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

Supporting Information for The Potential Energy Profile of the Decomposition of 1,1-Diamino-2,2-dinitroethylene (FOX-7) in Gas Phase

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Zero-point energy (a.u.), CCSD(T)-F12A potential energy (a.u.), optimized Cartesian coordinates (Å), and vibrational frequencies (cm^{-1}) of reactant, intermediates, transition states, and dissociation products.

FOX-7 Zero-Point Energy = 0.094733 CCSD(T)-F12A Energy = -597.74618012

O	0.54588632	1.17512751	-1.91710417	120.559	125.150	157.704
O	0.25878714	-2.25689714	-0.25357730	245.247	308.349	327.887
O	-0.25878714	2.25689714	-0.25357730	349.527	399.773	411.416
O	-0.54588632	-1.17512751	-1.91710417	488.100	493.673	495.904
N	0.09308473	1.21038014	-0.80332538	612.069	631.605	708.446
N	-0.09308473	-1.21038014	-0.80332538	725.512	809.565	819.372
N	0.12919683	-1.13099884	2.06383942	843.877	911.564	1079.356
N	-0.12919683	1.13099884	2.06383942	1097.685	1192.128	1245.464
C	0.00000000	0.00000000	-0.04895720	1350.218	1413.014	1493.570
C	0.00000000	0.00000000	1.36259797	1570.767	1638.355	1643.050
H	0.25899197	-1.99371704	1.55509765	1655.383	1713.284	3540.375
H	-0.06294309	-1.12854072	3.04887811	3544.051	3719.321	3721.336
H	0.06294309	1.12854072	3.04887811			
H	-0.25899197	1.99371704	1.55509765			

CO Zero-Point Energy = 0.005191 CCSD(T)-F12A Energy = -113.20498260

O	0.00000000	0.00000000	-0.47207219	2279.457
C	0.00000000	0.00000000	0.64808832	

CO2 Zero-Point Energy = 0.011987 CCSD(T)-F12A Energy = -188.41460910

O	0.00000000	0.00000000	-1.15459649	698.852	698.852	1414.713
C	0.00000000	0.00000000	0.00000000	2451.652		
O	0.00000000	0.00000000	1.15459649			

H Zero-Point Energy = 0.000000 CCSD(T)-F12A Energy = -0.49994621

H2 Zero-Point Energy = 0.010170 CCSD(T)-F12A Energy = -1.17478637

H	0.00000000	0.00000000	0.36951364	4466.072
H	0.00000000	0.00000000	-0.36951364	

NH2 Zero-Point Energy = 0.019245 CCSD(T)-F12A Energy = -55.82009135

N	0.00000000	0.00000000	0.20514761	1538.159	3412.754	3500.652
H	0.80299563	0.00000000	-0.43100341			
H	-0.80299563	0.00000000	-0.43100341			

NO Zero-Point Energy = 0.004731 CCSD(T)-F12A Energy = -129.77457252

N	0.00000000	0.00000000	0.60599794	2077.646
O	-0.00000000	-0.00000000	-0.52999794	

NO2 Zero-Point Energy = 0.009262 CCSD(T)-F12A Energy = -204.89571231

O	-1.08963531	0.00000000	0.13355284	794.291	1475.156	1797.978
N	0.00000000	0.00000000	-0.31788450			
O	1.08963531	0.00000000	0.13355284			

OH Zero-Point Energy = 0.008511 CCSD(T)-F12A Energy = -75.67408705

O	0.00000000	0.00000000	-0.09133811	3737.613
H	0.00000000	0.00000000	0.88307248	

I1 Zero-Point Energy = 0.092903 CCSD(T)-F12A Energy = -597.75132403

O	2.10936810	-0.62695472	0.25155898	98.098	132.414	157.792
O	-0.51623642	-3.08323802	-0.21890580	187.973	270.326	280.453
O	1.82893409	1.46750927	-0.17864052	368.643	398.174	429.195
N	-0.28227549	-2.02095414	-0.57091241	444.024	463.829	469.767
N	1.39537438	0.34167809	0.08760674	513.634	541.738	623.702
O	-0.41334518	-1.07873998	0.56137322	661.344	703.578	718.299

