Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Cartesian Coordinates (Å) and Energies (hartrees) for each Structure Optimized at the MCSCF(10,10)/cc-pVDZ Level

3-aza-benzvalene

Energy = −246.7154663140

Atom	X	Y	Z
C	-0.1815994766	-1.0485834775	0.0000613526
N	1.2346014003	-0.7167493816	-0.0000593858
C	1.2465782656	0.5407334927	-0.0001080355
C	-0.1503141451	1.0898872167	-0.0000264795
C	-1.0027650956	0.0266487648	-0.7399015920
C	-1.0026501406	0.0267149615	0.7400720917
H	-1.7641297465	0.0558601576	1.5017567301
H	-1.7643609125	0.0557961657	-1.5014695006
H	-0.4130168259	2.1378767017	-0.0000734290
H	2.1588363652	1.1248172012	-0.0001979232
H	-0.4696806882	-2.0885128026	0.0001421712

pyridine

Energy = −246.8335888420

Atom	X	Y	Z
C	-0.0104074848	-0.2982167003	-0.3694931026
C	-1.4163588156	-0.3615808957	-0.3910895238
N	-2.2014649621	0.6671736738	-0.2454980380
C	-1.6413575875	1.8733056397	-0.0622793872
C	-0.2532223107	2.0830697750	-0.0175317348
C	0.5959336354	0.9523875753	-0.1772521803
H	1.6725491428	1.0537902955	-0.1516232660
H	0.1480091135	3.0753596723	0.1332961260
H	-2.3250149953	2.7039883469	0.0537419859
H	0.5781207527	-1.1956585616	-0.4978468357
H	-1.9019250584	-1.3204795210	-0.5373228535

zezA

Energy = −246.6768613502

Atom	X	Y	Z
C	-0.1129303000	-1.2675036200	-0.3758114900
C	1.2051253300	-0.7347731000	0.0883987500
N	1.2626760000	0.5311181500	0.1107546100
C	0.0620713500	1.2733526200	-0.1518735300
C	-1.2228401900	0.7648659900	-0.0686515100
C	-1.1391999700	-0.6795949900	0.4010464000
H	-1.0844870800	-0.7937060000	1.4832979400
H	-2.0934307600	1.4054759700	-0.1129410700
H	-0.2282171800	-1.0840609100	-1.4457099400
H	2.1006922700	-1.3083677300	0.3047110700

zzeB			
Energy = −246.6763884978			
Atom	X	Y	Z
C	-0.1513292936	-1.1761728072	-0.3867517310
N	1.1813388529	-0.8954897085	0.0593319305
C	1.2519052092	0.3718339281	0.0722962284
C	0.0770982659	1.2972581348	-0.1647193077
C	-1.2210774734	0.8387665372	-0.0196876909
C	-1.1690517935	-0.6252106259	0.4195997298
H	-1.0514333953	-0.7426804568	1.4959027247
H	-2.0774765567	1.5015941075	-0.0160719934
H	0.2904752738	2.3467658139	-0.3295923050
H	-0.2595201724	-1.0601839536	-1.4636118768
H	2.2090295630	0.8344234303	0.3020734212

TSconA			
Energy = −246.6328210294			
Atom	X	Y	Z
C	-0.2346523702	-1.0716255906	-0.3757380427
C	1.1791242764	-0.6734460632	-0.0769009364
N	1.3162538330	0.5502888740	0.1982537691
C	0.0905920184	1.2719604498	0.0030489791
C	-1.0924425451	0.5502637975	-0.3043193750
C	-1.2153067274	-0.6932541080	0.6055527812
H	-0.8403935632	-0.5823023802	1.6200573995
H	-1.8989207677	0.9306522643	-0.9182717984
H	0.1778186777	2.3477116879	-0.0367349692
H	-0.5177965213	-1.4103674503	-1.3654123197
H	2.0374456894	-1.3344604811	-0.1190214876

