.93307	0.79904
C	2.57350	0.61655	1.25419
C	3.46923	1.63400	1.15999
C	2.24426	1.30265	-0.97252
H	2.41329	0.00541	2.12980
H	1.86565	1.38628	-1.97884
S	3.46451	2.35939	-0.39213
H	4.14221	1.99851	1.92125
Cu	0.28274	-0.49660	-0.24180



Copper 14

M06/def2-TZVP Geometry

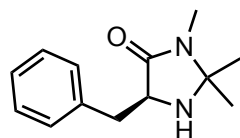
C	0.31620	2.26566	1.48066
Si	0.00328	1.09782	0.00001
C	0.31620	2.26570	-1.48063
C	1.58227	-0.00199	-0.00000
C	1.49469	-1.39321	0.00002
C	2.62434	-2.19856	0.00002
C	3.88499	-1.62570	-0.00001
C	4.00305	-0.24422	-0.00003
C	2.86589	0.54693	-0.00003
Cl	-3.78658	-1.20188	-0.00001
H	1.28291	2.77664	1.40197
H	-0.46465	3.03052	1.52433
H	0.29624	1.72029	2.42729
H	1.28289	2.77669	-1.40191
H	0.29627	1.72034	-2.42726
H	-0.46467	3.03053	-1.52429
H	0.50763	-1.85068	0.00003
H	2.51955	-3.27921	0.00004
H	4.77208	-2.25105	-0.00001
H	4.98692	0.21585	-0.00005
H	2.98295	1.62892	-0.00004
Cu	-1.93786	-0.07393	-0.00000



Copper 15

M06/def2-TZVP Geometry

Cl	-4.29948	0.78360	-0.77073
Cu	-2.33031	0.82050	-0.08063
O	-0.54308	0.68243	0.48342
C	0.29217	1.76893	0.58608
C	-0.13540	2.89768	-0.35449
C	0.29624	2.26035	2.03232
C	1.70742	1.34572	0.17469
C	2.00011	0.13112	-0.41340
C	3.27395	-0.26821	-0.79654
C	4.32404	0.60519	-0.60594
C	4.07627	1.84063	-0.02764
C	2.79807	2.19657	0.35471
I	0.49807	-1.28101	-0.85259
C	-0.20533	-2.05920	1.12821
F	0.57709	-1.57348	2.04899
F	-1.44438	-1.77340	1.35197
F	-0.05343	-3.36468	1.05021
H	-1.14323	3.22259	-0.08185
H	0.53335	3.76090	-0.30620
H	-0.16573	2.53465	-1.38544
H	0.90488	3.15395	2.18779
H	-0.73477	2.49638	2.30441
H	0.65130	1.46966	2.69682
H	3.43994	-1.24762	-1.23026
H	5.32700	0.31870	-0.89650
H	4.89356	2.53339	0.13514
H	2.63201	3.16687	0.80845

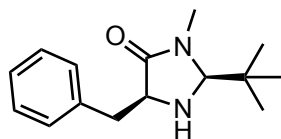


Amine 1

M06-2X/def2-TZVP Geometry

C	-0.67720	0.46392	1.43165
N	-0.90534	-0.93458	1.07184

C	-1.88911	-0.94724	-0.01548
N	-1.76626	0.39562	-0.60643
C	-1.14299	1.26641	0.21850
O	-0.99269	2.45853	0.04293
C	-2.44633	0.81065	-1.80613
C	-1.54658	-2.02571	-1.02836
C	-3.29102	-1.14858	0.55406
C	0.76897	0.78254	1.81804
C	1.76696	0.33795	0.77981
C	1.97024	1.08653	-0.37985
C	2.85279	0.64780	-1.35614
C	3.54629	-0.54461	-1.19146
C	3.35518	-1.29476	-0.04061
C	2.47173	-0.85348	0.93649
H	-1.32374	0.75027	2.26802
H	-0.03560	-1.31266	0.70878
H	-2.07590	0.26295	-2.67424
H	-3.52513	0.65727	-1.72545
H	-2.25022	1.87268	-1.94207
H	-0.57719	-1.81886	-1.48639
H	-1.50541	-2.99219	-0.52522
H	-2.30226	-2.08288	-1.81239
H	-4.05023	-1.06539	-0.22505
H	-3.49476	-0.40098	1.32157
H	-3.36132	-2.13715	1.00621
H	0.82593	1.86312	1.95957
H	0.98939	0.30410	2.77343
H	1.42928	2.01647	-0.50934
H	3.00374	1.24253	-2.24800
H	4.23664	-0.88286	-1.95321
H	3.89658	-2.22136	0.10114
H	2.32928	-1.43917	1.83827

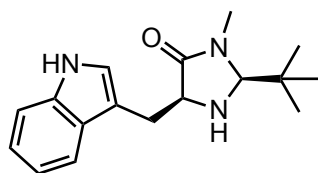


Amine 2

M06-2X/def2-TZVP Geometry

C	-0.05896	1.51318	1.34683
N	-0.65001	0.19589	1.55073
C	-1.76375	0.04442	0.61671
N	-1.52485	1.08010	-0.39500
C	-0.59241	1.98086	0.00144
O	-0.27141	2.99421	-0.58432

C	-2.43561	1.39688	-1.46883
C	-1.87702	-1.39743	0.07156
C	1.47069	1.53391	1.41183
C	2.10296	0.50674	0.50882
C	2.57861	-0.69646	1.02541
C	3.09902	-1.67693	0.18957
C	3.15065	-1.46328	-1.18001
C	2.68626	-0.26385	-1.70537
C	2.16689	0.71369	-0.86930
H	-0.44117	2.22196	2.09006
H	0.04783	-0.50592	1.33374
H	-3.46888	1.30783	-1.12544
H	-2.23857	2.42293	-1.77546
H	-2.29327	0.74149	-2.32928
H	1.78427	2.53940	1.12555
H	1.78228	1.36379	2.44345
H	2.54233	-0.86515	2.09636
H	3.46512	-2.60492	0.60977
H	3.55543	-2.22410	-1.83457
H	2.73085	-0.08786	-2.77257
H	1.80339	1.64803	-1.28116
H	-2.70845	0.27971	1.13049
C	-3.22409	-1.59966	-0.63078
H	-4.05364	-1.31217	0.01945
H	-3.30279	-1.03577	-1.55801
H	-3.34798	-2.65480	-0.88071
C	-1.83245	-2.36089	1.26403
H	-2.03575	-3.37622	0.91976
H	-0.86211	-2.36448	1.76002
H	-2.58652	-2.09539	2.00832
C	-0.74085	-1.71144	-0.90265
H	-0.77005	-1.05378	-1.77283
H	0.24659	-1.60690	-0.44659
H	-0.83317	-2.74187	-1.25148

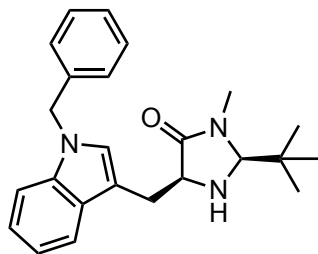


Amine 3

M06-2X/def2-TZVP Geometry

C	-0.98270	1.51963	1.50920
N	-1.57265	0.18691	1.52846
C	-2.25474	-0.03980	0.25527

N	-1.71731	1.00090	-0.62862
C	-1.07402	1.97171	0.06357
O	-0.67409	3.03037	-0.37750
C	-2.18849	1.25955	-1.96890
C	-2.09759	-1.49401	-0.24213
C	0.45418	1.58346	2.05208
C	1.34652	0.50143	1.53004
C	-0.64807	-1.80757	-0.61623
C	-2.99998	-1.74924	-1.45457
C	-2.56537	-2.42320	0.88437
C	1.71616	-0.61809	2.21847
N	2.47553	-1.43970	1.41894
C	2.61504	-0.85696	0.18443
C	1.91878	0.37015	0.21387
C	3.27571	-1.31675	-0.95417
C	3.23208	-0.51754	-2.07667
C	2.55498	0.71406	-2.06797
C	1.90344	1.16711	-0.93990
H	-1.59048	2.22329	2.08820
H	-0.82105	-0.48722	1.61658
H	-3.33344	0.14607	0.37576
H	-3.25760	1.04909	-2.04055
H	-2.00654	2.31119	-2.18512
H	-1.65770	0.65503	-2.70571
H	0.84405	2.57079	1.79392
H	0.41756	1.51971	3.14101
H	-0.59360	-2.80427	-1.05888
H	0.01563	-1.80081	0.25112
H	-0.25320	-1.08941	-1.33857
H	-4.02083	-1.40654	-1.26917
H	-2.63146	-1.26564	-2.35691
H	-3.04098	-2.82137	-1.65460
H	-3.59428	-2.19668	1.17349
H	-2.52896	-3.45908	0.54266
H	-1.94355	-2.33808	1.77510
H	1.49588	-0.89198	3.23852
H	2.89005	-2.30837	1.70381
H	3.80000	-2.26396	-0.95678
H	3.73257	-0.84194	-2.97973
H	2.55070	1.31948	-2.96481
H	1.38521	2.11737	-0.94534

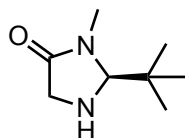


Amine 4

M06-2X/def2-TZVP Geometry

C	-2.66651	0.56637	-1.58894
N	-2.89290	0.46432	-0.15089
C	-2.81509	-0.94972	0.19653
N	-1.97274	-1.52516	-0.86517
C	-1.93316	-0.71516	-1.95788
O	-1.43268	-0.97662	-3.03204
C	-1.65941	-2.92764	-0.99138
C	-2.31905	-1.17186	1.64200
C	-1.88787	1.81266	-2.01053
C	-0.51194	1.84235	-1.42453
C	-2.62150	-2.60473	2.09391
C	-0.81961	-0.90242	1.76824
C	-3.09727	-0.22215	2.56117
C	0.60700	1.28807	-1.97600
N	1.67815	1.40771	-1.12345
C	1.25153	2.02069	0.02710
C	-0.11653	2.33499	-0.13419
C	1.94671	2.29946	1.20297
C	1.25118	2.92333	2.21955
C	-0.10326	3.26708	2.07321
C	-0.79006	2.98256	0.91011
C	2.98748	0.83707	-1.32383
C	3.21320	-0.44341	-0.54827
C	2.17006	-1.33686	-0.32904
C	2.40255	-2.52448	0.34937
C	3.67442	-2.83088	0.81438
C	4.71628	-1.93988	0.60171
C	4.48325	-0.75073	-0.07476
H	-3.62664	0.54721	-2.11784
H	-2.13129	0.93965	0.32258
H	-3.81916	-1.39433	0.11664
H	-0.85344	-3.22406	-0.31831
H	-2.53912	-3.53929	-0.77403
H	-1.34175	-3.10137	-2.01840
H	-1.82828	1.80570	-3.09935

H	-2.45519	2.69852	-1.71663
H	-2.05863	-3.35021	1.53478
H	-2.35577	-2.71747	3.14647
H	-3.68549	-2.83071	1.99266
H	-0.54013	0.10063	1.43559
H	-0.51748	-0.99319	2.81339
H	-0.23690	-1.61943	1.18972
H	-2.83047	0.82087	2.39136
H	-2.87468	-0.46195	3.60232
H	-4.17387	-0.32304	2.40798
H	0.71603	0.78674	-2.92590
H	2.98606	2.02007	1.32242
H	1.75730	3.14973	3.14865
H	-0.61351	3.76096	2.88966
H	-1.83712	3.24700	0.81080
H	3.74471	1.57447	-1.04736
H	3.09896	0.64906	-2.39349
H	1.17214	-1.09753	-0.68488
H	1.58665	-3.21614	0.51889
H	3.85080	-3.75744	1.34475
H	5.70909	-2.16645	0.96824
H	5.29671	-0.05133	-0.23311

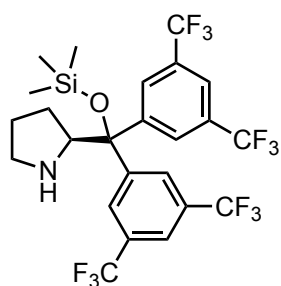


Amine 5

M06-2X/def2-TZVP Geometry

C	-1.71654	-1.57003	-0.17209
N	-0.26056	-1.62934	-0.23152
C	0.20091	-0.27669	-0.53409
N	-0.88762	0.58524	-0.05558
C	-2.05432	-0.11175	0.08027
C	-0.92765	2.01759	-0.23346
O	-3.14662	0.35520	0.30681
C	1.59669	0.01413	0.05688
C	2.52571	-1.14104	-0.33449
C	1.53885	0.15275	1.57797
C	2.17893	1.29747	-0.54607
H	-2.16583	-1.85632	-1.12734
H	-2.13023	-2.21448	0.60012
H	0.09249	-1.89226	0.68041
H	0.27634	-0.16550	-1.62716

H	-0.51895	2.29313	-1.20915
H	-1.97075	2.32484	-0.17661
H	-0.36626	2.53934	0.54255
H	2.53057	-1.28472	-1.41710
H	3.54463	-0.91447	-0.01631
H	2.22884	-2.08437	0.12197
H	2.53932	0.35175	1.96617
H	0.88670	0.97379	1.87815
H	1.17825	-0.75506	2.06601
H	1.65156	2.19184	-0.22098
H	3.22044	1.40284	-0.23742
H	2.15757	1.26211	-1.63761

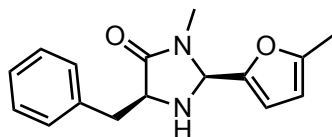


Amine 6

M06-2X/def2-TZVP Geometry

N	1.26045	2.57070	-1.90877
C	0.18987	1.59382	-1.80344
C	0.48622	0.59623	-2.93405
C	2.00832	0.64184	-3.11432
C	2.38396	2.07292	-2.71230
C	0.07265	0.98357	-0.37011
O	0.12379	2.04680	0.56176
C	-1.23006	0.21282	-0.15561
C	1.27403	0.09026	-0.09091
C	-1.43877	-0.35835	1.09923
C	-2.62142	-1.00916	1.39369
C	-3.63151	-1.11301	0.44616
C	-3.42182	-0.55538	-0.80017
C	-2.23257	0.10039	-1.10674
C	1.26097	-1.26571	-0.39788
C	2.41076	-2.02901	-0.26380
C	3.59393	-1.46529	0.18495
C	2.44992	0.65091	0.39282
Si	-0.95796	3.26688	0.93769
C	-1.61177	4.11472	-0.59141
C	-2.39389	2.62234	1.94007
C	0.07896	4.43596	1.94688

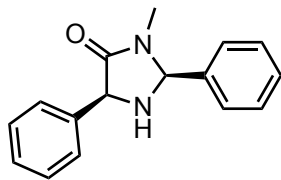
H	1.52408	2.96304	-1.01749
H	-0.76397	2.09393	-1.98405
H	-0.00750	0.94613	-3.84209
H	0.11546	-0.40812	-2.72857
H	2.49757	-0.07962	-2.46028
H	2.30316	0.40886	-4.13598
H	2.51276	2.70289	-3.59580
H	3.31961	2.09949	-2.14970
H	-0.66750	-0.27178	1.85682
C	-2.78868	-1.60458	2.76600
H	-4.55844	-1.61706	0.67876
H	-2.11333	0.51720	-2.09815
H	0.35257	-1.73971	-0.75053
C	2.34615	-3.48149	-0.64972
H	4.48884	-2.06231	0.28457
H	2.46559	1.69366	0.68109
H	-2.35744	3.50681	-1.10862
H	-2.10101	5.04673	-0.29746
H	-0.81213	4.35704	-1.29472
H	-3.07161	2.01085	1.34055
H	-2.06272	2.02742	2.79324
H	-2.96735	3.46912	2.32569
H	-0.51907	5.27618	2.30461
H	0.50348	3.92922	2.81505
H	0.90214	4.83946	1.35392
F	1.35418	-4.11462	-0.01407
F	2.11393	-3.62217	-1.96253
F	3.47881	-4.12958	-0.37496
C	3.59531	-0.12099	0.51900
C	4.84556	0.54633	1.02373
F	5.87679	-0.29630	1.09581
F	5.21153	1.55822	0.22382
F	4.66582	1.06712	2.24289
F	-2.54078	-0.70003	3.72141
F	-4.02229	-2.07088	2.96588
F	-1.93943	-2.61879	2.96453
C	-4.47800	-0.63399	-1.86884
F	-4.86599	0.58752	-2.25853
F	-4.01997	-1.25800	-2.96111
F	-5.56527	-1.28756	-1.45987



Amine 7

M06-2X/def2-TZVP Geometry

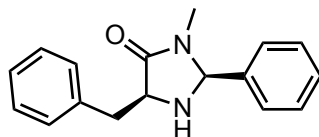
C	1.49326	-1.61482	-1.16616
N	0.23758	-1.02676	-1.62610
C	-0.82074	-1.39424	-0.68343
N	-0.11062	-1.94179	0.46731
C	1.20677	-2.12711	0.24088
O	2.01431	-2.61803	1.00245
C	-0.80107	-2.40320	1.64245
C	-1.67884	-0.23085	-0.31227
C	2.68217	-0.64840	-1.18763
C	2.41302	0.63750	-0.44892
C	2.43682	0.67700	0.94614
C	2.14984	1.85330	1.62338
C	1.83481	3.01005	0.92011
C	1.81035	2.98309	-0.46651
C	2.09757	1.80358	-1.14255
O	-3.02161	-0.38159	-0.44513
C	-3.60579	0.77247	-0.03685
C	-2.65244	1.65174	0.35636
C	-1.39200	0.99675	0.17904
C	-5.08573	0.83387	-0.10579
H	1.75495	-2.48823	-1.77244
H	0.31047	-0.01689	-1.64525
H	-1.47326	-2.17001	-1.10394
H	-0.06200	-2.83712	2.31275
H	-1.30659	-1.57252	2.13837
H	-1.54363	-3.16116	1.37953
H	3.52404	-1.17674	-0.73647
H	2.93895	-0.43205	-2.22593
H	2.68641	-0.22259	1.49656
H	2.17673	1.86844	2.70542
H	1.61489	3.92719	1.45093
H	1.57005	3.87898	-1.02435
H	2.08526	1.78976	-2.22710
H	-2.82625	2.64768	0.72736
H	-0.40720	1.38263	0.39691
H	-5.42772	1.80280	0.25167
H	-5.43483	0.69701	-1.13038
H	-5.53860	0.05524	0.50987