N	-2.23220522	0.89255463	0.25860014	807.400	842.464	943.865
N	-0.62955806	2.42280578	-0.37475642	1082.189	1113.977	1232.233
C	0.00323486	0.15970865	0.19335424	1339.988	1377.366	1493.963
C	-0.92162497	1.16813385	0.01340124	1593.686	1635.181	1652.445
H	-2.46367059	-0.06653325	0.45301465	1709.747	1915.959	3546.772
H	-2.92405188	1.42799847	-0.23676078	3620.685	3703.016	3725.141
H	-1.29139838	3.14849370	-0.16205131			
H	0.35421841	2.64917941	-0.42264337			

I2 Zero-Point Energy = 0.092929 CCSD(T)-F12A Energy = -597.75295273

O	1.50983102	-1.57016305	0.46439581	128.486	152.044	165.483
O	-0.91089031	-1.74158230	-1.14747141	174.003	264.892	289.413
O	2.17400021	0.36306464	-0.22206069	364.639	389.515	412.623
N	-1.39923454	-1.83418915	-0.12072822	417.490	464.758	499.112
N	1.29852716	-0.40631115	0.19023143	509.025	547.907	605.127
O	-0.92597482	-0.77753229	0.85352020	671.069	679.251	721.519
N	-1.67331492	1.74324146	0.30527086	819.936	866.785	950.280
N	0.40623027	2.29987071	-0.51728009	1079.362	1105.450	1233.513
C	-0.01501602	0.07777274	0.34201330	1320.886	1390.548	1498.977
C	-0.39618162	1.37105115	0.02831966	1589.294	1639.254	1652.449
H	-2.29496172	1.02532399	0.63616734	1698.411	1907.804	3543.656
H	-2.08013640	2.49084952	-0.22869929	3621.837	3706.520	3729.422
H	0.15144736	3.26717128	-0.42401678			
H	1.38037878	2.04393240	-0.60326069			

I3 Zero-Point Energy = 0.095104 CCSD(T)-F12A Energy = -597.73664445

O	1.97791378	1.06091645	-0.36825887	115.992	134.555	146.396
O	-2.11603342	-0.32795937	0.24286398	201.537	221.272	247.888
O	0.14367647	1.05792350	-1.50121462	390.968	400.250	424.832
O	-1.36438462	1.49106205	1.11996456	467.505	534.079	588.299

N	0.82764801	0.77479654	-0.54723801	634.351	659.482	749.509
N	-1.24121660	0.39891558	0.63279585	836.314	870.853	909.200
N	0.07211168	-1.86033742	-1.15531223	955.865	996.481	1023.195
N	0.59055306	-2.30841084	1.12888432	1131.702	1165.439	1293.330
C	0.18839134	-0.08671325	0.51334844	1311.038	1435.982	1459.266
C	0.27978417	-1.55788016	0.15850344	1509.809	1649.940	1742.549
H	-0.46420457	-1.21591482	-1.71611869	1743.218	1784.616	3227.411
H	-0.04011879	-2.83259617	-1.38966099	3511.653	3593.387	3697.641
H	0.61091106	-3.29180057	0.86533918			
H	0.68315249	0.11239727	1.45511991			

I4 Zero-Point Energy = 0.082714 CCSD(T)-F12A Energy = -467.97009029

O	-0.49324060	-2.35089318	0.00011226	96.548	105.563	201.249
H	1.94067348	2.18705638	-0.00243442	303.289	327.911	355.848
O	1.39654284	-1.31527038	0.00022515	392.861	423.100	451.839
H	2.03556221	0.42648741	-0.00084853	572.966	610.578	660.610
N	0.15825546	-1.34040797	0.00012728	683.239	706.116	752.302
O	-1.80489277	-0.06778593	-0.00022919	893.729	1026.176	1072.598
N	-0.59905175	2.25495185	0.00067823	1123.421	1336.852	1480.248
N	1.50037187	1.28483605	-0.00045912	1513.365	1623.876	1642.888
C	-0.57279061	-0.07003045	0.00001331	1693.357	1697.965	3520.765
C	0.17545245	1.16538529	-0.00004744	3595.834	3715.035	3744.391
H	-1.59518411	2.09650434	-0.00107192			
H	-0.22528792	3.18519724	-0.00147775			