TSconB			
Energy = −246.6452685022			
Atom	X	Y	Z
C	-0.2734587109	-0.9990864809	-0.3731431328
N	1.1255394845	-0.8320170808	-0.1333042187
C	1.2865016505	0.3909623799	0.1445476894
C	0.1090612527	1.3092204986	0.0437596241
C	-1.0779681665	0.6070080412	-0.2957685349
C	-1.2040275040	-0.6206954083	0.6470062665
H	-0.7866437149	-0.5081962076	1.6452418830
H	-1.8760105482	0.9660784507	-0.9308264945
H	0.2373520157	2.3820694248	-0.0070021957
H	-0.5824764461	-1.3985436818	-1.3296066366
H	2.2774006871	0.7751130642	0.3671067502

TSdisA			
Energy = −246.6447218545			
Atom	X	Y	Z
C	-0.0601591154	0.0520933818	0.0477439938
C	-1.4487893971	-0.2936068589	-0.3816099154
N	-2.2747988310	0.6722170289	-0.4498371110
C	-1.6475572304	1.8294360034	-0.0463647154
C	-0.1849264621	1.6054566074	0.3079429607
C	0.6649456344	1.0659617544	-0.8102824022
H	1.7393403373	1.1583960158	-0.8833271894
H	0.2688402873	2.1181107966	1.1469636519
H	-2.1531740009	2.7798624530	-0.0776577733
H	0.5067277709	-0.6304264154	0.6683846702
H	-1.7531929030	-1.3048614671	-0.6235520800

TSdisB			
Energy = −246.6426425495			
Atom	X	Y	Z
C	-0.1183253070	0.0850642067	0.0099609871
N	-1.4115957513	-0.3399738733	-0.4616945934
C	-2.1974039746	0.6550065245	-0.4848330707
C	-1.6315549586	1.9109504346	-0.0351085177
C	-0.1877402413	1.6310778120	0.3217005382
C	0.6467657979	1.0834016595	-0.8191197192
H	1.7227520706	1.1555119018	-0.8944422201
H	0.2818712352	2.1124984815	1.1700222916
H	-2.1242836828	2.8691978729	-0.0023981197
H	0.4200819489	-0.6274624280	0.6202771154
H	-3.2168182170	0.5473347278	-0.8379115814

TSzezA			
Energy = −246.6706773249			
Atom	X	Y	Z
C	-0.0692462335	-1.3266258734	-0.3813242590
C	1.2127430941	-0.6931232529	0.0540183847
N	1.2679566142	0.5664322872	0.1140161981
C	0.0636289618	1.2963340768	-0.1209689959
C	-1.2046625349	0.7638581508	-0.0087071510
C	-1.2346799939	-0.7017643536	0.3006909782
H	-1.5505173612	-1.0178433519	1.2901571545
H	-2.0746426673	1.4074128126	0.0036656469
H	0.2147640988	2.3548922838	-0.2774702487
H	-0.1608152673	-1.3351353987	-1.4692435678
H	2.1151766092	-1.2633931209	0.2560077700

TSzzeB			
Energy = −246.6717885260			
Atom	X	Y	Z
C	-0.1192479296	-1.2620387537	-0.3938771669
N	1.1832639594	-0.8632400157	0.0536171946
C	1.2500759924	0.3974498933	0.0485611688
C	0.0767507208	1.3040475444	-0.1762114005
C	-1.2055656087	0.8259703167	0.0463793931
C	-1.2438878449	-0.6351495777	0.3407428657
H	-1.5603964660	-0.9675303992	1.3233503800
H	-2.0488396629	1.4962991013	0.1579861234
H	0.2644455981	2.3608906226	-0.3158983279
H	-0.2107573458	-1.1938954830	-1.4778493525
H	2.1996006972	0.8684764008	0.2936438322