Amine 8

M06-2X/def2-TZVP Geometry

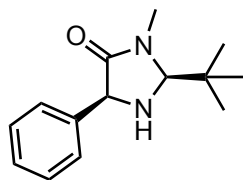
N	-0.03422	-0.07755	-1.21003
C	1.15878	0.69953	-0.88153
N	0.69389	1.69121	0.08086
C	-0.65731	1.84054	0.05430
C	-1.19531	0.76989	-0.89750
C	-2.35036	-0.03674	-0.36939
C	2.26795	-0.17091	-0.34597
C	1.57673	2.68356	0.64000
O	-1.29809	2.68195	0.64096
C	3.34023	-0.51860	-1.15555
C	4.33832	-1.35725	-0.67653
C	4.26936	-1.84711	0.61913
C	3.19989	-1.49859	1.43531
C	2.20296	-0.66463	0.95384
C	-3.16242	-0.72329	-1.26722
C	-4.19029	-1.53434	-0.81076
C	-4.41771	-1.66350	0.55281
C	-3.61425	-0.97906	1.45336
C	-2.58389	-0.16922	0.99548
H	-0.06140	-0.90166	-0.61831
H	1.51986	1.21851	-1.78040
H	-1.51116	1.29905	-1.80409
H	2.31057	2.21833	1.29933
H	2.10858	3.21740	-0.15310
H	0.96986	3.38951	1.20328
H	3.39101	-0.13359	-2.16723
H	5.16997	-1.62542	-1.31489
H	5.04840	-2.49718	0.99546
H	3.14573	-1.87556	2.44833
H	1.36926	-0.38206	1.58776
H	-2.98026	-0.62116	-2.33064
H	-4.81612	-2.06212	-1.51864
H	-5.22283	-2.29131	0.91189
H	-3.79407	-1.06833	2.51686
H	-1.97657	0.38266	1.70216



Amine 9

M06-2X/def2-TZVP Geometry

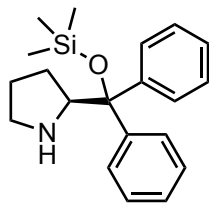
N	0.12181	-1.16743	-1.59164
C	-0.83568	-1.60703	-0.57321
N	-0.01134	-1.94156	0.58015
C	1.30723	-2.00180	0.28774
C	1.46255	-1.56127	-1.16370
C	-1.86293	-0.54266	-0.26721
C	-0.57830	-2.43473	1.80842
O	2.20162	-2.35006	1.02989
C	-3.18381	-0.70096	-0.66169
C	-4.11540	0.30006	-0.41429
C	-3.72608	1.46341	0.23215
C	-2.40415	1.62476	0.63211
C	-1.47600	0.62629	0.38489
H	0.06447	-0.15868	-1.66334
H	-1.35799	-2.51361	-0.90754
H	1.80537	-2.43580	-1.72630
H	-1.21705	-3.30114	1.61576
H	0.24273	-2.72883	2.45901
H	-1.17549	-1.66124	2.29382
H	-3.48380	-1.61064	-1.16881
H	-5.14329	0.17003	-0.72692
H	-4.45051	2.24365	0.42671
H	-2.09374	2.52991	1.13846
H	-0.44508	0.74999	0.70168
C	2.51756	-0.45768	-1.30868
H	2.66076	-0.24934	-2.37043
H	3.45203	-0.86099	-0.91529
C	1.30785	3.09164	0.80443
C	1.93121	2.05079	1.48233
C	2.34481	0.91677	0.79781
C	2.14243	0.80556	-0.57843
C	1.53027	1.86211	-1.24887
C	1.11100	2.99633	-0.56531
H	0.98649	3.97536	1.34053
H	2.09740	2.12254	2.54961
H	2.82153	0.10174	1.32932
H	1.38219	1.79720	-2.32171
H	0.63224	3.80374	-1.10421



Amine 10

M06-2X/def2-TZVP Geometry

N	0.34513	-0.57551	-1.02415
C	-0.62779	0.52064	-0.99221
C	0.07163	1.63699	-0.22113
N	1.35540	1.23213	-0.00826
C	1.65692	-0.02795	-0.69389
C	2.35530	2.19757	0.38441
O	-0.40656	2.69904	0.10276
C	2.52416	-1.02932	0.10060
C	3.97912	-0.55123	0.15994
C	2.51013	-2.36715	-0.64863
C	1.99400	-1.21217	1.52238
H	0.07637	-1.25727	-0.32465
H	-0.79587	0.90198	-2.00522
H	2.19596	0.20735	-1.62486
H	1.87005	3.17092	0.43675
H	2.78121	1.96676	1.36173
H	3.16156	2.22848	-0.35248
H	4.10564	0.33329	0.78072
H	4.60264	-1.33954	0.58523
H	4.35999	-0.32904	-0.83948
H	1.52262	-2.82668	-0.66272
H	2.82864	-2.23418	-1.68484
H	3.19965	-3.06261	-0.16735
H	0.96806	-1.58659	1.53971
H	2.61295	-1.93616	2.05526
H	2.01559	-0.27237	2.07625
C	-4.33615	-0.80068	0.71323
C	-3.27573	-0.44762	1.53815
C	-2.08570	-0.00059	0.98548
C	-1.94231	0.09753	-0.39634
C	-3.00827	-0.25429	-1.21452
C	-4.20141	-0.70218	-0.66373
H	-5.26698	-1.14542	1.14440
H	-3.38058	-0.51097	2.61346
H	-1.26513	0.29423	1.63104
H	-2.90095	-0.17657	-2.28981
H	-5.02611	-0.97154	-1.31073

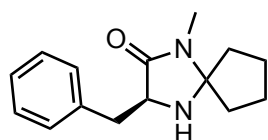


Amine 11

M06-2X/def2-TZVP Geometry

N	1.46732	-0.59226	-1.73687
C	0.09982	-0.90196	-1.34406
C	0.14452	-2.41783	-1.09667
C	1.32859	-2.92713	-1.94617
C	1.88571	-1.67072	-2.62798
C	-0.34120	-0.09362	-0.10739
O	0.50816	-0.36567	0.97544
C	-0.37383	1.41748	-0.36309
C	-1.75169	-0.55725	0.26991
C	-0.44207	2.26322	0.74355
C	-0.49705	3.63738	0.58810
C	-0.48967	4.19744	-0.68444
C	-0.44040	3.36783	-1.79177
C	-0.38834	1.98646	-1.63146
C	-2.83062	-0.25709	-0.55933
C	-4.10367	-0.71420	-0.25726
C	-4.31874	-1.47362	0.88574
C	-3.25124	-1.76694	1.71996
C	-1.97374	-1.31292	1.41399
Si	2.11920	-0.14897	1.31229
C	3.14158	-1.64933	0.86831
C	2.86567	1.40389	0.59116
C	2.11761	0.00787	3.17697
H	1.55415	0.32188	-2.16337
H	-0.61813	-0.70293	-2.15324
H	0.31858	-2.60805	-0.03812
H	-0.80191	-2.88428	-1.36389
H	2.08615	-3.37985	-1.30838
H	1.02611	-3.67356	-2.67864
H	1.45125	-1.56505	-3.63171
H	2.97165	-1.68673	-2.73139
H	-0.44826	1.82523	1.73452
H	-0.54691	4.27574	1.46096
H	-0.52851	5.27169	-0.80866
H	-0.44304	3.79062	-2.78827
H	-0.36712	1.36232	-2.51637
H	-2.67848	0.35512	-1.44071

H	-4.93121	-0.47035	-0.91107
H	-5.31298	-1.82745	1.12558
H	-3.40961	-2.35274	2.61655
H	-1.14025	-1.53913	2.06392
H	4.07795	-1.63695	1.43180
H	2.61281	-2.56945	1.12871
H	3.37620	-1.67395	-0.19495
H	2.83534	1.41373	-0.49726
H	2.36146	2.29964	0.95637
H	3.91334	1.45808	0.90011
H	1.53122	0.87168	3.49669
H	1.68537	-0.88052	3.64213
H	3.13216	0.12829	3.56272

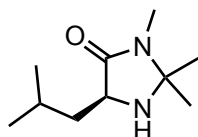


Amine 12

M06-2X/def2-TZVP Geometry

C	-0.17616	0.76410	1.42630
N	-0.75916	-0.48406	0.93568
C	-1.70490	-0.11230	-0.12036
N	-1.20940	1.17857	-0.59917
C	-0.37050	1.76361	0.28686
C	1.28496	0.64654	1.86230
O	0.11685	2.87268	0.20801
C	-1.72140	1.86741	-1.75579
C	-3.13004	-0.06138	0.44431
C	-3.54071	-1.53841	0.53255
C	-2.65192	-2.28814	-0.49781
C	-1.80855	-1.20254	-1.17985
C	2.16782	0.02917	0.80831
C	2.51299	-1.31895	0.87342
C	3.28700	-1.90668	-0.11907
C	3.72817	-1.14840	-1.19346
C	3.39355	0.19784	-1.26655
C	2.61956	0.78309	-0.27503
H	-0.75695	1.14016	2.27557
H	-0.01554	-1.02968	0.50888
H	1.62560	1.65664	2.09612
H	1.33045	0.05384	2.77705
H	-1.29609	2.86944	-1.75412
H	-1.43328	1.35838	-2.67704
H	-2.81045	1.94243	-1.72026

H	-3.15777	0.45508	1.40382
H	-3.77450	0.48107	-0.25124
H	-3.35029	-1.91965	1.53387
H	-4.60208	-1.67180	0.32867
H	-2.00409	-2.99786	0.01526
H	-3.24037	-2.85204	-1.21976
H	-2.33779	-0.79754	-2.04536
H	-0.82735	-1.54255	-1.51651
H	2.17402	-1.91274	1.71540
H	3.54876	-2.95471	-0.04882
H	4.33490	-1.60143	-1.96671
H	3.74123	0.79716	-2.09832
H	2.35773	1.83296	-0.33296

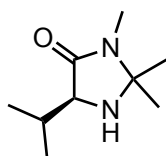


Amine 13

M06-2X/def2-TZVP Geometry

N	-0.15384	-1.01162	-0.17529
C	-1.61171	-0.88339	-0.09239
N	-1.82717	0.57203	-0.12332
C	-0.70893	1.25924	0.22553
C	0.40571	0.22721	0.37362
C	-2.27976	-1.56641	-1.27210
C	-2.10402	-1.46922	1.22914
C	-3.12508	1.19126	-0.20035
O	-0.61664	2.45505	0.39718
C	1.69133	0.66497	-0.30206
C	2.82066	-0.36590	-0.24508
C	3.12868	-0.79359	1.18624
C	4.06570	0.19958	-0.92129
H	0.10387	-1.06177	-1.15729
H	0.58102	0.10576	1.44824
H	-1.99350	-1.07987	-2.20618
H	-1.97367	-2.61233	-1.30442
H	-3.36572	-1.53225	-1.18023
H	-1.56927	-1.01700	2.06504
H	-3.17200	-1.29165	1.36307
H	-1.92397	-2.54349	1.24255
H	-2.98108	2.26505	-0.09391
H	-3.60115	0.98677	-1.16079
H	-3.78247	0.84223	0.60015
H	1.47163	0.91033	-1.34756

H	2.01313	1.59678	0.17174
H	2.50259	-1.25549	-0.79905
H	3.35310	0.07842	1.80702
H	2.29050	-1.32851	1.63413
H	3.99638	-1.45450	1.21203
H	4.43144	1.07203	-0.37380
H	4.86831	-0.53876	-0.94970
H	3.85561	0.51242	-1.94569

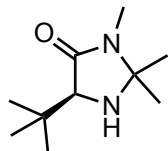


Amine 14

M06-2X/def2-TZVP Geometry

N	0.12181	-1.16743	-1.59164
C	-0.83568	-1.60703	-0.57321
N	-0.01134	-1.94156	0.58015
C	1.30723	-2.00180	0.28774
C	1.46255	-1.56127	-1.16370
C	-1.86293	-0.54266	-0.26721
C	-0.57830	-2.43473	1.80842
O	2.20162	-2.35006	1.02989
C	-3.18381	-0.70096	-0.66169
C	-4.11540	0.30006	-0.41429
C	-3.72608	1.46341	0.23215
C	-2.40415	1.62476	0.63211
C	-1.47600	0.62629	0.38489
H	0.06447	-0.15868	-1.66334
H	-1.35799	-2.51361	-0.90754
H	1.80537	-2.43580	-1.72630
H	-1.21705	-3.30114	1.61576
H	0.24273	-2.72883	2.45901
H	-1.17549	-1.66124	2.29382
H	-3.48380	-1.61064	-1.16881
H	-5.14329	0.17003	-0.72692
H	-4.45051	2.24365	0.42671
H	-2.09374	2.52991	1.13846
H	-0.44508	0.74999	0.70168
C	2.51756	-0.45768	-1.30868
H	2.66076	-0.24934	-2.37043
H	3.45203	-0.86099	-0.91529
C	1.30785	3.09164	0.80443
C	1.93121	2.05079	1.48233

C	2.34481	0.91677	0.79781
C	2.14243	0.80556	-0.57843
C	1.53027	1.86211	-1.24887
C	1.11100	2.99633	-0.56531
H	0.98649	3.97536	1.34053
H	2.09740	2.12254	2.54961
H	2.82153	0.10174	1.32932
H	1.38219	1.79720	-2.32171
H	0.63224	3.80374	-1.10421

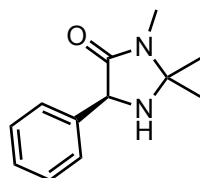


Amine 15

M06-2X/def2-TZVP Geometry

N	0.23030	-1.21380	-0.11003
C	1.60913	-0.71656	-0.05279
N	1.38785	0.71636	0.07998
C	0.13629	1.10746	-0.26362
C	-0.65837	-0.15482	-0.58387
C	2.32024	-1.28383	1.16778
C	2.39314	-1.02605	-1.33173
C	2.43723	1.65092	0.39513
O	-0.25743	2.25325	-0.31324
C	-2.05631	-0.20952	0.06806
C	-2.97845	0.80248	-0.61289
C	-1.95231	0.09130	1.56234
C	-2.61995	-1.61721	-0.13386
H	0.16979	-2.05063	-0.67444
H	-0.79579	-0.17230	-1.67626
H	1.78059	-0.99840	2.07018
H	2.33626	-2.37219	1.10206
H	3.35125	-0.93103	1.23016
H	1.86278	-0.63593	-2.20185
H	3.38970	-0.58316	-1.30386
H	2.51293	-2.10530	-1.44402
H	2.01383	2.65054	0.32415
H	2.81464	1.49150	1.40663
H	3.26788	1.56482	-0.30933
H	-3.07973	0.57962	-1.67832
H	-3.97343	0.75260	-0.16553
H	-2.59533	1.81603	-0.50918
H	-1.23875	-0.58349	2.03866

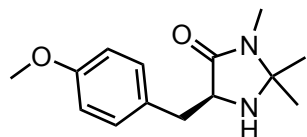
H	-1.63235	1.12115	1.73034
H	-2.92449	-0.04326	2.04046
H	-2.01948	-2.36067	0.39229
H	-3.63951	-1.67030	0.25249
H	-2.65223	-1.87850	-1.19568



Amine 16

M06-2X/def2-TZVP Geometry

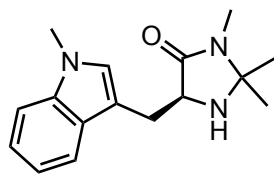
N	0.88018	-0.94313	-1.11585
C	1.85181	-0.81546	-0.02170
N	1.90751	0.63275	0.21078
C	0.85041	1.29051	-0.32402
C	0.03424	0.25122	-1.10373
C	1.34850	-1.53902	1.22556
C	3.20390	-1.35872	-0.45223
C	2.82375	1.26266	1.12717
O	0.60374	2.47122	-0.21015
H	1.38473	-0.98085	-1.99226
H	-0.09980	0.62940	-2.11909
H	0.36873	-1.15876	1.51428
H	1.26090	-2.60526	1.01724
H	2.03909	-1.40362	2.05937
H	3.91852	-1.32590	0.37030
H	3.09312	-2.39822	-0.76276
H	3.60207	-0.77573	-1.28458
H	3.85593	1.13671	0.79627
H	2.58261	2.32364	1.15194
H	2.72208	0.85317	2.13496
C	-3.89686	-0.33578	0.56698
C	-3.42394	0.94568	0.31552
C	-2.15551	1.13321	-0.21272
C	-1.34239	0.03606	-0.49173
C	-1.82091	-1.24501	-0.24430
C	-3.09221	-1.42928	0.28442
H	-4.88730	-0.47985	0.97899
H	-4.04547	1.80509	0.53205
H	-1.78231	2.13182	-0.40006
H	-1.18772	-2.09288	-0.46889
H	-3.45365	-2.43215	0.47353



Amine 17

M06-2X/def2-TZVP Geometry

N	-1.73994	-0.65534	-1.19456
C	-2.39211	0.61673	-0.86866
N	-2.18216	0.74918	0.58258
C	-1.84634	-0.42447	1.16371
C	-1.68870	-1.44245	0.03656
C	-1.73499	1.75897	-1.62368
C	-3.88358	0.53193	-1.18256
C	-2.53442	1.92102	1.34159
O	-1.70993	-0.63711	2.35165
H	-0.78544	-0.45134	-1.47519
H	-2.55171	-2.11461	0.09243
H	-1.78166	1.55726	-2.69421
H	-2.24724	2.70254	-1.43294
H	-0.68979	1.85715	-1.32330
H	-4.02298	0.41541	-2.25666
H	-4.32387	-0.33028	-0.68036
H	-4.40826	1.43153	-0.85729
H	-1.91489	2.77283	1.05603
H	-3.58509	2.18565	1.20019
H	-2.36659	1.69229	2.39251
C	-0.41774	-2.28114	0.18779
H	-0.43737	-3.08051	-0.55475
H	-0.45982	-2.74081	1.17663
C	3.14698	0.10173	-0.27815
C	2.46697	0.09212	0.93557
C	1.32752	-0.69168	1.08137
C	0.84604	-1.47416	0.03817
C	1.54642	-1.45322	-1.16960
C	2.67945	-0.67863	-1.33367
O	4.26680	0.82844	-0.52371
H	2.81255	0.68093	1.77284
H	0.80096	-0.69263	2.02858
H	1.19745	-2.06252	-1.99649
H	3.22543	-0.66626	-2.26762
C	4.77843	1.61816	0.52506
H	5.05581	1.00293	1.38530
H	4.05440	2.37398	0.84178
H	5.66435	2.10949	0.13192