I5 Zero-Point Energy = 0.077667 CCSD(T)-F12A Energy = -392.76681364

H	0.47434202	3.11657971	-0.00534432	82.413	168.177	252.810
O	-1.08669066	-1.37836420	-0.07772176	286.062	417.285	439.758
H	-1.66810170	2.22443787	-0.24171308	562.326	602.330	624.477
O	0.85660676	-2.27813841	0.19528774	688.859	787.297	798.974

H	1.82279117	-0.08028495	0.25132516	858.741	963.747	1085.048
N	0.12715784	-1.31204752	0.07785905	1103.982	1157.952	1336.294
N	-1.24664664	1.32400523	-0.10976983	1409.113	1452.383	1545.704
N	0.94618588	2.21626895	0.07361623	1651.825	1661.117	3309.049
C	0.75562661	-0.04340824	0.12672334	3497.138	3612.103	3753.263
C	0.10007516	1.23516973	0.01817022			
H	-1.79613115	0.48710281	-0.20113416			

I6 Zero-Point Energy = 0.078527 CCSD(T)-F12A Energy = -392.72909976

H	-0.47855888	2.66686273	0.01637907	149.235	190.973	278.234
O	-1.60202645	-0.76282589	0.23482565	293.868	386.642	408.055
H	2.62147248	1.02364113	-0.10071296	458.762	504.611	590.213
O	-0.31394068	-2.29712131	-0.57123795	679.109	711.323	763.226
H	1.87049563	2.55608834	0.01957596	822.317	943.258	1071.800
N	-0.48392492	-1.20977663	-0.05869741	1084.159	1205.290	1383.479
N	-0.48968064	1.68436604	0.22308958	1494.059	1555.796	1601.940
N	1.78249387	1.57302520	-0.17027035	1634.722	1671.579	3535.861
C	0.63252296	-0.44219408	0.25433438	3620.115	3714.275	3733.032
C	0.61454605	0.93878462	0.09117356			
H	-1.36280761	1.18170178	0.31571446			

I7 Zero-Point Energy = 0.064093 CCSD(T)-F12A Energy = -541.73896046

O	0.23386076	1.52329117	-1.64302362	105.932	128.944	224.990
O	0.08121519	-2.15223714	-0.02046313	244.719	281.877	375.519
O	-0.09854938	2.32241579	0.32646862	413.772	446.393	488.873
O	-0.30007326	-1.06935098	-1.83984296	496.006	618.688	644.633
N	0.03961768	1.40635087	-0.46330795	782.110	809.073	823.364
N	-0.07319742	-1.11737440	-0.66489962	915.143	1103.897	1191.808
N	0.07275141	-0.90580422	2.39094603	1318.120	1393.297	1437.412
H	0.02078168	-0.65458503	3.36507324	1570.603	1663.076	1724.853

C	-0.00314954	0.08461716	0.12776313	1772.198	3505.820	3665.953
C	0.02482218	0.00193654	1.46660749			
H	0.14649943	-1.88010243	2.11487294			

I11 Zero-Point Energy = 0.074628 CCSD(T)-F12A Energy = -338.24286965

H	0.00000000	-1.93376657	0.59648433	129.564	289.827	378.403
H	0.00000000	1.33303015	2.26059706	417.265	507.472	551.728
O	0.00000000	1.14044662	-1.35318216	604.985	606.459	749.783
H	0.00000000	1.93376657	0.59648433	802.637	813.892	841.872
H	0.00000000	-1.33303015	2.26059706	1057.478	1132.719	1343.009
O	0.00000000	-1.14044662	-1.35318216	1438.006	1509.275	1619.064
N	0.00000000	-1.16917614	1.26838744	1769.311	1872.660	3478.213
N	0.00000000	1.16917614	1.26838744	3490.346	3683.519	3686.093
C	0.00000000	0.00000000	-0.89838233			
C	0.00000000	0.00000000	0.69030028			