3,4-diaza-benzvalene			
Energy = −262.687219999			
Atom	X	Y	Z
C	-0.1148126595	0.0632534895	0.0597705138
N	-1.4875720542	-0.3403444293	-0.2411117579
N	-2.1236388163	0.6679480140	-0.4775395562
C	-1.2137085943	1.8051824872	-0.3487699961
C	-0.1536329494	1.4553400161	0.7040026765
C	0.1959405537	1.3383295681	-0.7353468002
H	0.9907703450	1.6903747723	-1.3704493716
H	0.2765283987	1.9295671971	1.5695095627
H	-1.5901106880	2.8006621626	-0.5210249173
H	0.6144284093	-0.6941103688	0.2983778147

pyridazine			
Energy = −262.787905644			
Atom	X	Y	Z
C	-0.0772849181	-0.2507687104	-0.3534786991
N	-1.4048860034	-0.3583077971	-0.3880878683
N	-2.1507893894	0.6704835455	-0.2142075934
C	-1.6154340895	1.8707444042	0.0050045037
C	-0.2258199219	2.0978602766	0.0615157362
C	0.5931531002	0.9682764270	-0.1293280449
H	1.6724016273	1.0184056361	-0.1077776185
H	0.1735572743	3.0857349313	0.2414160047
H	-2.3245900813	2.6749852748	0.1394459894
H	0.4647897667	-1.1722951715	-0.5106940380

TSconA′

Energy = −262.597450819

Atom	X	Y	Z
C	0.0330564603	0.0812747518	-0.0269456376
N	1.4141502674	0.2142561328	0.3474318209
N	1.6637519821	1.3857828896	0.5968088608
C	0.5819673295	2.3258854663	0.3493887801
C	-0.6642151940	1.8051171407	-0.0391244397
H	-0.6219314367	0.6750689680	1.8980665430
H	-1.3759436376	2.2777318311	-0.7030933605
H	0.8891648570	3.3598351908	0.3191988273
H	-0.1626688172	-0.2396146717	-1.0416751866

TSdisA′

Energy = −262.606104319

Atom	X	Y	Z
C	-0.1090163887	0.0892316296	0.0839662507
N	-1.4228523455	-0.2879911748	-0.3984456464
N	-2.2032176208	0.6669442892	-0.4384675361
C	-1.6262308911	1.8402669547	0.0039891207
C	-0.1832266341	1.6258382729	0.3805012813
C	0.6581538950	1.0776100881	-0.7494735277
H	1.7341965081	1.1381629599	-0.8216787669
H	0.2594733901	2.1266412435	1.2308784613
H	-2.1949914858	2.7535289654	0.0345692655
H	0.3966917429	-0.6541908986	0.6834184278

zezA′

Energy = −262.627070911

Atom	X	Y	Z
C	0.1430786560	-0.0707148007	-0.0263765456
N	1.4318356946	0.1758169949	0.5655010731
N	1.6435574545	1.3848878792	0.5155660270
C	0.5771938334	2.2964546491	0.1092729844
C	-0.7734257745	2.0029974134	0.2099325569
C	-0.9115879305	0.5662920445	0.6703237584
H	-0.9944828520	0.4220202363	1.7448732713
H	-1.5334129036	2.7738246327	0.1855215333
H	0.9450449115	3.2957076355	-0.0732366433
H	0.1785356574	0.1105577725	-1.0984065700

TSezA′			
Energy = −262.624575354			
Atom	X	Y	Z
C	0.1430786560	-0.0707148007	-0.0263765456
N	1.4318356946	0.1758169949	0.5655010731
N	1.6435574545	1.3848878792	0.5155660270
C	0.5771938334	2.2964546491	0.1092729844
C	-0.7734257745	2.0029974134	0.2099325569
C	-0.9115879305	0.5662920445	0.6703237584
H	-0.9944828520	0.4220202363	1.7448732713
H	-1.5334129036	2.7738246327	0.1855215333
H	0.9450449115	3.2957076355	-0.0732366433
H	0.1785356574	0.1105577725	-1.0984065700