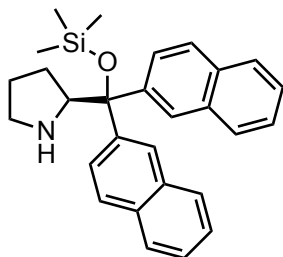


Amine 18

M06-2X/def2-TZVP Geometry

N	-1.60842	-1.63530	-0.20551
C	-2.11651	-0.57452	-1.09020
N	-2.23601	0.58855	-0.20538
C	-2.05897	0.29133	1.09696
C	-1.65896	-1.17293	1.17864
C	-2.58165	1.90918	-0.66330
C	-1.13216	-0.30051	-2.21897
C	-3.48793	-0.96301	-1.63701
O	-2.17798	1.04860	2.04064
C	-0.33035	-1.33651	1.94471
C	0.87489	-0.96478	1.13927
C	1.76623	-1.85155	0.60384
N	2.70948	-1.20329	-0.15602
C	2.43470	0.13876	-0.12630
C	1.29116	0.33601	0.68078
C	3.10333	1.19075	-0.75324
C	2.60513	2.46237	-0.55791
C	1.47750	2.68509	0.25000
C	0.82033	1.64287	0.87241
C	3.81984	-1.80613	-0.84932
H	-0.64153	-1.81745	-0.44833
H	-2.43916	-1.69058	1.74487
H	-2.70615	2.53742	0.21690
H	-1.78663	2.32316	-1.28752
H	-3.51474	1.90033	-1.23008
H	-0.18628	0.06568	-1.81204
H	-0.95451	-1.22280	-2.77453
H	-1.52807	0.43943	-2.91557
H	-4.16163	-1.19118	-0.81068
H	-3.92155	-0.16309	-2.23962
H	-3.38970	-1.85265	-2.25855
H	-0.41149	-0.72636	2.84729
H	-0.23442	-2.37698	2.26021
H	1.80434	-2.92525	0.71296
H	3.97828	1.01753	-1.36691
H	3.09600	3.30428	-1.02852
H	1.12392	3.69781	0.39344
H	-0.03874	1.83255	1.50379

H	3.77210	-1.58804	-1.91784
H	3.77956	-2.88408	-0.71080
H	4.76946	-1.43672	-0.45738

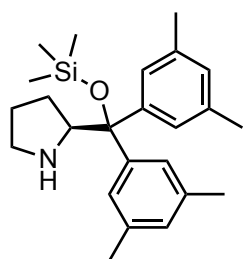


Amine 19

M06-2X/def2-TZVP Geometry

C	0.88593	3.06561	2.71160
N	1.12003	2.16842	1.58391
C	0.01290	1.22198	1.58516
C	-1.20140	2.10971	1.90186
C	-0.62099	3.33852	2.63391
C	-0.11318	0.48292	0.23821
C	1.08842	-0.41202	-0.07616
C	-1.35987	-0.40184	0.30052
O	-0.28766	1.40600	-0.80248
Si	0.62220	2.61892	-1.48090
C	0.21495	4.28798	-0.74583
C	2.46526	2.31558	-1.47440
C	0.03100	2.61094	-3.25633
C	-1.38760	-1.50200	1.19608
C	-2.49694	-2.28721	1.30732
C	-3.64967	-2.03113	0.52427
C	-3.62337	-0.94177	-0.38079
C	-2.45732	-0.14035	-0.46951
C	-4.81598	-2.82769	0.61127
C	-5.90718	-2.55330	-0.16445
C	-5.88274	-1.46732	-1.06687
C	-4.76863	-0.68276	-1.17193
C	2.03524	-0.78182	0.83732
C	3.11523	-1.63297	0.48324
C	3.20499	-2.11769	-0.84368
C	2.19935	-1.74194	-1.77082
C	1.17786	-0.92190	-1.39926
C	4.10703	-2.01054	1.41889
C	5.13899	-2.82849	1.05101
C	5.22871	-3.30973	-0.27259
C	4.28293	-2.96212	-1.19670

H	1.13248	2.59145	3.67180
H	1.48954	3.96946	2.61743
H	2.02425	1.71549	1.62536
H	0.11427	0.46977	2.38123
H	-1.68495	2.40665	0.97184
H	-1.93518	1.56850	2.49645
H	-1.05110	3.47731	3.62427
H	-0.81168	4.24508	2.06154
H	0.50383	5.08094	-1.44008
H	-0.85961	4.37919	-0.56953
H	0.73451	4.44619	0.19838
H	2.94211	3.10219	-2.06599
H	2.72062	1.35665	-1.92807
H	2.88825	2.34728	-0.47175
H	-1.04845	2.76766	-3.30822
H	0.51278	3.40085	-3.83636
H	0.25439	1.65637	-3.73725
H	-0.50668	-1.73050	1.78418
H	-2.50677	-3.12692	1.99214
H	-2.43913	0.69281	-1.15992
H	-4.82795	-3.66033	1.30471
H	-6.79518	-3.16760	-0.09097
H	-6.75266	-1.25974	-1.67645
H	-4.74473	0.15109	-1.86339
H	1.98492	-0.44275	1.86606
H	2.25562	-2.12316	-2.78366
H	0.41080	-0.64059	-2.11048
H	4.03505	-1.63979	2.43476
H	5.89235	-3.11103	1.77482
H	6.05004	-3.95668	-0.55183
H	4.34507	-3.32956	-2.21411



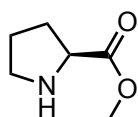
Amine 20

M06-2X/def2-TZVP Geometry

C	-1.30987	-2.28518	2.96364
N	-1.38671	-1.33148	1.86105
C	-0.01415	-0.93537	1.57602

C	0.75771	-2.26021	1.67688
C	-0.10504	-3.15797	2.58952
C	0.11432	-0.25795	0.19720
C	-0.67025	1.05550	0.10094
C	1.59830	0.03907	-0.04016
O	-0.31929	-1.13598	-0.80829
Si	-1.75385	-1.85720	-1.22307
C	-3.27604	-0.82517	-0.89303
C	-1.57683	-2.06581	-3.07488
C	-1.92882	-3.56126	-0.47426
C	2.32016	-0.65833	-0.99255
C	3.68348	-0.41658	-1.17744
C	4.30750	0.53432	-0.38685
C	3.60021	1.25465	0.57739
C	2.24786	0.99951	0.73714
C	-1.12089	1.76545	1.20246
C	-1.81460	2.97034	1.05379
C	-2.04152	3.45411	-0.22305
C	-1.58309	2.76948	-1.35092
C	-0.89776	1.58047	-1.17218
C	-2.29815	3.71331	2.26935
C	-1.85203	3.31234	-2.72734
C	4.44519	-1.18365	-2.22372
C	4.30245	2.29038	1.41233
H	-1.12692	-1.78655	3.92577
H	-2.23786	-2.85247	3.04964
H	-1.98364	-0.54063	2.06919
H	0.38115	-0.24337	2.33361
H	0.85645	-2.69847	0.68441
H	1.76090	-2.09714	2.06651
H	0.43209	-3.49286	3.47531
H	-0.43372	-4.04417	2.04880
H	-3.26482	0.09932	-1.47230
H	-4.15626	-1.40091	-1.19255
H	-3.38391	-0.56702	0.15937
H	-1.46884	-1.09742	-3.56792
H	-0.69644	-2.66475	-3.31711
H	-2.44976	-2.56513	-3.50079
H	-2.26859	-3.51165	0.55943
H	-2.65028	-4.14584	-1.05070
H	-0.97567	-4.09495	-0.50096
H	1.81467	-1.39733	-1.60061
H	5.36642	0.73002	-0.52266
H	1.68452	1.57208	1.46614
H	-0.93468	1.40431	2.20813
H	-2.58036	4.38727	-0.35131

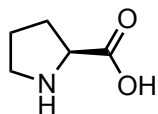
H	-0.52916	1.03484	-2.03367
H	-2.79912	4.63949	1.99184
H	-3.00158	3.10767	2.84376
H	-1.46653	3.96232	2.93093
H	-1.59514	4.37064	-2.78893
H	-1.27800	2.77560	-3.48122
H	-2.91068	3.21808	-2.97905
H	5.49752	-0.90281	-2.23290
H	4.38064	-2.25792	-2.04283
H	4.03447	-0.99663	-3.21751
H	5.11093	1.84122	1.99204
H	4.74458	3.06414	0.78230
H	3.61405	2.77117	2.10599



Amine 21

M06-2X/def2-TZVP Geometry

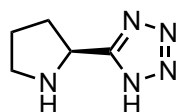
N	1.38127	-0.94454	0.69704
C	0.37800	0.10873	0.74310
C	0.98671	1.29880	-0.04828
C	2.40860	0.83254	-0.37842
C	2.24529	-0.67842	-0.45329
C	-0.94168	-0.31983	0.13001
O	-1.87408	0.63009	0.26682
O	-1.14355	-1.37231	-0.41287
C	-3.15104	0.32164	-0.28926
H	0.93787	-1.85314	0.63247
H	0.16415	0.39766	1.77532
H	0.42208	1.46541	-0.96687
H	0.95547	2.22275	0.52417
H	2.78953	1.26968	-1.29997
H	3.09064	1.08271	0.43480
H	3.18669	-1.21878	-0.35652
H	1.77753	-0.95935	-1.40718
H	-3.56331	-0.56909	0.18245
H	-3.06476	0.14588	-1.36060
H	-3.77896	1.18505	-0.09210



Proline

M06-2X/def2-TZVP Geometry

N	0.82438	-0.94722	0.76825
C	-0.08539	0.18427	0.69389
C	0.68199	1.28455	-0.09162
C	2.06729	0.67132	-0.32728
C	1.76794	-0.82055	-0.34263
C	-1.38377	-0.15927	-0.00690
O	-2.24351	0.87465	0.00258
O	-1.64461	-1.21445	-0.51463
H	0.31177	-1.82029	0.73169
H	-0.35597	0.53556	1.69306
H	0.18677	1.48127	-1.04327
H	0.71356	2.22249	0.45739
H	2.53013	1.02557	-1.24683
H	2.73121	0.89786	0.50734
H	2.64818	-1.43844	-0.16752
H	1.32575	-1.10671	-1.30700
H	-3.04540	0.58974	-0.45896

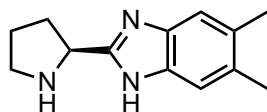


Tetrazole-derived amine

M06-2X/def2-TZVP Geometry

N	-1.24543	-1.04699	-0.51683
C	-0.58251	0.26609	-0.63302
C	-1.35269	1.20515	0.31447
C	-2.75778	0.61117	0.30354
C	-2.45453	-0.88533	0.31366
C	0.86213	0.15555	-0.27457
N	1.43310	-0.96620	0.17253
N	2.72070	-0.72411	0.43007
N	2.91443	0.50652	0.14612
N	1.77893	1.09017	-0.29739
H	-1.48932	-1.39678	-1.43222
H	-0.64413	0.65123	-1.65393
H	-0.92520	1.14263	1.31730
H	-1.29326	2.24127	-0.01037

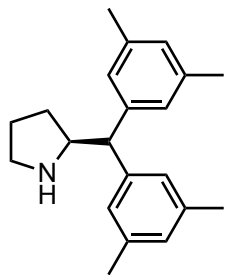
H	-3.36402	0.93220	1.14927
H	-3.27861	0.88442	-0.61726
H	-3.26539	-1.50151	-0.07197
H	-2.24189	-1.21654	1.33324
H	1.00199	-1.86842	0.29995



Benzimidazole-derived amine

M06-2X/def2-TZVP Geometry

N	3.33920	0.98125	-0.62569
C	2.74917	-0.35979	-0.79242
C	3.43962	-1.24915	0.24803
C	3.71725	-0.24982	1.36832
C	4.16763	0.98932	0.59754
C	1.26398	-0.30533	-0.55249
N	0.61679	0.88900	-0.44322
C	-0.71640	0.60914	-0.24605
C	-0.78772	-0.79132	-0.25097
N	0.47162	-1.33396	-0.44253
C	-1.84192	1.40489	-0.06467
C	-3.06289	0.77658	0.11215
C	-3.15293	-0.63894	0.10829
C	-2.02179	-1.41444	-0.07155
C	-4.49294	-1.29604	0.30155
C	-4.30608	1.60028	0.30948
H	3.87702	1.24595	-1.43715
H	2.90748	-0.73095	-1.80676
H	2.81295	-2.08862	0.54014
H	4.37921	-1.62858	-0.15913
H	2.79377	-0.03974	1.91282
H	4.46413	-0.59070	2.08298
H	5.23241	0.91135	0.35590
H	4.01722	1.91099	1.16040
H	1.09899	1.77229	-0.47804
H	-1.77625	2.48616	-0.06182
H	-2.08594	-2.49559	-0.07479
H	-4.39834	-2.38038	0.27663
H	-4.94081	-1.01770	1.25841
H	-5.19950	-1.00049	-0.47764
H	-5.04615	1.39691	-0.46794
H	-4.78321	1.37840	1.26686
H	-4.07608	2.66445	0.28599

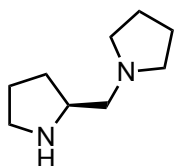


Amine 24

M06-2X/def2-TZVP Geometry

N	1.51164	2.59190	-0.16026
C	0.23673	1.96747	0.18448
C	-0.78763	3.05431	-0.19336
C	0.01883	4.37247	-0.21683
C	1.40014	3.96814	0.30357
C	0.06240	0.64133	-0.56158
C	-1.29844	-0.00068	-0.37510
C	1.18730	-0.31320	-0.19997
C	1.16047	-1.03159	0.99579
C	2.21323	-1.85745	1.36058
C	3.31012	-1.96247	0.50442
C	3.36323	-1.26408	-0.69237
C	2.29077	-0.43795	-1.03126
C	-1.76621	-0.86152	-1.36984
C	-2.98401	-1.51138	-1.25463
C	-3.75092	-1.29166	-0.10923
C	-3.31629	-0.44461	0.89695
C	-2.08367	0.19594	0.75127
C	4.53944	-1.39466	-1.62111
C	2.17815	-2.64338	2.64289
C	-3.48482	-2.43050	-2.33468
C	-4.14717	-0.20368	2.12790
H	2.29706	2.09549	0.24387
H	0.18074	1.77700	1.26841
H	-1.21660	2.83721	-1.17257
H	-1.61198	3.08489	0.51703
H	0.10590	4.74394	-1.23700
H	-0.43486	5.15668	0.38715
H	1.42247	4.04186	1.40142
H	2.20661	4.58267	-0.09605
H	0.17061	0.88507	-1.62251
H	0.29485	-0.95280	1.64491
H	4.13764	-2.60805	0.78110
H	2.32417	0.12998	-1.95522
H	-1.15355	-1.02686	-2.25034

H	-4.70740	-1.79426	-0.00703
H	-1.74754	0.85668	1.54239
H	4.91548	-0.41419	-1.91657
H	5.35328	-1.94684	-1.15304
H	4.25501	-1.92246	-2.53361
H	2.12250	-3.71459	2.43955
H	3.07940	-2.47020	3.23308
H	1.31524	-2.37076	3.24875
H	-3.71210	-3.41842	-1.93086
H	-4.40202	-2.04194	-2.78132
H	-2.74637	-2.54829	-3.12632
H	-3.58780	-0.45159	3.03162
H	-4.43701	0.84617	2.20218
H	-5.05521	-0.80480	2.11548

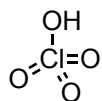


Amine 25

M06-2X/def2-TZVP Geometry

N	1.53463	1.06523	-0.34587
C	1.22098	-0.35655	-0.53443
C	2.54032	-1.09908	-0.22738
C	3.56307	0.01527	0.03193
C	2.68621	1.14837	0.54741
C	0.08992	-0.82953	0.37531
N	-1.11546	-0.04312	0.21483
C	-2.16612	-0.40024	1.15705
C	-3.39024	0.34960	0.63366
C	-3.14169	0.44933	-0.89004
C	-1.74957	-0.16276	-1.09322
H	0.72055	1.55789	0.00389
H	0.92386	-0.52123	-1.57361
H	2.41873	-1.71284	0.66873
H	2.83950	-1.76299	-1.03650
H	4.34320	-0.27841	0.73288
H	4.03428	0.32362	-0.90205
H	3.16152	2.12704	0.47451
H	2.43314	0.97086	1.60374
H	-0.10521	-1.90189	0.18582
H	0.41488	-0.73697	1.41711
H	-2.34810	-1.48934	1.13926

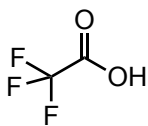
H	-1.88358	-0.12353	2.17357
H	-4.31745	-0.16656	0.87687
H	-3.43678	1.34346	1.07649
H	-3.89448	-0.08289	-1.46926
H	-3.15404	1.48874	-1.21368
H	-1.83384	-1.22499	-1.38254
H	-1.16773	0.34873	-1.85961



Perchloric acid (HClO₄)

M06-2X/def2-TZVP Geometry

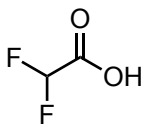
O	-0.70524	1.26429	0.00000
Cl	-0.13385	-0.01284	0.00000
O	-0.34439	-0.75644	1.17712
O	-0.34442	-0.75645	-1.17710
O	1.43939	0.33965	-0.00002
H	1.91287	-0.51007	-0.00003



TFA

M06-2X/def2-TZVP Geometry

O	-1.41415	-1.29587	0.00000
C	-0.29259	-0.90409	0.00000
C	0.08632	0.59288	0.00000
O	0.80808	-1.64844	0.00000
F	0.80808	0.88535	1.07872
F	0.80808	0.88535	-1.07872
F	-1.00056	1.34074	0.00000
H	0.54588	-2.58126	0.00000

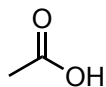


DFA

M06-2X/def2-TZVP Geometry

C	0.70274	-0.15121	0.35616
C	-0.75686	0.18186	0.02638
O	-1.52125	-0.89312	0.23478
O	-1.14301	1.24561	-0.34032

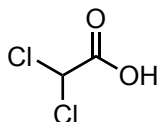
F	1.12175	-1.13613	-0.46799
F	1.46264	0.92997	0.15097
H	0.81440	-0.48745	1.38953
H	-2.43513	-0.66093	0.01274



AcOH

M06-2X/def2-TZVP Geometry

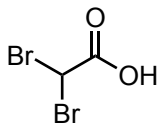
O	-0.62367	1.19822	0.00001
C	-0.08987	0.12601	-0.00001
C	1.38834	-0.12349	-0.00001
O	-0.78808	-1.02736	0.00002
H	1.65728	-0.70731	0.87972
H	1.65739	-0.70883	-0.87874
H	1.91523	0.82481	-0.00084
H	-1.72669	-0.79065	-0.00019



DCA

M06-2X/def2-TZVP Geometry

C	-0.24823	0.00000	-0.53163
C	1.21393	0.00003	-0.11002
O	1.36850	0.00001	1.21106
O	2.10444	0.00003	-0.90611
Cl	-1.04730	-1.46503	0.04779
Cl	-1.04735	1.46500	0.04779
H	-0.28678	0.00000	-1.61423
H	2.31821	0.00002	1.39958

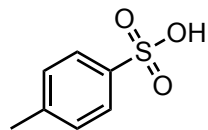


DBA

M06-2X/def2-TZVP Geometry

C	0.00000	0.19660	-0.56864
C	-0.00008	1.64054	-0.10717
O	-0.00014	1.76607	1.21822
O	-0.00019	2.55231	-0.87985
Br	1.60944	-0.69226	0.02245
Br	-1.60935	-0.69242	0.02244