I12 Zero-Point Energy = 0.071650 CCSD(T)-F12A Energy = -338.22253947

H	-1.98094197	1.99803631	0.00000000	68.364	76.055	140.684
H	1.47715957	2.33433886	0.00000000	146.297	210.550	463.018
O	1.13747694	-1.59429340	0.00000000	527.532	539.132	637.892
H	1.77957741	0.63878460	0.00000000	659.178	697.348	776.967
H	-0.66926188	3.10342241	0.00000000	1062.338	1144.098	1321.350
O	-1.13275707	-2.02009555	0.00000000	1403.289	1461.893	1649.643
N	-0.98840509	2.13915271	0.00000000	1671.815	2438.546	3474.301
N	1.10962678	1.38754024	0.00000000	3489.440	3690.054	3715.795
C	-0.01113719	-1.75307674	0.00000000			
C	-0.18334702	1.07751361	0.00000000			

I13 Zero-Point Energy = 0.058062 CCSD(T)-F12A Energy = -149.79960686

H	2.00122548	0.00000000	-0.37406471	445.443	490.525	540.315

H	-1.12430632	0.00000000	1.10002003	623.904	770.585	1061.357
N	-1.10924991	0.00000000	0.08310862	1143.329	1303.188	1439.587
H	-2.00122548	0.00000000	-0.37406471	1644.673	1674.597	3457.089
H	1.12430632	0.00000000	1.10002003	3470.168	3714.894	3718.564
C	0.00000000	0.00000000	-0.65795602			
N	1.10924991	0.00000000	0.08310862			

I14 Zero-Point Energy = 0.033156 CCSD(T)-F12A Energy = -148.61284001

H	-0.54061195	1.77431493	-0.51274096	560.849	578.015	749.745
C	0.00000000	0.00000000	-0.00886153	916.824	919.784	1320.394
N	-0.05698614	-1.21172625	0.07702921	2256.220	3623.470	3635.528
H	0.54061195	-1.77431493	-0.51274096			
N	0.05698614	1.21172625	0.07702921			

I15 Zero-Point Energy = 0.032452 CCSD(T)-F12A Energy = -148.47277214

H	1.18070460	-0.78957987	0.56492167	517.915	911.402	931.537
C	0.00000000	0.00000000	-0.89581203	950.084	1149.391	1264.920
N	-0.73146035	-0.07070941	0.26513065	1480.120	3520.250	3525.911
H	-1.18070460	0.78957987	0.56492167			
N	0.73146035	0.07070941	0.26513065			

I16 Zero-Point Energy = 0.044791 CCSD(T)-F12A Energy = -149.17054583

H	-0.30390860	2.05493784	0.09146615	301.694	450.682	509.768
H	1.05925161	-1.29342158	-0.24658442	686.197	994.945	1116.598
N	0.09359684	-1.13476406	0.00609230	1277.615	1619.959	1837.839
H	-0.54602156	-1.89933868	-0.09372642	3555.211	3584.269	3735.552
N	0.22452758	1.19772223	-0.00428665			
C	-0.38242910	0.11835326	0.05708362			

I17 Zero-Point Energy = 0.043994 CCSD(T)-F12A Energy = -149.15901756

H	1.04529648	1.45372824	0.07701226	318.617	427.405	483.831
H	1.08777139	-1.30315341	-0.12333225	667.489	890.289	1098.077
N	0.10269329	-1.13897180	0.03648390	1213.875	1623.119	1926.346
H	-0.51600418	-1.90645644	-0.15015280	3413.765	3545.138	3712.374
N	0.04211138	1.26692653	0.02536113			
C	-0.38419432	0.11576556	0.00141493			

I18 Zero-Point Energy = 0.016130 CCSD(T)-F12A Energy = -93.29163183

H	0.00000000	0.00000000	-1.42409970	555.045	555.045	2152.276
N	0.00000000	0.00000000	-0.42648466	3821.278		
C	0.00000000	0.00000000	0.73472086			

I21 Zero-Point Energy = 0.083252 CCSD(T)-F12A Energy = -467.95038340

O	-0.55895289	-2.30476784	0.00000000	94.460	113.860	264.318
H	1.95410958	2.25141074	0.00000000	297.962	331.027	348.556
O	1.38011405	-1.32831078	0.00000000	426.531	465.208	578.007
H	2.05890884	0.50297738	0.00000000	612.308	672.251	697.341
N	0.14226993	-1.31436312	0.00000000	741.534	802.019	826.616
O	-1.78754674	-0.06400597	0.00000000	873.069	1091.828	1114.518
N	-0.69979061	2.21008243	0.00000000	1173.455	1347.381	1416.681
N	1.51389163	1.34999413	0.00000000	1471.875	1579.805	1596.849
C	-0.48884209	-0.06001528	0.00000000	1645.911	1720.684	3363.833
C	0.17076256	1.26533756	0.00000000	3569.163	3586.891	3737.025
H	-2.01776763	0.90053116	0.00000000			
H	-0.30076495	3.14144690	0.00000000			

I22 Zero-Point Energy = 0.074754 CCSD(T)-F12A Energy = -338.25145815

O	1.22584118	-1.26410581	0.00000000	113.094	232.901	312.596
H	1.06183203	2.42711611	0.00000000	429.465	466.100	570.818
H	-1.43504690	2.11369800	0.00000000	581.750	626.758	767.149

H	1.91404650	0.90775167	0.00000000	833.325	840.201	869.373
H	-1.71917702	-0.82646028	0.00000000	1082.201	1148.472	1257.648
O	-0.99340565	-1.48121772	0.00000000	1406.149	1487.533	1618.620
N	-1.31459149	1.10544411	0.00000000	1767.963	1902.675	3544.127
N	1.05006447	1.42444217	0.00000000	3606.206	3612.269	3751.347
C	0.12823037	-0.78685426	0.00000000			
C	-0.09985391	0.72537381	0.00000000			

I23 Zero-Point Energy = 0.021531 CCSD(T)-F12A Energy = -188.92573256

O	-0.15952126	-1.17794212	0.00000000	556.953	652.744	1127.773
H	0.49992910	1.73841915	0.00000000	1281.108	1974.147	3862.791
O	-0.18905272	1.06556111	0.00000000			
C	0.38142622	-0.13986925	0.00000000			

I24 Zero-Point Energy = 0.021216 CCSD(T)-F12A Energy = -188.92281854

O	-0.19792445	-1.10871431	0.00000000	616.305	626.309	1132.545
H	-1.00727575	1.15687585	0.00000000	1319.127	1941.715	3681.120
O	-0.03392249	1.15152441	0.00000000			
C	0.39804129	-0.09552292	0.00000000			

I25 Zero-Point Energy = 0.083661 CCSD(T)-F12A Energy = -467.94525199

O	-0.41235181	-2.28032191	0.02798893	97.798	140.232	292.741
H	1.81562808	2.37895220	0.07556398	340.019	364.915	405.884
O	1.48503827	-1.21833744	0.14715139	439.771	465.504	527.121
H	2.02222478	0.66306779	0.04244998	630.083	667.660	685.077
N	0.25948581	-1.24213671	0.05501667	739.792	755.865	866.214
O	-1.75715417	-0.21087896	-0.09353616	870.745	1100.833	1120.645
N	-0.80158858	2.24214507	0.08861664	1157.479	1348.477	1377.357
N	1.43444479	1.46678035	-0.10225011	1451.569	1564.621	1608.384
C	-0.47272313	-0.04541573	-0.01953970	1634.749	1712.986	3513.917