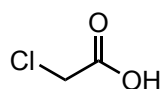
H	0.00000	0.18263	-1.65022
H	-0.00024	2.71134	1.42677



p-TSA

M06-2X/def2-TZVP Geometry

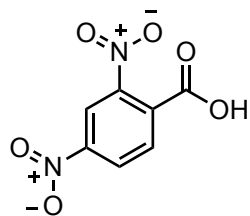
C	-0.13049	0.00685	-0.07479
C	0.54894	1.21357	-0.07805
C	1.93568	1.20431	-0.02925
C	2.64326	0.00777	0.02156
C	1.93110	-1.19320	0.01845
C	0.54988	-1.20396	-0.03298
C	4.14505	-0.00579	0.05633
S	-1.88851	-0.00094	-0.12495
O	-2.34564	1.30393	-0.48373
O	-2.32505	-1.16771	-0.80672
O	-2.28600	-0.23150	1.39991
H	-0.00395	2.14172	-0.13491
H	2.47527	2.14323	-0.03680
H	2.47171	-2.13157	0.05088
H	-0.00412	-2.13315	-0.05193
H	4.54566	-0.39156	-0.88301
H	4.54718	0.99406	0.20988
H	4.50961	-0.65102	0.85630
H	-2.41223	0.62822	1.82550



MCA

M06-2X/def2-TZVP Geometry

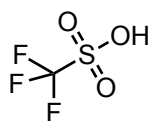
O	0.92500	1.31793	-0.00002
C	0.93720	0.12713	-0.00001
C	-0.25912	-0.79916	0.00004
O	2.06258	-0.61133	0.00002
Cl	-1.78605	0.07336	-0.00002
H	-0.20927	-1.43459	0.88198
H	-0.20926	-1.43470	-0.88183
H	2.81213	0.00153	0.00003



DNBA

M06-2X/def2-TZVP Geometry

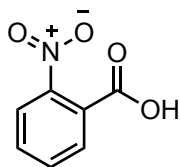
C	0.93127	-0.74727	0.00790
C	0.43050	0.54800	0.03175
C	-0.92112	0.81911	0.01397
C	-1.77968	-0.26247	-0.00555
C	-1.33465	-1.57027	-0.00435
C	0.03140	-1.80473	0.00112
C	2.39270	-1.08565	-0.06046
O	3.00265	-0.44156	-1.05870
O	2.90989	-1.90080	0.64204
H	-1.29052	1.83397	0.02840
H	-2.05059	-2.37898	-0.01101
H	0.41675	-2.81523	-0.00437
H	3.94258	-0.67641	-1.03792
N	1.34630	1.69830	0.16423
O	2.36046	1.51358	0.79321
O	0.99693	2.73996	-0.33326
N	-3.23622	-0.00244	-0.01386
O	-3.59040	1.15090	0.00823
O	-3.96592	-0.96393	-0.04325



Triflic acid

M06-2X/def2-TZVP Geometry

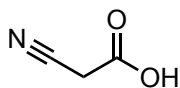
C	-0.98337	0.00290	-0.00187
S	0.84979	-0.13632	0.07305
O	1.23316	1.05116	-0.88374
F	-1.51353	-0.89970	0.80024
F	-1.34569	1.21499	0.39678
F	-1.40710	-0.19356	-1.23494
O	1.23124	0.19018	1.40038
O	1.20289	-1.34081	-0.57241
H	1.36204	1.86379	-0.37015



2-NO₂-benzoic acid

M06-2X/def2-TZVP Geometry

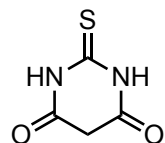
C	1.07960	-1.68228	0.00778
C	0.07182	-0.72820	-0.00573
C	0.44007	0.61029	-0.02139
C	1.76013	1.01337	0.00985
C	2.75355	0.04583	0.03616
C	2.41309	-1.29869	0.02715
N	-0.58394	1.66078	-0.16993
O	-1.55437	1.38944	-0.83678
O	-0.36246	2.72808	0.35125
C	-1.34203	-1.21716	0.06038
O	-2.04268	-0.59855	1.01796
O	-1.76424	-2.11661	-0.60479
H	0.80019	-2.72744	0.01096
H	1.98977	2.06921	-0.00374
H	3.79239	0.34598	0.05135
H	3.18743	-2.05385	0.03888
H	-2.94952	-0.93716	0.98571



CNAcOH

M06-2X/def2-TZVP Geometry

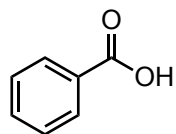
O	0.75659	1.33040	-0.00002
C	0.85689	0.14385	0.00000
C	-0.28747	-0.85173	0.00001
O	2.02515	-0.51647	-0.00004
C	-1.59504	-0.20986	0.00003
N	-2.63682	0.26310	0.00004
H	-0.18870	-1.49466	-0.87626
H	-0.18868	-1.49466	0.87628
H	2.73488	0.14259	-0.00007



TBA

M06-2X/def2-TZVP Geometry

C	-1.03513	0.00000	-0.00017
N	-0.29922	1.15658	-0.00015
C	1.08071	1.28578	-0.00005
C	1.86565	-0.00000	0.00042
C	1.08071	-1.28578	0.00001
N	-0.29922	-1.15658	-0.00015
O	1.59890	-2.36829	-0.00014
O	1.59890	2.36828	-0.00008
S	-2.67052	0.00000	0.00007
H	-0.83052	2.01761	-0.00016
H	2.52271	-0.00002	-0.87077
H	2.52153	0.00001	0.87253
H	-0.83053	-2.01761	-0.00018



Benzoic acid

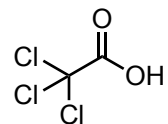
M06-2X/def2-TZVP Geometry

C	2.55389	-0.04503	0.00001
C	1.82975	-1.22978	0.00007
C	0.44369	-1.19577	0.00006
C	-0.21408	0.03000	0.00002
C	0.51127	1.21728	-0.00009
C	1.89544	1.17851	-0.00007
C	-1.69747	0.12282	0.00001
O	-2.30162	-1.08048	-0.00021
O	-2.31916	1.15004	0.00017
H	2.34614	-2.18063	0.00013
H	-0.13091	-2.11154	0.00014
H	-0.02816	2.15528	-0.00011
H	2.46261	2.09994	-0.00014
H	-3.25439	-0.91286	0.00023
H	3.63602	-0.07498	0.00005

H-Cl
HCl

M06-2X/def2-TZVP Geometry

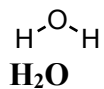
H	0.00000	0.00000	-1.20633
Cl	0.00000	0.00000	0.07096



TCA

M06-2X/def2-TZVP Geometry

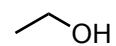
O	-2.01428	1.00308	0.00000
C	-1.33409	0.02846	0.00000
C	0.21326	0.05480	0.00000
O	-1.78005	-1.22523	0.00000
Cl	0.78093	-0.78304	1.45229
Cl	0.78093	-0.78304	-1.45229
Cl	0.78093	1.71148	0.00000
H	-2.74775	-1.19420	0.00000



H₂O

M06-2X/def2-TZVP Geometry

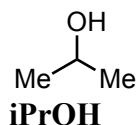
O	0.00000	0.00000	0.11617
H	-0.00000	0.76445	-0.46468
H	-0.00000	-0.76445	-0.46468



EtOH

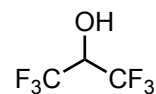
M06-2X/def2-TZVP Geometry

O	-1.14330	-0.39501	0.00000
H	-1.98167	0.07320	-0.00000
C	-0.08438	0.54799	0.00000
C	1.21630	-0.22171	-0.00000
H	-0.14157	1.19092	0.88547
H	-0.14157	1.19092	-0.88547
H	2.06641	0.46088	0.00000
H	1.27662	-0.85677	0.88366
H	1.27662	-0.85677	-0.88367



M06-2X/def2-TZVP Geometry

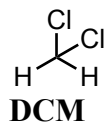
O	0.06692	1.36071	-0.16145
H	0.91547	1.74544	0.07572
C	-0.00220	0.04238	0.36728
C	-1.32693	-0.53172	-0.09023
C	1.17698	-0.79347	-0.10239
H	0.00584	0.09015	1.46386
H	-1.34945	-0.58129	-1.18012
H	-1.47067	-1.53539	0.31058
H	-2.14841	0.10164	0.24256
H	1.18096	-0.84766	-1.19239
H	1.12098	-1.80635	0.29901
H	2.12276	-0.35537	0.22445



HFIP

M06-2X/def2-TZVP Geometry

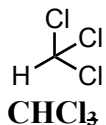
O	0.00003	1.86948	-0.18643
H	0.00013	1.94691	0.77640
C	-0.00001	0.52632	-0.54117
C	1.27978	-0.15170	-0.04328
C	-1.27979	-0.15168	-0.04327
H	-0.00002	0.46235	-1.63035
F	1.39030	-0.04147	1.28475
F	1.32777	-1.44163	-0.35868
F	2.33750	0.44405	-0.58652
F	-1.39010	-0.04184	1.28480
F	-1.32797	-1.44152	-0.35906
F	-2.33752	0.44434	-0.58620



M06-2X/def2-TZVP Geometry

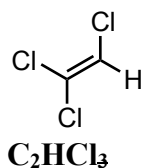
C	-0.00000	0.00000	0.76575
H	0.89613	-0.00000	1.37429

H	-0.89613	0.00000	1.37429
Cl	0.00000	1.46772	-0.21597
Cl	-0.00000	-1.46772	-0.21597



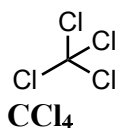
M06-2X/def2-TZVP Geometry

C	-0.00009	0.00015	0.45722
H	0.00006	0.00009	1.53940
Cl	-1.12375	1.24399	-0.08399
Cl	1.63930	0.35112	-0.08397
Cl	-0.51552	-1.59517	-0.08396



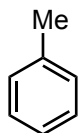
M06-2X/def2-TZVP Geometry

C	-0.42519	-0.11077	0.00000
Cl	-0.33570	1.59396	-0.00000
Cl	-2.01159	-0.77273	0.00000
C	0.63235	-0.90953	-0.00000
H	0.51349	-1.98212	0.00000
Cl	2.24397	-0.34452	0.00000



M06-2X/def2-TZVP Geometry

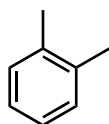
C	0.00000	0.00000	0.00000
Cl	1.01872	1.01872	1.01872
Cl	-1.01872	-1.01872	1.01872
Cl	-1.01872	1.01872	-1.01872
Cl	1.01872	-1.01872	-1.01872



toluene

M06-2X/def2-TZVP Geometry

C	-0.90762	0.00281	-0.01098
C	-0.19558	-1.19438	-0.00835
C	1.19136	-1.19990	0.00192
C	1.89319	-0.00201	0.00793
C	1.19600	1.19728	0.00187
C	-0.19219	1.19656	-0.00826
C	-2.41157	0.00099	0.00872
H	-0.73718	-2.13343	-0.01687
H	1.72574	-2.14139	0.00176
H	2.97533	-0.00402	0.01315
H	1.73327	2.13711	0.00162
H	-0.73010	2.13751	-0.01671
H	-2.81234	0.93651	-0.38003
H	-2.81213	-0.81852	-0.58808
H	-2.78412	-0.12190	1.02810

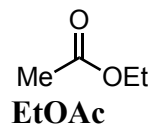


xylene

M06-2X/def2-TZVP Geometry

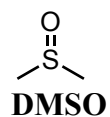
C	-0.47170	0.70101	0.00000
C	0.74274	1.37742	0.00001
C	1.95033	0.69258	0.00000
C	1.95033	-0.69258	-0.00000
C	0.74274	-1.37742	-0.00000
C	-0.47170	-0.70101	-0.00000
C	-1.76926	1.45967	-0.00001
H	0.74071	2.46130	0.00001
H	2.88377	1.24034	0.00000
H	2.88376	-1.24034	-0.00001
H	0.74070	-2.46130	-0.00001
C	-1.76926	-1.45967	0.00001
H	-2.37182	1.21405	-0.87749
H	-2.37193	1.21388	0.87735
H	-1.59336	2.53409	0.00011
H	-1.59337	-2.53409	-0.00009
H	-2.37183	-1.21404	0.87748

H -2.37192 -1.21389 -0.87736



M06-2X/def2-TZVP Geometry

C	-2.13106	-0.87753	0.00003
C	-1.03007	0.14410	-0.00007
O	0.17708	-0.44128	0.00010
O	-1.18428	1.33394	-0.00029
C	1.30109	0.44839	-0.00003
C	2.55058	-0.39780	0.00021
H	-2.03789	-1.51423	0.87921
H	-3.09163	-0.37264	0.00025
H	-2.03821	-1.51399	-0.87936
H	1.24014	1.09004	0.88003
H	1.24023	1.08967	-0.88035
H	3.43166	0.24377	0.00012
H	2.58496	-1.03325	0.88467
H	2.58505	-1.03362	-0.88398



M06-2X/def2-TZVP Geometry

S	0.00000	0.23087	-0.44340
O	-0.00000	1.46198	0.38610
C	-1.34113	-0.79424	0.18279
H	-1.32228	-1.77017	-0.30061
H	-1.23271	-0.88318	1.26309
H	-2.26726	-0.27610	-0.05639
C	1.34113	-0.79424	0.18279
H	1.32228	-1.77017	-0.30061
H	2.26726	-0.27610	-0.05639
H	1.23271	-0.88318	1.26309



M06-2X/def2-TZVP Geometry

C	-0.86237	-0.64342	-0.00016
O	-1.93862	-0.09229	0.00032
H	-0.76297	-1.74213	-0.00035
N	0.34102	-0.02202	-0.00089
C	1.58146	-0.75670	0.00030
H	2.17562	-0.51659	-0.88527
H	2.17429	-0.51617	0.88668
H	1.37500	-1.82587	0.00043
C	0.42113	1.42116	0.00006
H	0.95501	1.77322	-0.88599
H	-0.58895	1.82144	-0.00111
H	0.95246	1.77231	0.88805

Me-CN

MeCN

M06-2X/def2-TZVP Geometry

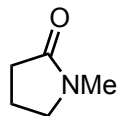
C	0.00000	0.00000	0.28210
N	0.00000	0.00000	1.42741
C	-0.00000	-0.00000	-1.17532
H	-0.00000	1.02399	-1.54420
H	0.88680	-0.51199	-1.54420
H	-0.88680	-0.51199	-1.54420



THF

M06-2X/def2-TZVP Geometry

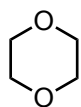
C	1.12421	-0.46915	-0.15948
O	0.00014	-1.19182	0.30110
C	-1.12404	-0.46944	-0.15967
C	-0.77290	1.01009	0.05056
C	0.77258	1.01036	0.05031
H	1.99539	-0.80134	0.40183
H	1.28858	-0.67940	-1.22436
H	-1.28801	-0.67950	-1.22465
H	-1.99527	-0.80203	0.40132
H	-1.19341	1.63953	-0.73195
H	-1.15759	1.36284	1.00593
H	1.19258	1.63961	-0.73262
H	1.15748	1.36368	1.00539



NMP

M06-2X/def2-TZVP Geometry

C	0.17981	0.86595	-0.00687
C	-1.33430	0.90004	0.13653
C	-1.77660	-0.52597	-0.19136
C	-0.53749	-1.37312	0.13117
H	-1.55428	1.17341	1.17115
H	-1.75845	1.66721	-0.50659
H	-2.65199	-0.85028	0.36673
H	-2.00259	-0.60924	-1.25435
H	-0.55349	-1.74593	1.16281
H	-0.43167	-2.23330	-0.53263
C	1.93206	-0.86002	-0.01136
H	2.14461	-1.57561	-0.80798
H	2.55447	0.02287	-0.14032
H	2.16704	-1.32778	0.94932
N	0.55564	-0.44309	-0.05948
O	0.92700	1.81737	-0.04255



Dioxane

M06-2X/def2-TZVP Geometry

O	-0.00000	-1.37218	-0.29407
C	1.16264	-0.73284	0.19398
C	1.16264	0.73284	-0.19398
O	0.00000	1.37218	0.29407
C	-1.16264	0.73284	-0.19398
C	-1.16264	-0.73284	0.19398
H	1.20364	-0.82176	1.28773
H	2.01883	-1.25131	-0.23740
H	2.01883	1.25131	0.23740
H	1.20364	0.82176	-1.28773
H	-2.01883	1.25131	0.23740
H	-1.20364	0.82176	-1.28773
H	-2.01883	-1.25131	-0.23740
H	-1.20364	-0.82176	1.28773



PhH

M06-2X/def2-TZVP Geometry

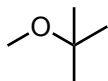
C	-0.33147	-1.34837	0.00000
C	1.00207	-0.96119	0.00001
C	1.33350	0.38712	-0.00000
C	0.33141	1.34839	0.00000
C	-1.00202	0.96124	0.00000
C	-1.33348	-0.38718	-0.00001
H	-0.58979	-2.39948	-0.00001
H	1.78311	-1.71055	-0.00001
H	2.37294	0.68901	-0.00002
H	0.58986	2.39946	-0.00001
H	-1.78316	1.71050	0.00001
H	-2.37296	-0.68894	0.00000

Me-NO₂

CH₃NO₂

M06-2X/def2-TZVP Geometry

N	0.17425	0.00000	-0.00997
O	0.72455	1.07490	0.00256
O	0.72437	-1.07500	0.00256
C	-1.31599	0.00009	-0.00337
H	-1.61473	-0.00076	1.04242
H	-1.65019	0.90576	-0.49594
H	-1.65027	-0.90479	-0.49734



MTBE

M06-2X/def2-TZVP Geometry

C	-2.01626	0.00666	-0.14994
O	-0.77675	0.00853	-0.80976
C	0.39505	-0.00069	0.00773
C	0.38901	-1.18880	0.96669
C	0.52631	1.31303	0.77599
C	1.53511	-0.13750	-0.99069
H	-2.19399	-0.92820	0.39059
H	-2.11821	0.84274	0.54906
H	-2.77868	0.10929	-0.92022
H	0.19556	-2.11230	0.41839

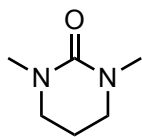
H	1.35935	-1.27382	1.45733
H	-0.36662	-1.07859	1.74558
H	0.46142	2.15515	0.08581
H	-0.24938	1.42102	1.53478
H	1.49064	1.35303	1.28444
H	1.50758	0.69065	-1.69929
H	2.49859	-0.13387	-0.48006
H	1.43249	-1.06951	-1.54706

Me-OH

MeOH

M06-2X/def2-TZVP Geometry

C	0.66173	-0.02046	0.00000
H	1.08259	0.98329	-0.00109
H	1.02057	-0.54596	-0.88994
H	1.02073	-0.54413	0.89097
O	-0.74380	0.12246	0.00000
H	-1.14390	-0.75008	0.00001