C	0.08180849	1.32621425	0.00912176	3538.562	3596.156	3725.280
H	-1.89865436	-1.18275811	-0.07860215			
H	-0.37505520	3.16627776	0.09429457			

I26 Zero-Point Energy = 0.074653 CCSD(T)-F12A Energy = -338.24227307

O	1.20032774	1.22398454	0.04901060	93.989	294.701	347.611
H	1.05304071	-2.41955940	0.09922323	433.506	452.317	526.930
H	-1.35511034	-2.20539913	0.06328113	558.469	617.483	644.170
H	1.88788631	-0.90901122	0.04036797	823.952	837.372	909.452
H	-0.76053969	2.39508066	-0.05120169	1099.458	1144.540	1224.730
O	-1.01780061	1.46375344	-0.06354905	1361.226	1481.704	1620.087
N	-1.32790438	-1.18699942	0.06037318	1770.851	1858.927	3501.618
N	1.03809749	-1.43320518	-0.08531520	3614.895	3742.270	3824.175
C	0.09723692	0.74943612	-0.00346308			
C	-0.13978032	-0.75231824	0.00072898			

I27 Zero-Point Energy = 0.067606 CCSD(T)-F12A Energy = -262.97183914

C	0.07656230	-0.46347210	0.00000000	178.029	274.344	324.682
H	-0.07390480	-2.52789945	0.00000000	448.654	573.886	615.915
H	1.96791564	-0.94875241	0.00000000	669.519	812.895	821.730
H	-1.56332105	-1.63380629	0.00000000	1061.410	1076.748	1125.839
H	0.78248796	1.51020408	0.00000000	1403.951	1489.373	1499.884
O	-0.18988680	1.79261972	0.00000000	1615.485	1780.962	3002.982
N	1.31539367	-0.17364965	0.00000000	3564.153	3611.994	3737.292
N	-0.55691599	-1.64802186	0.00000000			
C	-0.91163382	0.74310595	0.00000000			

I28 Zero-Point Energy = 0.068054 CCSD(T)-F12A Energy = -263.00459387

C	0.00000000	0.00000000	0.40856317	171.928	192.912	258.278
H	0.83161188	1.79295119	1.00447112	332.780	460.058	590.419

H	0.83161188	-1.79295119	1.00447112	602.588	640.482	722.880
H	-0.83161188	1.79295119	1.00447112	837.169	1158.553	1226.063
H	-0.83161188	-1.79295119	1.00447112	1310.692	1374.797	1643.764
O	0.00000000	0.00000000	-2.07133405	1665.287	2217.803	3576.541
N	0.00000000	-1.23337250	1.11233341	3576.743	3660.764	3665.840
N	0.00000000	1.23337250	1.11233341			
C	0.00000000	0.00000000	-0.91194700			

I31 Zero-Point Energy = 0.082903 CCSD(T)-F12A Energy = -467.96536489

O	-0.46676769	-2.35630342	0.00000000	100.574	119.705	291.606
H	1.99507190	2.07700722	0.00000000	327.488	377.871	381.190
O	1.48520402	-1.34725923	0.00000000	440.458	478.633	521.666
H	1.79417932	-0.37733918	0.00000000	583.196	636.297	650.013
N	0.13326764	-1.29572384	0.00000000	767.371	786.795	826.026
O	-1.76090062	-0.03880782	0.00000000	874.327	1089.263	1122.326
N	-0.54656766	2.28877877	0.00000000	1171.794	1293.022	1461.412
N	1.53647589	1.17290225	0.00000000	1536.870	1612.593	1718.198
C	-0.55215879	-0.06905395	0.00000000	1760.253	1765.180	2800.375
C	0.25770256	1.21474094	0.00000000	3561.614	3609.852	3741.794
H	-1.54210459	2.13508893	0.00000000			
H	-0.17603130	3.22095034	0.00000000			