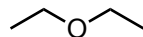


DMPU

M06-2X/def2-TZVP Geometry

C	-1.23135	1.30971	0.19831
C	-0.00004	2.00168	-0.34632
C	1.23129	1.30980	0.19840
C	0.00003	-0.83441	-0.07803
H	-1.32510	1.49421	1.27805
H	0.00002	1.93946	-1.43606
H	2.13364	1.70597	-0.27265
H	-2.13371	1.70584	-0.27277
H	-0.00013	3.05397	-0.06191
H	1.32494	1.49427	1.27814
N	-1.17405	-0.11183	-0.07444
N	1.17405	-0.11174	-0.07443
C	2.41825	-0.83414	0.08072
H	2.26028	-1.87327	-0.18723
H	3.17646	-0.39779	-0.57222
H	2.78043	-0.78387	1.11364
C	-2.41823	-0.83421	0.08075
H	-2.26011	-1.87349	-0.18653
H	-2.78072	-0.78335	1.11354

H	-3.17631	-0.39829	-0.57264
O	0.00008	-2.05366	-0.12279



Et₂O

M06-2X/def2-TZVP Geometry

C	-0.40929	-2.36741	0.00000
C	0.51624	-1.17268	0.00000
O	-0.26199	-0.00000	0.00000
C	0.51624	1.17268	0.00000
C	-0.40929	2.36741	0.00000
H	0.16437	-3.29439	0.00000
H	-1.04662	-2.35081	0.88369
H	-1.04662	-2.35081	-0.88369
H	1.16756	-1.18637	-0.88463
H	1.16756	-1.18637	0.88463
H	1.16756	1.18637	-0.88463
H	1.16756	1.18637	0.88463
H	0.16437	3.29439	0.00000
H	-1.04662	2.35081	-0.88369
H	-1.04662	2.35081	0.88369

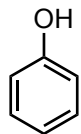


hexane

M06-2X/def2-TZVP Geometry

C	0.66386	0.37290	0.00000
H	0.71110	1.02956	-0.87562
H	0.71110	1.02956	0.87562
C	-0.66386	-0.37290	-0.00000
H	-0.71110	-1.02956	-0.87562
H	-0.71110	-1.02956	0.87562
C	-1.87473	0.55169	0.00000
H	-1.82628	1.20648	0.87503
H	-1.82628	1.20648	-0.87503
C	1.87473	-0.55169	0.00000
H	1.82628	-1.20648	0.87503
H	1.82628	-1.20648	-0.87503
C	-3.19436	-0.20876	-0.00000
H	-4.04915	0.46804	-0.00000
H	-3.27378	-0.84870	-0.88093
H	-3.27378	-0.84869	0.88093
C	3.19436	0.20876	-0.00000
H	4.04915	-0.46804	-0.00000

H	3.27378	0.84870	-0.88093
H	3.27378	0.84869	0.88093



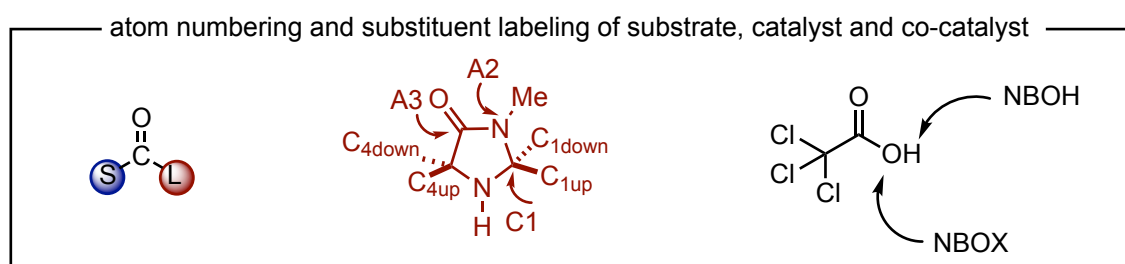
Phenol

M06-2X/def2-TZVP Geometry

C	-0.00000	0.93447	-0.00000
C	1.21088	0.25175	-0.00000
C	1.21420	-1.13295	0.00000
C	0.02140	-1.84643	0.00000
C	-1.18142	-1.15674	0.00000
C	-1.19822	0.23112	-0.00000
H	2.13042	0.82135	-0.00000
H	2.15951	-1.66025	0.00000
H	0.03099	-2.92771	0.00000
H	-2.11855	-1.69832	0.00000
H	-2.14012	0.76853	-0.00000
O	0.04783	2.29482	-0.00000
H	-0.84586	2.65049	-0.00000

Parameters Collected

The parameters calculated and considered for the systems are reported in separate tables encompassed in the accompanying excel spreadsheets. Sterimol parameters L, B1 and B5, respectively, represent the length, minimum and maximum widths of the considered substituent and are calculated using the Bondi radii.^{12,13} IR stretching frequencies, intensities and NBO charges have been found to be useful descriptors of electronic and steric properties,¹⁴ hence these have been calculated. Global parameters including highest occupied molecular orbital (HOMO)/lowest unoccupied molecular orbital (LUMO) energies and polarizability were also collected for each reaction component. Solvent topological and connectivity descriptors were acquired from DFT optimized geometries and calculated with the molecular descriptors application available in Maestro using default settings.



Carbonyl that engages in iminium and enamine formation

Carbonyls have a number of overlapping features and these have been parameterized as follows. Sterimol values of the small (S) and large (L) substituents were collected. NBO charges from the common C, O, S and L unit were calculated and acquired, in addition to HOMO, LUMO and polarizabilities.

Other reaction components

Limited structural overlap across this diverse set of reaction components necessitated us to only consider the HOMO, LUMO and polarizability as DFT descriptors.

Secondary amine catalyst

NBO charges, Sterimol values of each substituent (C1, A2, A3 and C4), vibrations and intensities of the N-H bond, global properties such as LUMO, HOMO and polarizability were calculated and collected.

Solvent parameter tables

2D descriptors (e.g., common topological and connectivity as exemplified by molecular shape, size and number of heteroatoms) are used to describe structurally disparate solvent molecules and have been defined elsewhere.¹⁵

Co-catalyst parameter tables

NBO charges from the common H-X subunit (where X is O, Cl, N) are calculated and collected. LUMO, HOMO and polarizability were also collected as descriptors.

Data curation

Relevant data were manually extracted from the following sources:

- (1) Ouellet, S. G.; Tuttle, J. B.; MacMillan, D. W. C. Enantioselective organocatalytic hydride reduction. *J. Am. Chem. Soc.* **2005**, *127*, 32–33.
- (2) Suri, J. T.; Mitsumori, S.; Albertshofer, K.; Tanaka, F.; Barbas, C. F. Dihydroxyacetone variants in the organocatalytic construction of carbohydrates: Mimicking tagatose and fucose aldolases. *J. Org. Chem.* **2006**, *71*, 3822–3828.
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- (12) Marigo, M.; Fielenbach, D.; Braunton, A.; Kjærsgaard, A.; Jørgensen, K. A. Enantioselective formation of stereogenic carbon - Fluorine centers by a simple catalytic method. *Angew. Chem., Int. Ed.* **2005**, *44*, 3703–3706.
- (13) Franzén, J. *et al.* A general organocatalyst for direct α -functionalization of aldehydes: Stereoselective C-C, C-N, C-F, C-Br, and C-S bond-forming reactions. Scope and mechanistic insights. *J. Am. Chem. Soc.* **2005**, *127*, 18296–18304.
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- (28) Brown, S. P. *Iminium and enamine activation: methods for enantioselective organocatalysis*; California Institute of Technology, Pasadena, 2005.
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- (30) Larsen, C. H. M. *Investigating imidazolidinone catalysts: enantioselective organocatalytic Diels–Alder reactions, conjugate additions to access non-natural α -amino acids, and bimodal catalyst activation for the development of organo-cascade reactions*; California Institute of Technology, Pasadena, 2005.

Out-of-sample

- (1) Bertelsen, S.; Dinér, P.; Johansen, R. L.; Jørgensen, K. A. Asymmetric organocatalytic β -hydroxylation of α,β -unsaturated aldehydes. *J. Am. Chem. Soc.* **2007**, *129*, 1536–1537.
- (2) List, B. Direct catalytic asymmetric α -amination of aldehydes. *J. Am. Chem. Soc.* **2002**, *124*, 5656–5657.

Out-of-sample synergistic

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Thesis Mining

We supplemented our dataset curated from scientific journals with experimental data obtained from Ph.D. theses that have been made available to the public. Considering the goal of this effort was to gather negative data, our general approach was based on the premise that screening data gathered during the development of a published method would likely be included in the author's thesis as part of their Ph.D. requirements. Therefore, one could in principle search for the author's Ph.D. thesis from the relevant repository. Using this focused search criteria, we extracted relevant data from sources 27 to 30 as outlined on page S343 via <https://thesis.library.caltech.edu/cgi/search/simple>.

Model development

Measured $\Delta\Delta G^\ddagger$ values were calculated using the formula $\Delta\Delta G^\ddagger = -RT\ln(er)$ where R is the gas constant, T is temperature, and er is the enantiomeric ratio. From the survey of reactions, we categorized the data set by catalyst structure (steric blocking or hydrogen bonding) wherein reactions catalyzed by imidazolidinone and diphenylprolinol ethers are binned by +ee and proline type catalysts as a -ee. Linear regression models were developed using an in-house script implemented in MATLAB[®] (version R2018b), to obtain the predicted $\Delta\Delta G^\ddagger$. Forward stepwise linear regression was employed for model development with previously reported algorithms,¹⁶ with small changes in input as a consequence of the number of parameters screened to describe the system under study. These changes included the removal of parameters that measure similar features i.e. collinear parameters were automatically removed, defined by 0.3 collinear criteria. With the truncated parameter set in hand, the algorithm proceeds by performing single parameter regression with each descriptor (x). The 20 descriptors with the highest R² values are used as a start point for building two parameter correlations. These are constructed by adding a second parameter to the previously identified 20 univariate correlations to generate 20x models. As before, the 20 two parameter models with the highest R² values are taken forward to generate three parameter correlations. This sequence is performed until the user terminates parameter addition or the R² does not increase. Because mechanistic analysis is a secondary goal of the workflow, we try to limit the number of parameters included in an equation and we purposely do not include cross-terms in our model search.

As the model search process can produce a large pool of model candidates, we truncated the models on the recorded statistics as well as the number of included parameters (in more detail below).

The generalized model structure consists of a constant term, first-ordered parameters (P) and their coefficients (β). In some cases, interactions between parameters would also lead to cross terms ($P_j \cdot P_k$).

$$\Delta\Delta G^\ddagger = const. + \sum_i \beta_i P_i$$

The predictions provided by the models would then be fitted to the measured results to visualize and further evaluate the model performances. In the resulting equations (shown below in generalized form), the slope would have the same value as R², and the intercept corresponds to the variance in experimental results in which the included parameters could not account for.

$$(measured\Delta\Delta G^\ddagger) = slope \cdot (predicted\Delta\Delta G^\ddagger) + intercept$$

Normalized parameters were employed so that the coefficients would be reflective of the importance of each descriptor. Normalization is the operation of extracting the mean value (μ) then dividing by the standard deviation (σ).

$$P_{norm} = \frac{P - \mu_P}{\sigma_P}$$

A good linear correlation (R^2 close to 1.0 and intercept close to 0.0) between the predicted $\Delta\Delta G^\ddagger$ and the measured $\Delta\Delta G^\ddagger$ indicates that the obtained model adequately approximates the system under study.

Model validation

Models were validated using external and cross-validation techniques. Cross-validation generally refers to the statistical method of excluding part of the dataset as validations, predicting their values using the remaining set of data, evaluating the predictions, and repeating the process to reduce variability. Such analysis is generally employed to test the stability of a model and identify if overfitting occurs. Leave-one-out cross-validation is where only one data point would be removed each time and predicted by the remaining set. All validation predictions would then be combined and fitted to the measured values, the R^2 value of the resulting fit is called Q^2 .

Another method to test model robustness is k -fold cross-validation. In this validation method, the dataset is divided randomly into k subsets with same/similar sizes, each set would then be predicted out by the other $k-1$ subsets, and the goodness of fit would be tested based on these predictions. However, it is important to note that the k -fold statistics is dependent on the partitioning of the dataset, and that there's a necessity of executing the process multiple times for average results.

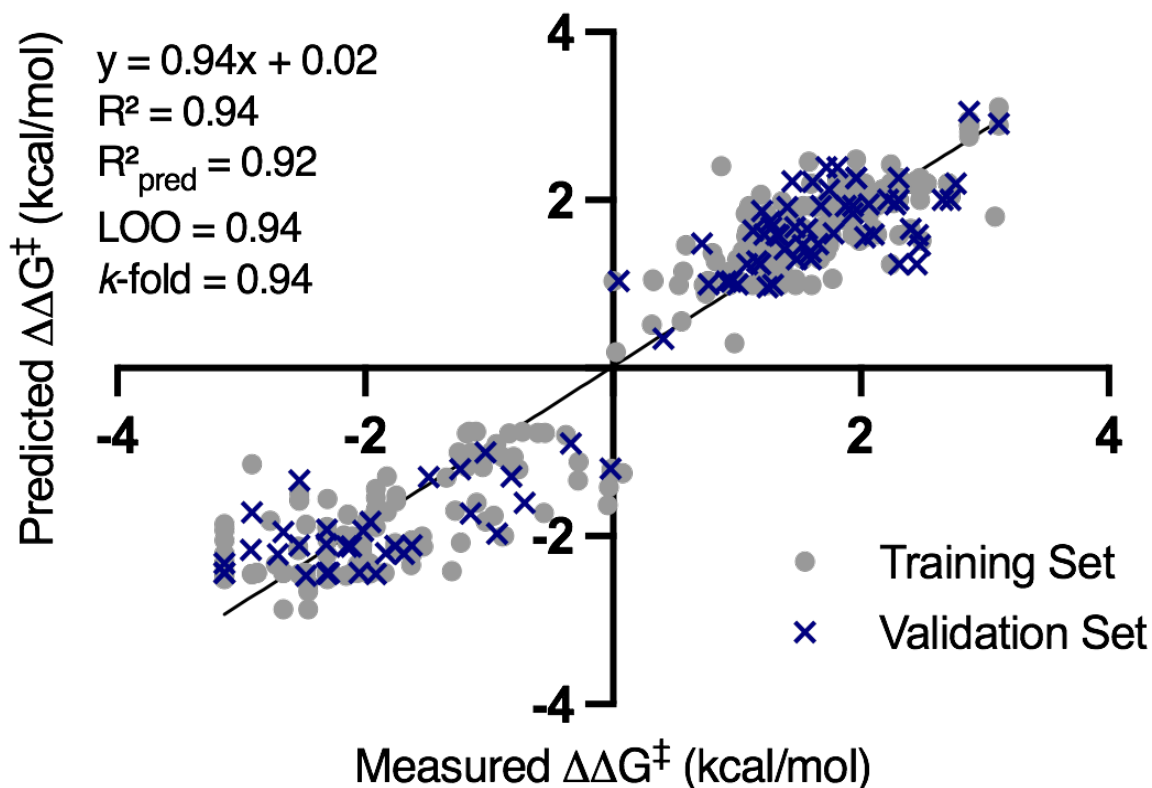
The 452 reactions were split into 80:20 TS:VS sets for external validation. The split was partitioned based on the response values using the MATLAB “*equidistant*” function. This process can be described as pseudorandom as it is generated using a deterministic algorithm.

As another model test, we have created models wherein the descriptors (1 substrate, 2 reactant, 7 cat, 3 solvent) are replaced with dummy values (random numbers on a normal distribution) to create a meaningless reaction barcode. The statistical scores are much worse ($R^2 = 0.69$, $Q^2 = 0.65$, $LOO = 0.63$, 10-fold CV = 0.62), suggesting that the DFT descriptors are correlating something meaningful.

All data associated with model construction and predictions are encompassed in the accompanying excel spreadsheet. We also include key plots below.

Secondary amine model (with validations)

$$\begin{aligned} \Delta\Delta G^\ddagger = & 0.31 + 0.27L_S - 0.21HOMO + 0.17pol + 0.39iNH \\ & + 1.60NBO_{C1} - 0.49NBO_{A2} + 1.43B5_{C1up} - 0.57B5_{C1down} + \\ & 0.42LUMO - 0.11HOMO - 0.03KS + 0.30CI + 0.182DShape \end{aligned}$$



KS = kier alpha modified shape index

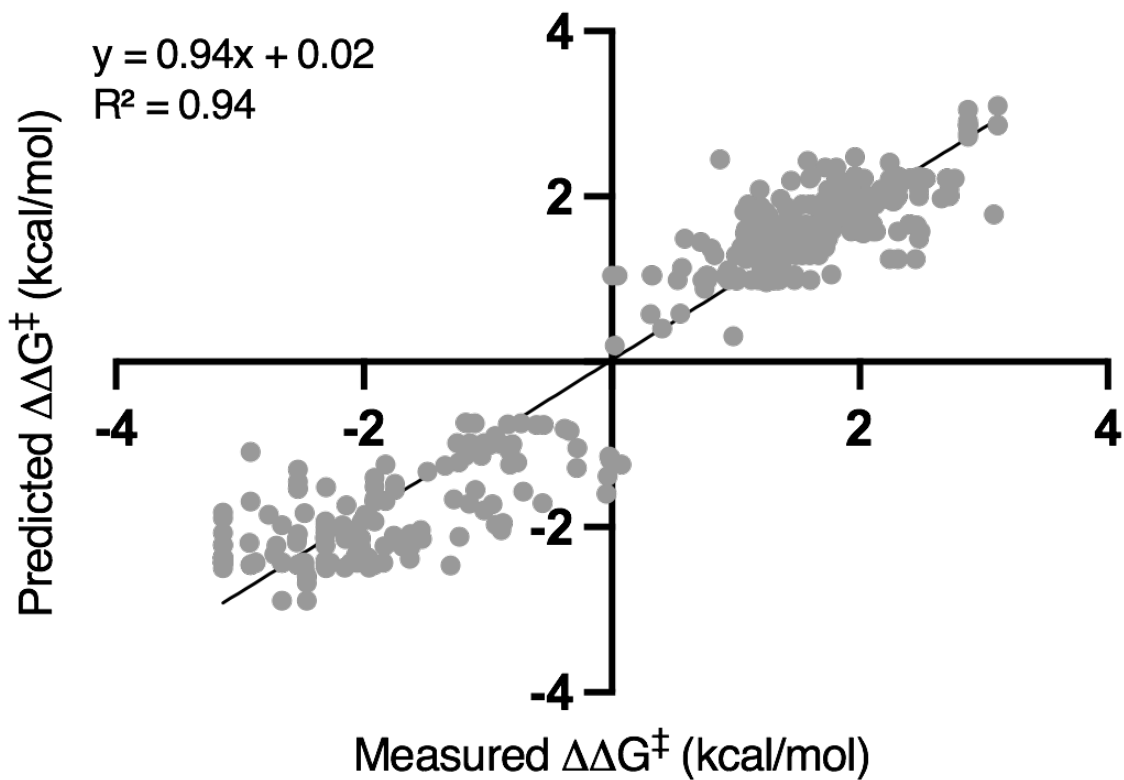
CI = averaged valence connectivity index chi-5

2DShape = Petitjean 2D shape

See page S341 for the definition of the additional descriptors.

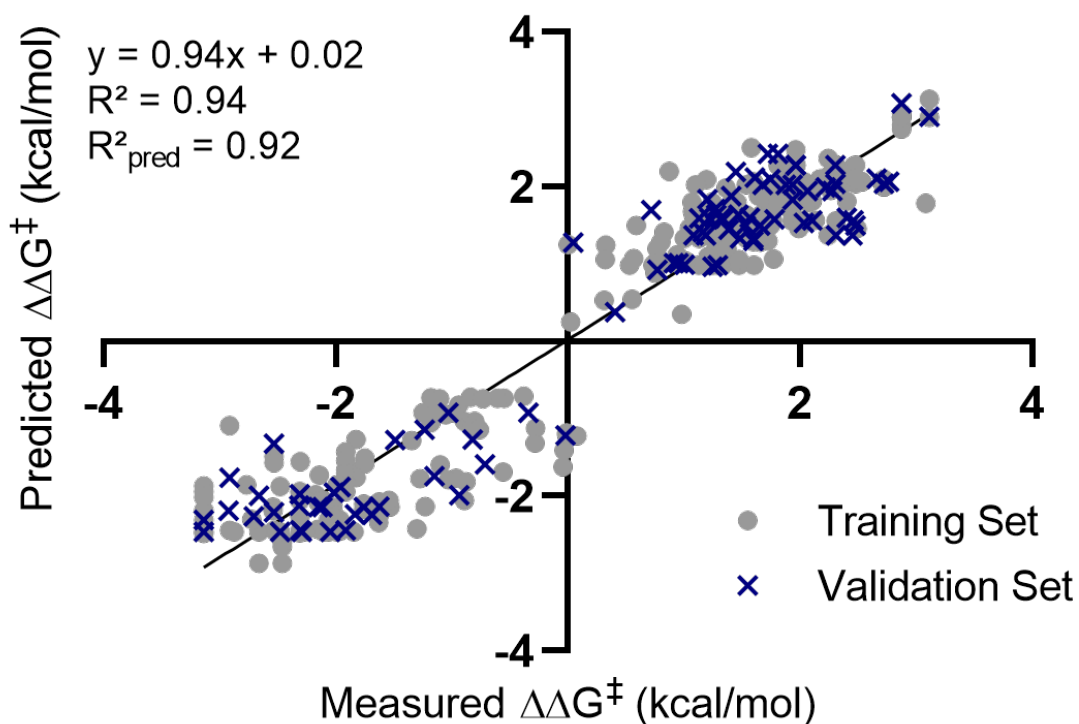
Secondary amine model (all data as training)

$$\Delta\Delta G^\ddagger = 0.31 + 0.28L_S - 0.23HOMO + 0.17pol + 0.39iNH + 1.55NBO_{C1} - 0.55NBO_{A2} + 1.48B5_{C1up} - 0.58B5_{C1down} + 0.47LUMO - 0.11HOMO - 0.04KS + 0.31CI + 0.192DShape$$

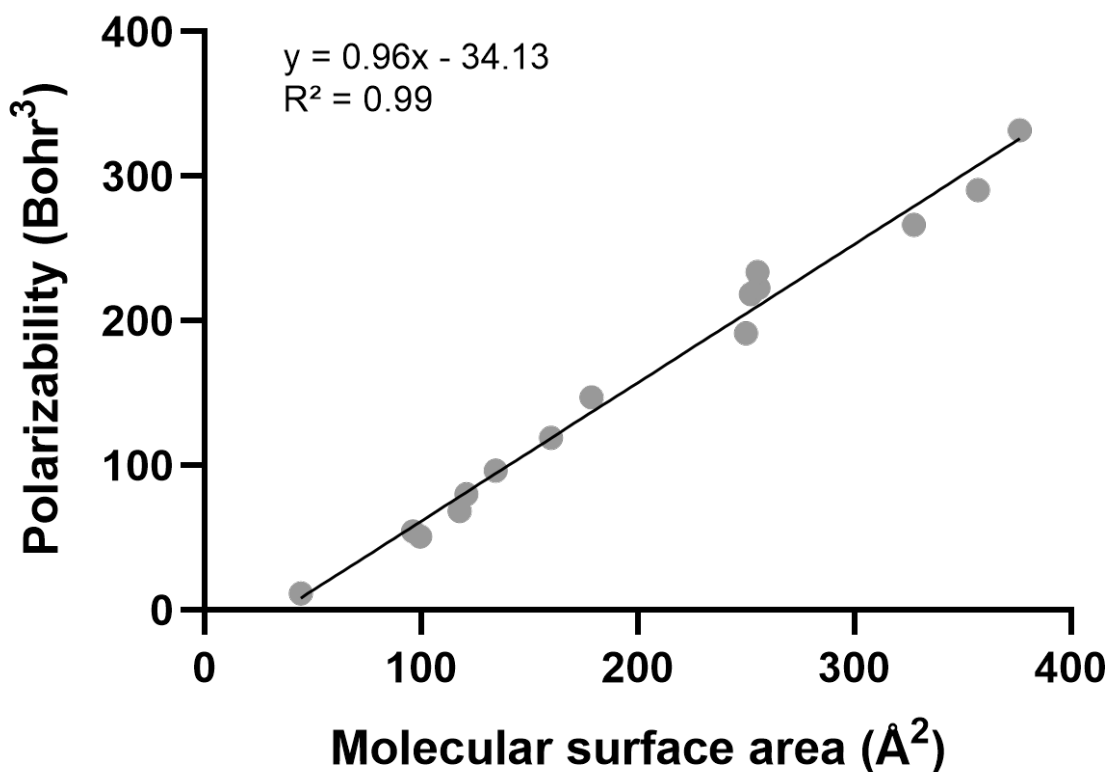


For some examples, the reactions were performed with mixed solvent systems. We reasoned that because solute-solvent interactions with polar substances will likely dominate over those with non-polar molecules, we collected topological, two-dimensional descriptors from the solvent with the largest dielectric constant. To test this impact of adding a second solvent (often non-polar) to the reaction we averaged the three solvent descriptors (kier alpha modified shape index, averaged valence connectivity index chi-5, and Petitjean 2D shape) taken from both solvents. Ultimately, modeling the solvent mixtures with averaged parameters is not critical since the statistical models obtained are almost identical.

$$\Delta\Delta G^\ddagger = 0.31 + 0.26L_S - 0.23HOMO + 0.18pol + 0.35iNH + 1.67NBO_{C1} - 0.42NBO_{A2} + 1.37B5_{C1up} - 0.56B5_{C1down} + 0.37LUMO - 0.10HOMO + 0.02KS + 0.28CI + 0.152DShape$$



As part of our analysis in connecting the model terms to transition state features, we suggested that the polarizability likely acts as a proxy for chemical size. To probe this further we correlated polarizability against molecular surface area (MSA) for a subset of reactants and show that there is a strong positive correlation. We choose not to include MSA as a parameter for all the reactants since it requires importing structures into an additional program and performing another calculation. For precise structures of the reactants included in this correlation please see the accompanying excel spreadsheet.

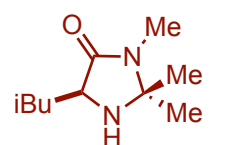
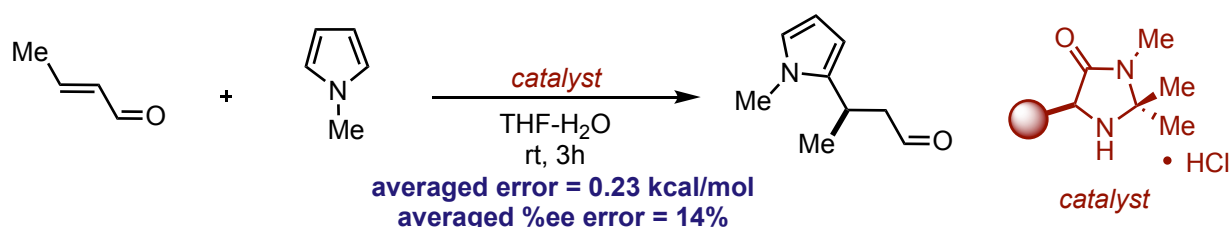


Out-of-sample predictions

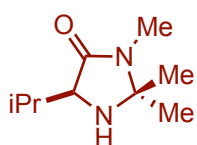
We evaluated the model's ability to transfer the mechanistic principles leading to enantioselective catalysis captured by the statistical models to reactive intermediates generated from a second achiral catalyst. Treating the test reactions as virtual predictions prediction accuracy was determined by both enantioselectivity values and the average absolute $\Delta\Delta G^\ddagger$ error ($\Delta\Delta G^\ddagger$ error = absolute(model measured – experimentally measured/ no. of examples).

Using the secondary amine catalyst model:

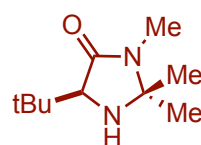
We next validated the secondary amine model by testing its ability to extrapolate to new reaction types involving a single catalyst. As described in the main text, when tested against two different reactions, the model predicted the experimental data exceptionally well. Assessing the model's ability to predict low ee data would provide a different test of the model's capabilities. To accomplish this, we removed the only extensive catalyst screening data that was available (obtained from a Ph.D. thesis) from the training set and used these as the out-of-sample prediction platform. The model was retrained using the same parameters (but without these 7 catalyst data points) and, the resulting model was applied to predict the results of the catalyst screen. As shown below, the model also provided decent predictions for this catalyst screen despite the limited training data in that enantioselectivity range i.e. 0–70% ee.



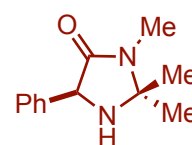
experiment 33% ee
predicted 33% ee



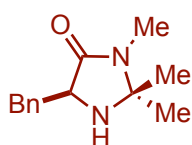
experiment 26% ee
predicted 46% ee



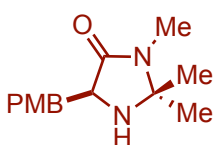
experiment 68% ee
predicted 24% ee



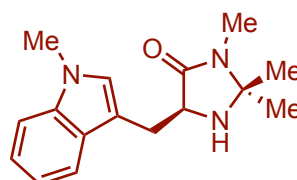
experiment 2% ee
predicted 15% ee



experiment 66% ee
predicted 70% ee



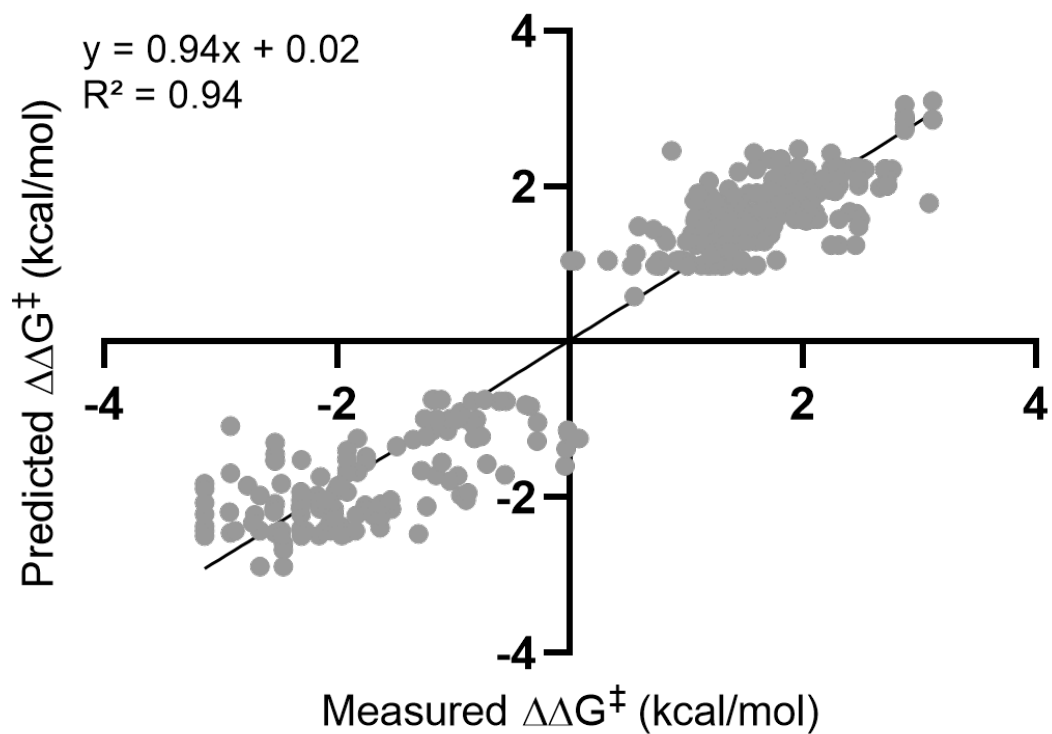
experiment 56% ee
predicted 65% ee



experiment 66% ee
predicted 76% ee

Secondary amine model used to predict the catalyst set

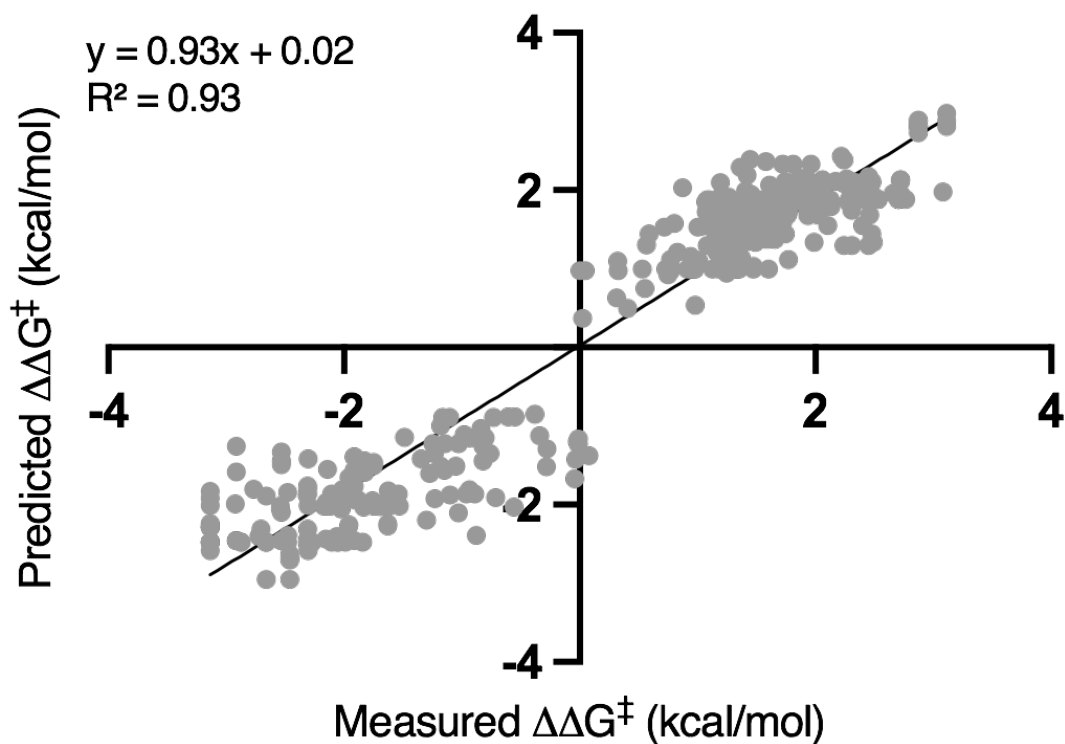
$$\Delta\Delta G^\ddagger = 0.31 + 0.28L_s - 0.23HOMO + 0.17pol + 0.39iNH + 1.51NBO_{C1} - 0.56NBO_{A2} + 1.48B5_{C1up} - 0.58B5_{C1down} + 0.47LUMO - 0.11HOMO - 0.05KS + 0.31CI + 0.192DShape$$



Adjusted secondary amine model

As part of the exploration on predicting out-of-sample, we discovered replacing the HOMO with a HOMO-LUMO term could lead to a more generalizable model.

$$\Delta\Delta G^\ddagger = 0.31 + 0.33L_s + 0.08\text{HOMO-LUMO} + 0.21\text{pol} + 0.30\text{iNH} \\ + 1.76\text{NBO}_{C1} - 0.25\text{NBO}_{A2} + 1.42\text{B5}_{C1\text{up}} - 0.59\text{B5}_{C1\text{down}} + \\ 0.35\text{LUMO} - 0.08\text{HOMO} + 0.03\text{KS} + 0.28\text{CI} + 0.20\text{DShape}$$