I32 Zero-Point Energy = 0.056013 CCSD(T)-F12A Energy = -262.38488244

C	-0.67005082	0.89936809	0.10062149	168.027	305.243	372.709
H	-0.48981462	-2.37280515	-0.15976770	465.006	486.947	604.545
H	1.75308826	0.31159612	0.00893333	646.893	831.680	912.403
H	1.74137758	-1.40405017	-0.10136789	1087.629	1130.690	1378.373
C	-0.11204954	-0.52247977	0.01640157	1622.531	1771.271	1989.000
O	-0.02186188	1.87539374	0.09659353	3499.136	3606.231	3720.220
N	1.25024689	-0.55367457	0.11373546			

N -0.94814521 -1.46434410 -0.09869039

I33 Zero-Point Energy = 0.021067 CCSD(T)-F12A Energy = -205.53183943

O	-0.22106955	1.06963313	0.00000000	593.320	707.988	913.935
N	0.48678715	0.15014492	0.00000000	1347.700	1846.555	3842.107
O	-0.23747189	-1.03481390	0.00000000			
H	0.44289415	-1.71901461	0.00000000			

I34 Zero-Point Energy = 0.065714 CCSD(T)-F12A Energy = -392.21299054

O	-0.45206936	-2.20189031	-0.45952387	101.959	139.873	248.447
H	-2.13007045	1.64243992	0.01237385	285.152	301.665	413.244
H	1.38154945	1.99198967	-0.29902869	465.271	516.337	563.051
H	-0.05342837	2.95981475	-0.37011534	601.323	709.882	888.589
N	-0.23187283	-1.52404297	0.48947677	940.634	1069.263	1101.839
O	1.69372296	-0.30267497	0.04579769	1155.965	1444.610	1624.688
N	0.38857996	2.08279173	-0.16407169	1753.418	1770.274	1891.227
N	-1.59922628	0.77899577	0.10801964	3511.474	3618.215	3742.590
C	0.50724628	-0.27812443	0.13801886			
C	-0.34609582	0.95819118	0.01763460			

I41 Zero-Point Energy = 0.068211 CCSD(T)-F12A Energy = -263.04757113

H	0.48109524	2.41749733	0.07482044	67.852	251.594	313.373
H	-1.77381857	-0.29880642	-0.05723218	484.643	530.068	593.959
H	-1.79649217	1.43785899	-0.02590482	638.239	901.338	918.531
O	-0.04357685	-1.82229932	-0.04805564	1052.044	1072.953	1153.944
H	1.74412836	-0.86977849	0.02526070	1374.037	1446.350	1614.017
C	0.07015111	0.55255268	0.02563529	1758.966	1861.539	3047.975
N	-1.28399967	0.57712123	0.01455609	3506.267	3617.821	3750.090
N	0.92024026	1.49853024	0.06017974			
C	0.64463524	-0.84208642	-0.00040980			

I42 Zero-Point Energy = 0.077414 CCSD(T)-F12A Energy = -392.82643468

H	-2.46427089	0.87789754	0.00000000	130.556	270.115	270.252
O	-0.59210938	-1.99621272	0.00000000	393.130	406.809	419.517
H	0.88931588	2.18742494	0.00000000	466.134	558.660	604.409
O	1.86459034	0.34730076	0.00000000	697.867	714.388	753.060
H	-0.78030404	2.75352122	0.00000000	772.930	951.182	1070.590
N	0.60476396	-1.56467139	0.00000000	1129.331	1250.546	1317.395
N	-1.65797329	0.27373848	0.00000000	1442.460	1479.527	1599.397
N	-0.10824303	2.00686609	0.00000000	1663.381	1749.842	3004.244
C	0.76262718	-0.20825188	0.00000000	3533.966	3637.822	3709.365
C	-0.43385593	0.73059182	0.00000000			
H	-1.66896348	-0.77093219	0.00000000			