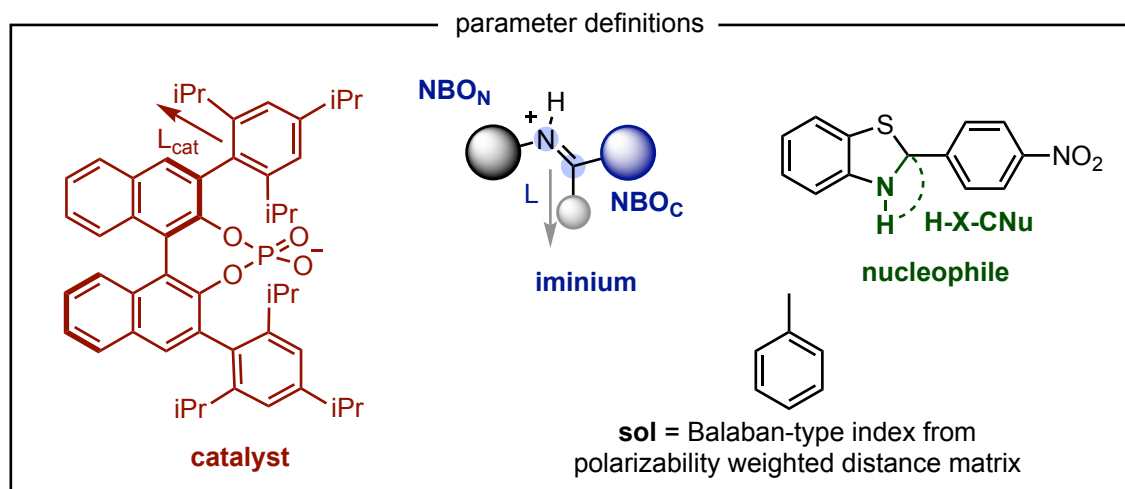
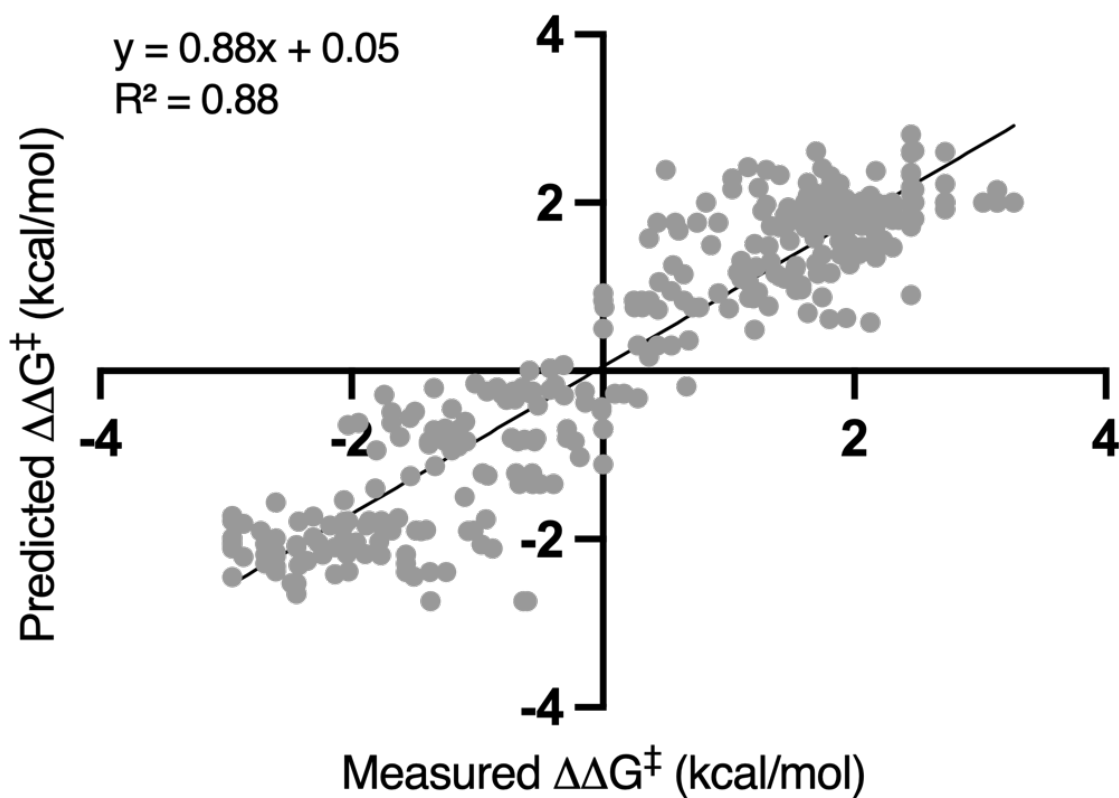
Using the chiral phosphoric acid catalyzed published model:

Because the nucleophile terms were not sensitive to the change in method required to optimize the iron complex, we could deploy the published dataset without any modification. This included using all the available data as the training set, re-creating the statistical model in MATLAB, and using this as a platform to extrapolate to multi-catalysis. Initially, reaction performance was evaluated using the comprehensive model to determine the mechanistic pathway under operation, these predictions could then be further refined with the specific models (*Z*-imine). This two-tiered workflow is imperative as the process avoids mechanistic assumptions, ensuring that the results of the test reactions are unknown. Below we show the statistical models utilized and describe the necessary model parameters required for prediction. To be specific we collected the H-X-CNu, and B5Nu from the achiral iron complex.

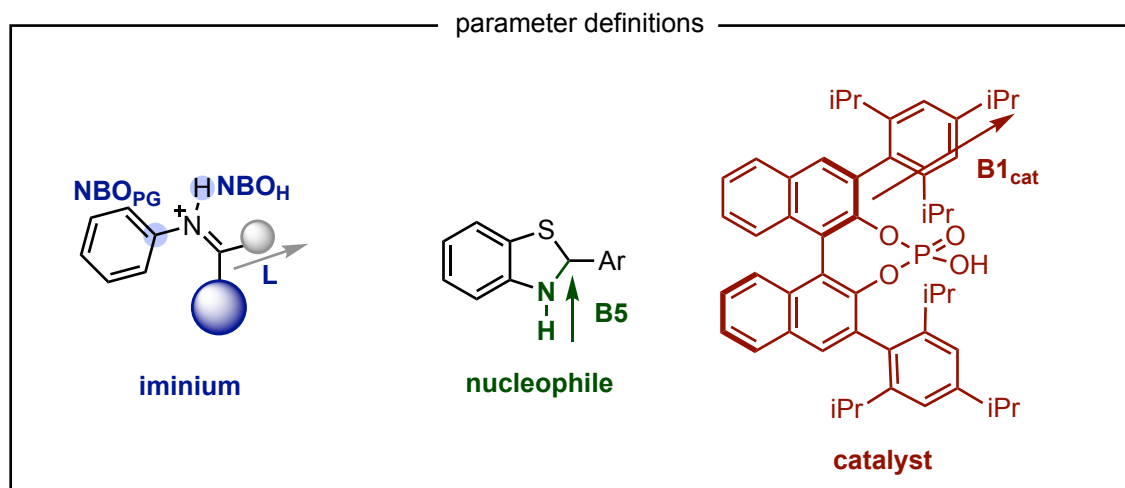
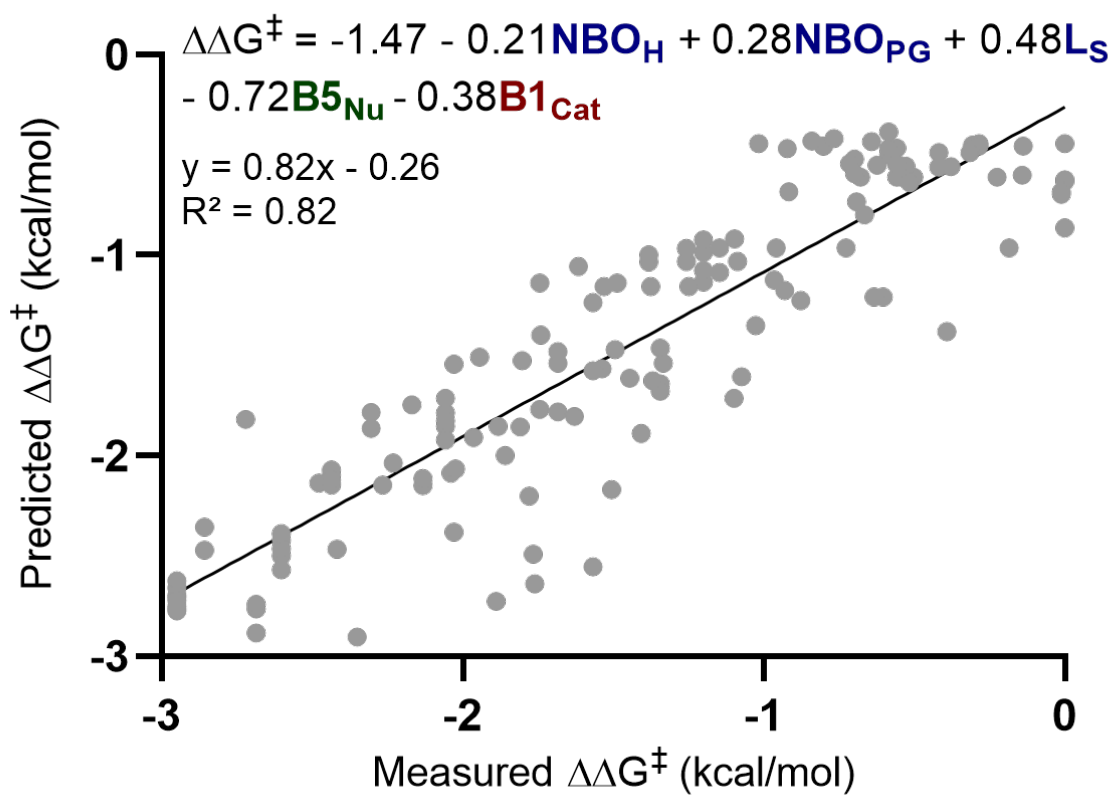
Comprehensive model

$$\Delta\Delta G^\ddagger = 0.42 + 0.30\text{sol} - 0.86\text{NBO}_N - 0.83\text{NBO}_C + 0.40\text{L}_S + 0.63\text{H-X-C}_{\text{Nu}} + 0.23\text{L}_{\text{Cat}}$$

$$y = 0.88x + 0.05$$
$$R^2 = 0.88$$



Z-imine model

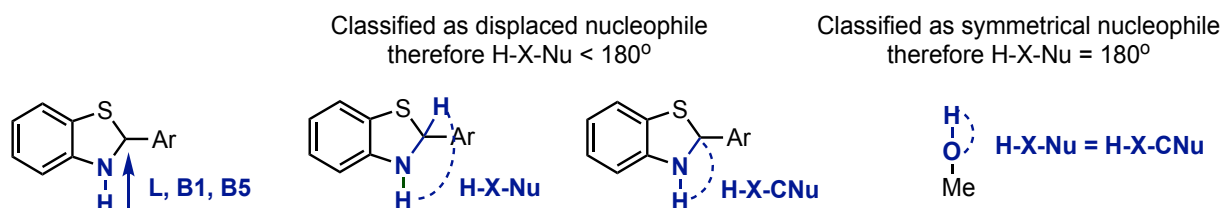


More details about imine parameters

We derive parameters from both the *E* and *Z* iminium, since both configurations are important in dictating the enantioselectivity. As outlined in the previous publication, *E*-iminium descriptors are employed for comprehensive model and *Z*-iminium descriptors for the focused model. From these DFT optimized structures NBO charges and Sterimol values of specific substituents are required. Sterimol values were calculated using the Bondi radii from the small substituent (S). NBO charges were calculated for the molecule and the necessary charges collected from specific atoms on the iminium (e.g. N, C, H and the first atom of the protecting group PG).

More details about nucleophile parameters

Sterimol B5 value of the entire nucleophile unit and the H-X-CNu angle measurement are necessary for prediction. For most nucleophiles, such as alcohols, the H-bond that holds the nucleophile to the catalyst is in line with the nucleophilic site. Inspired by the work of Goodman, “angle” measurements have been used to numerically describe this feature.¹⁷ Nucleophiles with this geometric feature are classified as linear therefore geometrically assigned an “angle” of 180° i.e., H-X-Nu is 180° even when X=Nu. However, in some cases, the bond may be displaced to one side and these molecules have smaller H-X-Nu angles. A second angle measurement, H-X-CNu, is employed for displaced nucleophiles to describe a larger angle. This angle is defined from the H, X and the atom that is attached to the nucleophilic site if the nucleophilic site is not carbon. H-X-Nu = H-X-CNu if Nu = C.



More details about catalyst and solvent parameters

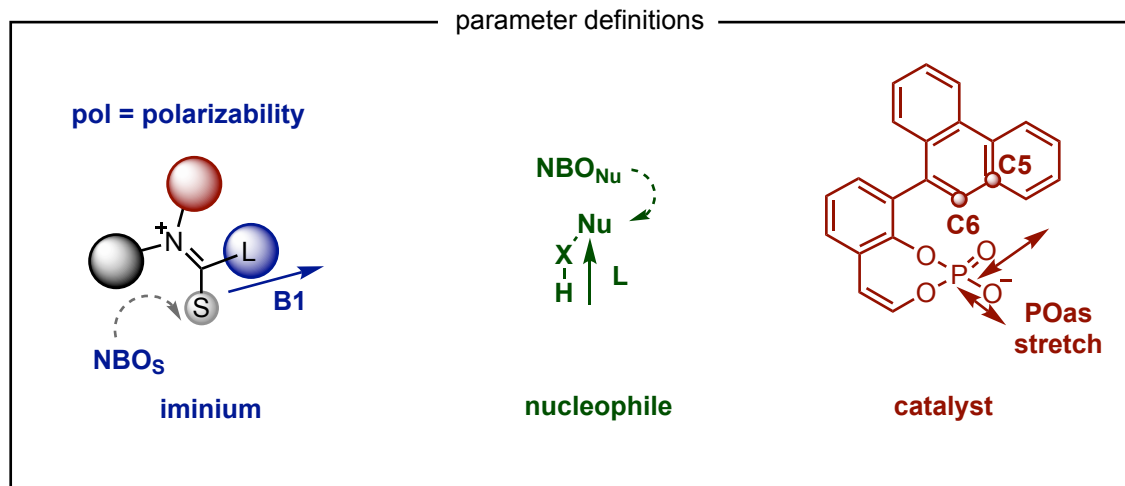
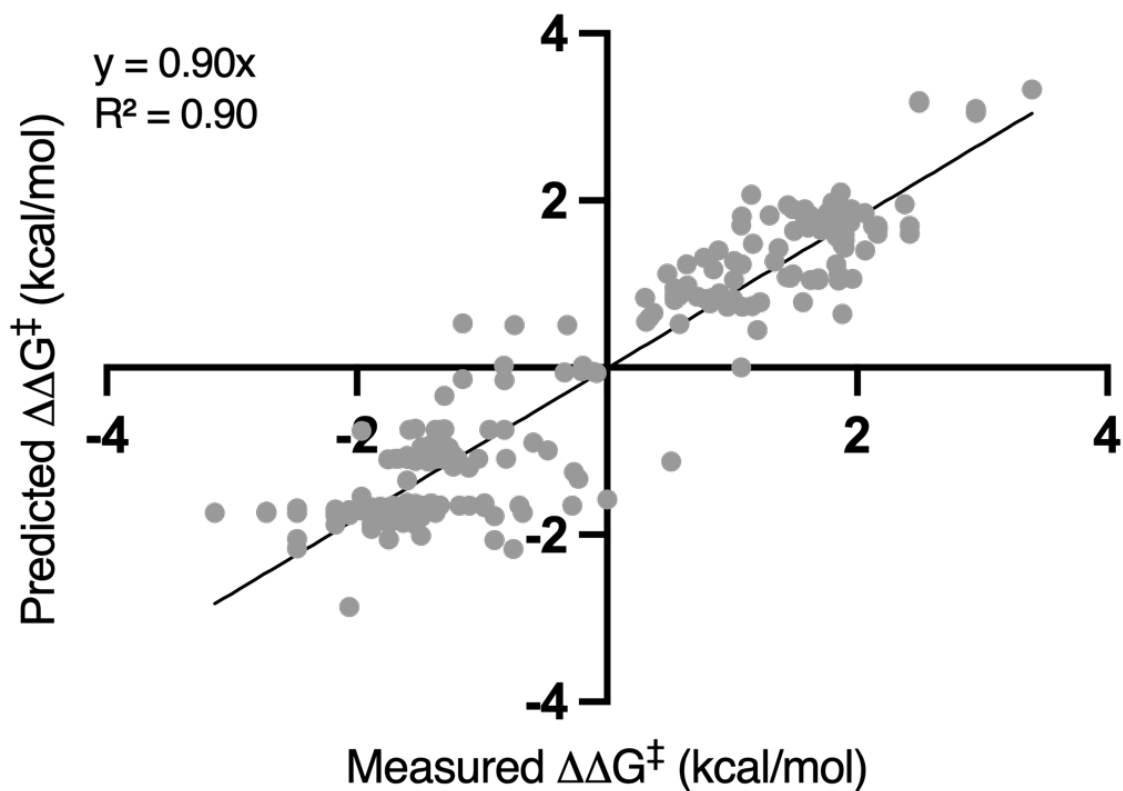
Solvent descriptors were acquired from the molecular descriptors application available in Maestro using default settings. Sterimol parameters were acquired for the whole catalyst aromatic group and the 2-substituent as defined above.

More detailed parameter descriptions can be found in ref 10.

Using the chiral phosphate catalyzed published model:

We expected that the NBO charges would be highly sensitive to the change in method required to optimize the gold-activated allenamides. Thus, all iminium components required to build the previously reported model were optimized at the M06/def2TZVP level and the necessary parameters acquired from these structures. Employing these parameters in combination with the previously published nucleophile and catalyst descriptors, the model was re-created in MATLAB using all the available data as the training set. The resulting model was then used to predict the enantioselectivity outcome when organometallic intermediates (Gold intermediate 1 to 3) were used as the electrophilic component in an [Au(I)]-Catalyzed Dearomatization of β -Naphthols with Allenamides.

$$\Delta\Delta G^\ddagger = -0.08 - 0.35\text{NBO}_S + 0.02\text{B1}_L + 0.19\text{pol} + 0.69\text{NBO}_{\text{Nu}} - 0.30\text{L}_{\text{Nu}} - 0.77\text{B5}_{\text{C5}} + 0.34\text{L}_{\text{C6}} + 0.25\text{PO}_{\text{as}}$$



More details on the iminium parameters

From the ground state DFT optimized iminium structure NBO charges and Sterimol values of the necessary substituent (SubR, SubEWG, SubL, and SubS) in addition to polarizability were calculated and collected. Specifically, the NBO of the first atom on the small group (S) and the Sterimol L value of the large group (L) was gathered.



More details on the nucleophile parameters

Sterimol B5 value of the entire nucleophile unit and the NBO charge of the nucleophilic site were necessary for prediction.

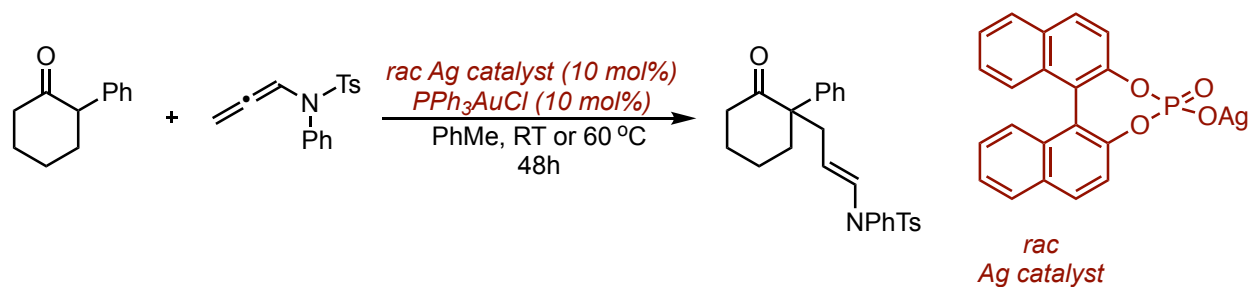
More details on the model catalyst parameters

The vibration term POas (the asymmetric P–O stretching frequency) and Sterimol values from the C5 and C6 positions were calculated and collected from simple model phosphoric acid structures.

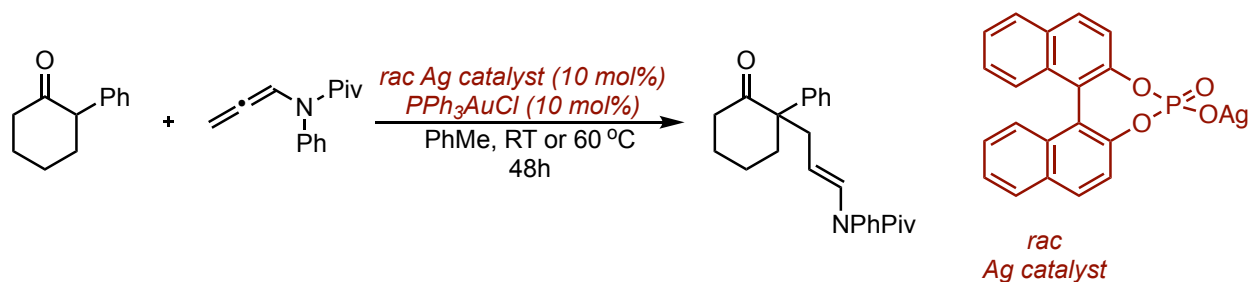
More detailed parameter descriptions can be found in ref 11.

Unsuccessful reactions

Attempted reactions involving 2-phenylcyclohexanone were unsuccessful i.e. gave no conversion to the product under the mult catalysis conditions. Despite the fact that naphthols which are operationally similar and work well (i.e. thought to proceed through the same mechanism).



We also changed the allenamide structure to one which has been reported to work in combination with 2-phenylcyclohexanone under chiral acid only conditions see X. Yang and F. D. Toste, *Chem. Sci.* 2016, 7, 2653–2656.

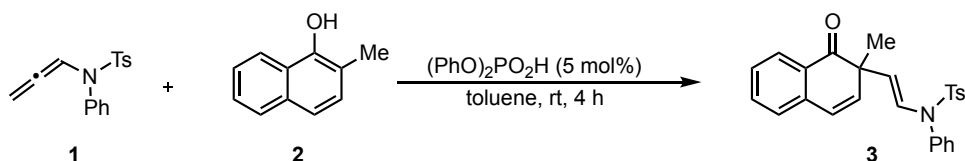


However, under the gold catalysis conditions we noted significant decomposition of the Piv-substituted allenamide and no product was observed.

General experimental information

All commercial reagents were used as received; all solvents are HPLC grade dried and degassed with Solvent Purification System (SPS). The *N*-phenyl-*N*-sulfonylallenamide **1**,¹⁸ (*R*)-phosphoric acids¹⁹ and the chiral silver phosphates²⁰ were obtained following known procedures. Flash chromatography was carried out using 230-400 mesh silica gel and dry-packed columns. Thin layer chromatography was carried out using Merck TLC Silica gel 60 F254 aluminum sheets. Components were visualized by UV light ($\lambda = 254$ nm) and stained with phosphomolybdic dip. NMR spectra were recorded at 298 K on a Bruker Avance 400dir Ultrashield apparatus. CDCl₃ was used as internal standard for ¹³C NMR and ¹H NMR spectra. Chemical shifts are given in ppm and coupling constants in Hz. High performance liquid chromatography (HPLC) was performed on Agilent Technologies chromatographs (1100 and 1200 Series), using Daicel Chiralpak AD-H columns. Optical rotation measurements were carried out on a Jasco P-2000 polarimeter.

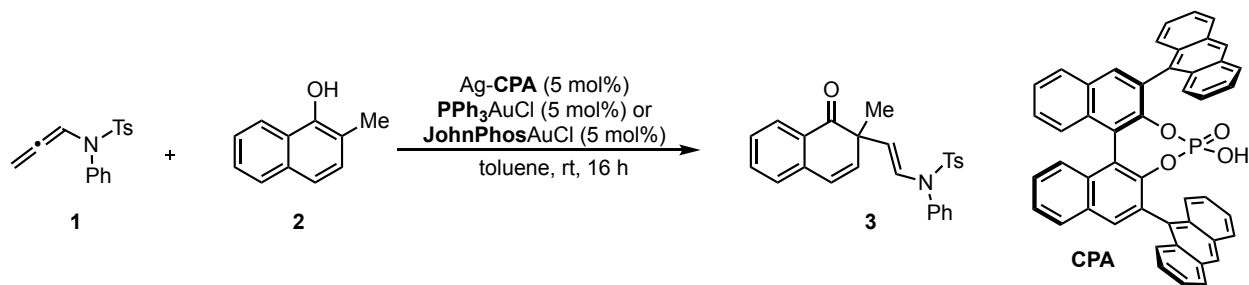
General procedure for synthesis of *rac*-3



Scheme S1. Synthesis of *rac*-3

Under N₂ atmosphere, an oven dried flask was charged with 1 mL of anhydrous toluene, the *N*-phenyl-*N*-sulfonylallenamide **1** (42.8 mg, 0.15 mmol, 1.5 eq), the naphthol **2** (15.8 mg, 0.1 mmol, 1.0 eq), and Diphenyl phosphate (2.5 mg, 0.01 mmol, 10 mol%) were added and the reaction was kept stirring at room temperature for 4 hours. Then, the reaction mixture was directly transferred into silica gel column chromatography (Petroleum ether:AcOEt = 10:1) to afford compound *rac*-**3**.

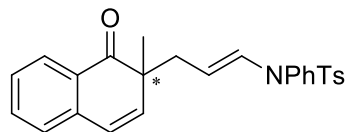
General procedure for enantioselective synergistic reactions



Scheme S2. Synthesis of **3** using the synergistic protocol.

Under N₂ atmosphere, an oven dried flask was charged with 1 mL of anhydrous toluene, PPh₃-AuCl (2.5 mg, 0.005 mmol, 5 mol%) or JohnPhos-AuCl (2.6 mg, 0.005 mmol, 5 mol%) and Ag-(R)-CPA (4.0 mg, 0.005 mmol, 5 mol%). After stirring for 15 min in the dark, the *N*-phenyl-*N*-sulfonylallenamide **1** (42.8 mg, 0.15 mmol, 1.5 eq) and the naphthol **2** (15.8 mg, 0.1 mmol, 1.0 eq) were added and the reaction was kept stirring at room temperature until **2** was completely consumed (TLC) (around 16 h). Then, the reaction mixture was directly transferred into silica gel column chromatography (Petroleum ether:AcOEt = 10:1) to afford the desired compound **3**.

Characterization data



Orange oil. 30.0 mg, 68% yield. $[\alpha]_D^{23} = -15.8$ ($c = 0.1$, CH_2Cl_2)

HPLC: 76% ee (Daicel Chiralpak AD-H, hexane/*i*-PrOH = 90:10, flow rate 1.0 mL/min, $\lambda = 254$ nm): minor isomer: $t_R = 18.8$ min; major isomer: $t_R = 21.9$ min.

^1H NMR (400 MHz, CDCl_3) δ 7.80 (d, $J = 7.7$ Hz, 1H), 7.52 (td, $J = 7.5, 1.2$ Hz, 1H), 7.44 (d, $J = 8.3$ Hz, 2H), 7.34 – 7.15 (m, 5H), 7.13 – 7.00 (m, 3H), 6.86 (d, $J = 13.9$ Hz, 1H), 6.45 (d, $J = 9.8$ Hz, 1H), 6.36 (d, $J = 7.4$ Hz, 2H), 5.92 (d, $J = 9.8$ Hz, 1H), 4.02 (m, 1H), 2.55 – 2.43 (m, 1H), 2.48 (s, 3H), 2.16 (m, 1H), 1.22 (s, 3H).

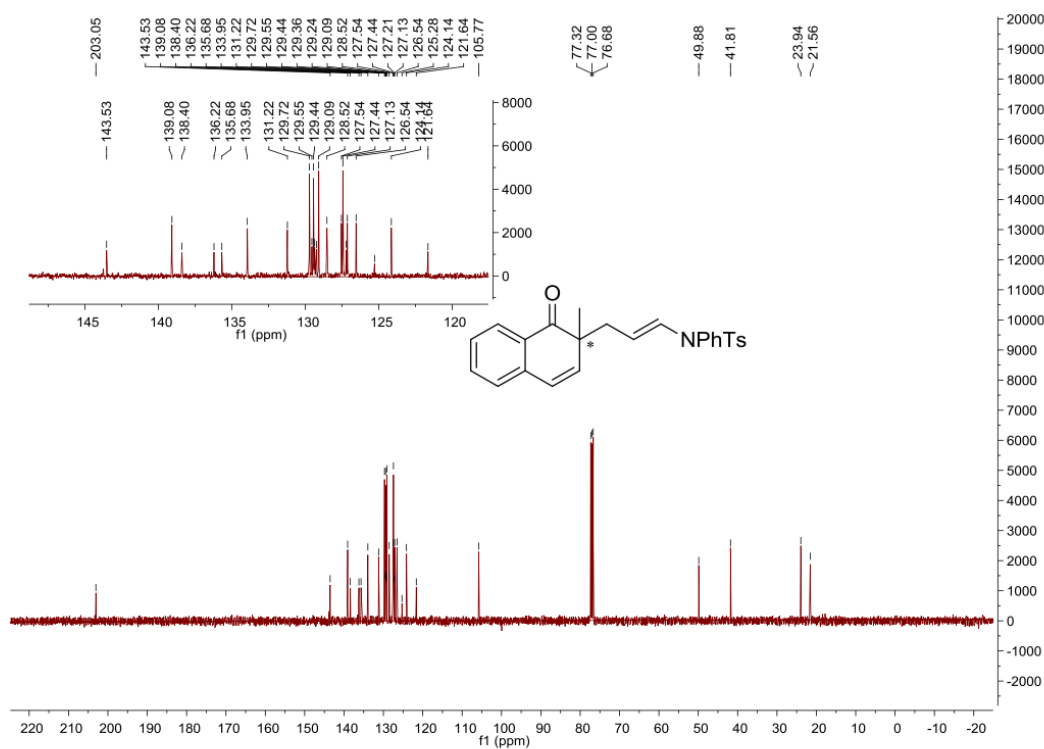
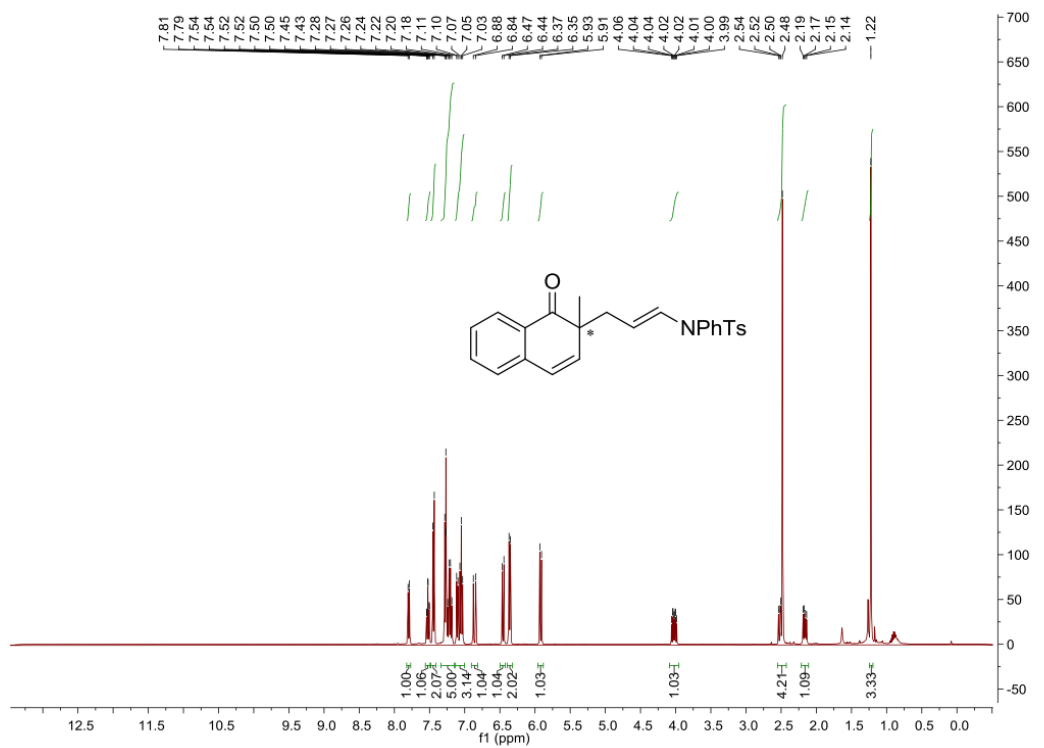
^{13}C NMR (101 MHz, CDCl_3) δ 203.05, 143.53, 139.08, 138.40, 136.22, 135.68, 133.95, 131.22, 129.72, 129.55, 129.44, 129.36, 129.24, 129.09, 128.52, 127.54, 127.44, 127.21, 127.13, 126.54, 125.28, 124.14, 121.64, 105.77, 49.88, 41.81, 23.94, 21.56.

IR (neat) 3067, 3029, 2969, 2930, 1671, 1654, 1597, 1490, 1359, 1306, 1269, 1165, 1116, 1090, 1025, 946, 906 cm^{-1}

HRMS (ESI) m/z $[\text{M}+\text{Na}]^+$ ($\text{C}_{27}\text{H}_{25}\text{NO}_3\text{SNa}$), calcd.: 466.1453; found: 466.1449.

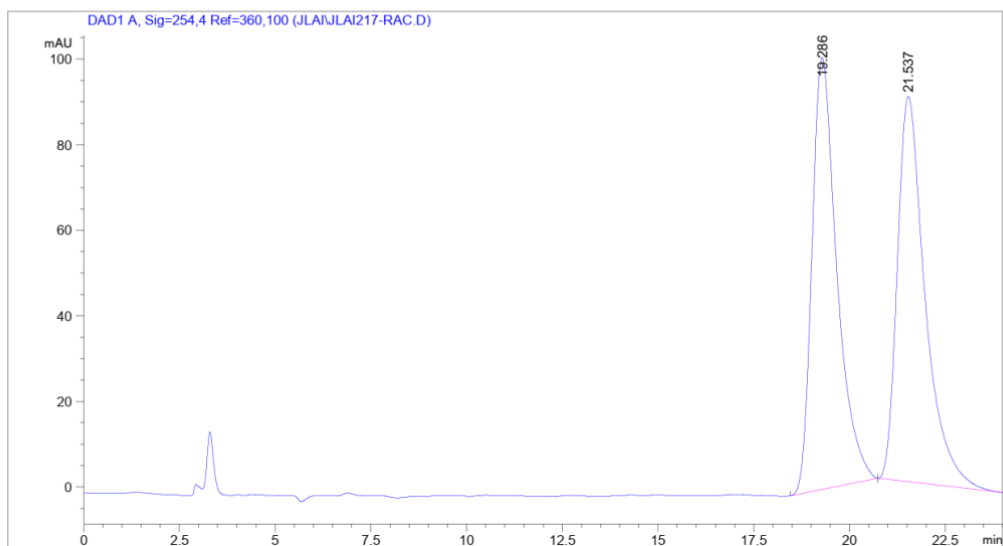
NMR spectra

NMR of 3



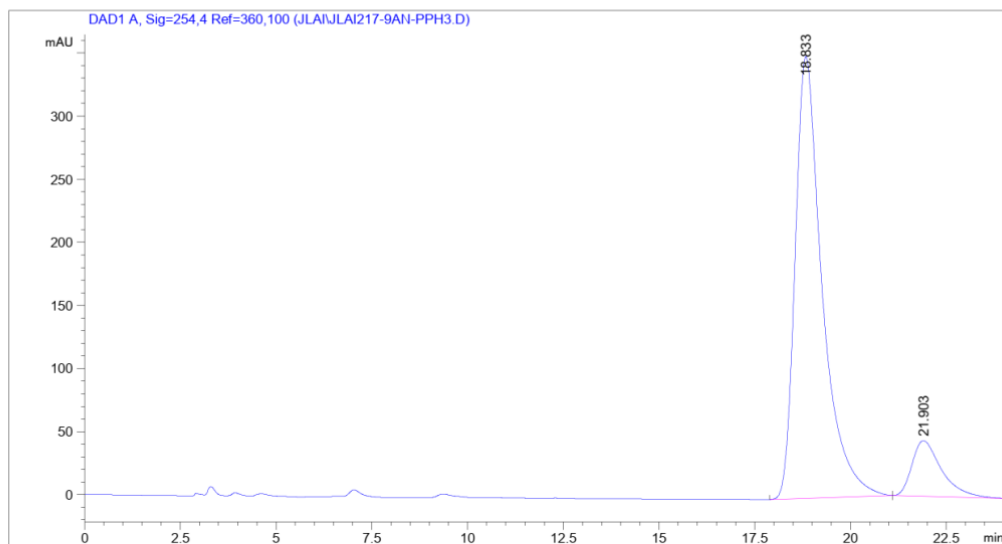
HPLC chromatograms

HPLC of *rac* 3



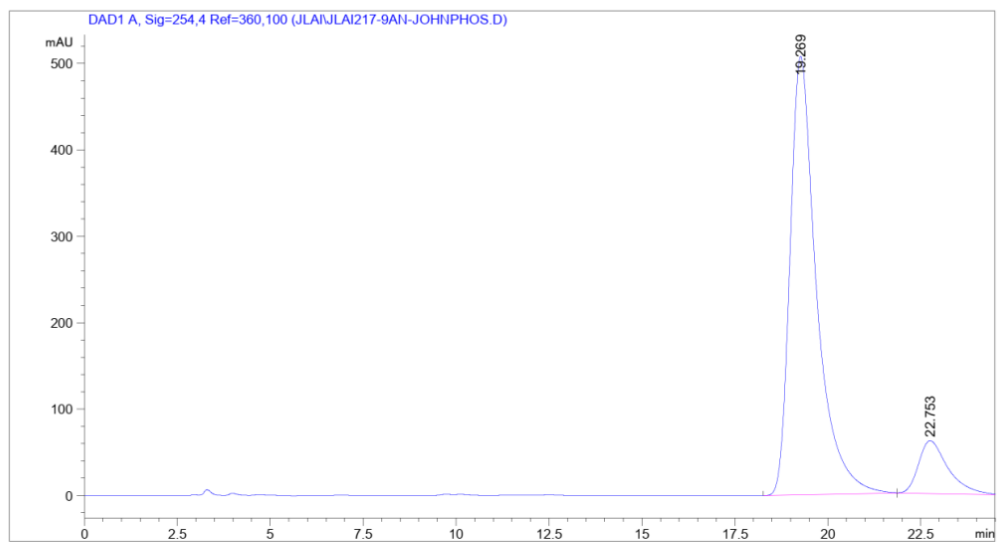
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.286	BB	0.6773	4562.80615	100.95540	50.1561
2	21.537	BB	0.7496	4534.41309	90.02364	49.8439

HPLC of **3** (from reaction catalyzed by CPA-Ag and PPh₃-AuCl)



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.833	BB	0.7254	1.71448e4	350.08804	87.8554
2	21.903	BB	0.8038	2370.00391	44.04052	12.1446

HPLC of 3 (from reaction catalyzed by CPA-Ag and JohnPhos-AuCl)



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.269	BB	0.7339	2.51391e4	507.49442	88.0991
2	22.753	BB	0.8271	3395.90894	61.22491	11.9009

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