I43 Zero-Point Energy = 0.078029 CCSD(T)-F12A Energy = -392.83124639

H	-2.40966985	0.91644371	0.00000000	95.350	252.988	308.323
O	-0.59913854	-2.02494809	0.00000000	347.010	403.363	451.603
H	0.86448381	2.27013795	0.00000000	480.594	569.777	597.449
O	1.85156337	0.32932908	0.00000000	705.118	756.613	785.975
H	-0.80403590	2.78875454	0.00000000	831.568	1037.747	1082.724
N	0.61967687	-1.54708756	0.00000000	1174.153	1235.046	1384.839
N	-1.64529997	0.24940692	0.00000000	1473.407	1606.502	1697.353
N	-0.11992811	2.05453585	0.00000000	1708.935	1762.645	2631.660
C	0.74149797	-0.17041093	0.00000000	3547.365	3602.119	3736.776
C	-0.47014220	0.76138062	0.00000000			
H	-1.27947821	-1.25391694	0.00000000			

I44 Zero-Point Energy = 0.073316 CCSD(T)-F12A Energy = -392.76291416

H	-2.00871605	1.99451443	-0.18236636	56.862	84.438	123.193
O	-1.46958248	-1.57448125	0.21243479	154.821	172.429	206.747

H	1.72640904	2.04437176	0.10124972	294.103	308.259	457.060
O	1.94352264	-1.02252891	0.12486684	484.292	597.815	657.927
H	0.53672497	3.24266303	-0.27007602	691.081	715.614	940.969
N	-0.24709225	-1.75244440	-0.40827823	977.552	1108.037	1247.830
N	-1.39536563	1.20549218	0.02440222	1440.955	1557.648	1620.214
N	0.75783416	2.30259750	0.02770213	1901.952	2335.513	3376.021
C	0.83333672	-1.33804845	-0.04486137	3436.433	3551.749	3697.853
C	-0.17103426	1.35778030	0.11625653			
H	-1.64760705	-0.60840978	0.13105230			

I45 Zero-Point Energy = 0.026874 CCSD(T)-F12A Energy = -243.59233356

N	0.51834164	-0.47977143	0.00000000	219.888	237.361	569.999
O	-0.35232513	-1.56767817	0.00000000	721.140	956.463	1335.318
H	0.25314776	-2.31417125	0.00000000	1537.157	2340.054	3884.511
O	-0.18671489	1.78472709	0.00000000			
C	0.07171649	0.65608289	0.00000000			

I46 Zero-Point Energy = 0.078151 CCSD(T)-F12A Energy = -392.81697394

H	-2.51091825	0.90540640	0.00000000	108.692	274.433	322.337
O	-0.44049693	-2.05089235	0.00000000	332.811	353.592	437.415
H	1.63626241	1.38471316	0.00000000	449.433	586.141	639.493
O	1.85026503	0.41760441	0.00000000	705.612	764.720	771.812
H	-0.83974151	2.68803730	0.00000000	830.446	860.171	1096.137
N	0.70441722	-1.50895963	0.00000000	1139.281	1247.955	1313.589
N	-1.71961546	0.28730840	0.00000000	1427.982	1533.405	1563.777
N	-0.08730298	2.00840663	0.00000000	1596.721	1753.564	3371.353
C	0.69225400	-0.17365725	0.00000000	3556.428	3565.802	3717.737
C	-0.47437346	0.78953544	0.00000000			
H	-1.83062423	-0.71564834	0.00000000			

I47 Zero-Point Energy = 0.072256 CCSD(T)-F12A Energy = -392.71920887

H	-1.44466808	3.04424423	0.00000000	54.830	81.526	124.831
O	-1.57263670	-1.97662177	0.00000000	131.220	244.833	292.050
H	1.78763025	0.20455139	0.00000000	303.717	359.053	419.548
O	1.90320432	-0.81232536	0.00000000	437.796	493.279	508.385
H	1.35665803	2.61047177	0.00000000	681.272	869.335	909.440
N	-0.38734668	-1.63682889	0.00000000	1008.158	1118.496	1260.482
N	-1.36801144	2.03644507	0.00000000	1412.545	1519.656	1618.850
N	1.01815658	1.64830768	0.00000000	1865.908	2587.226	2746.870
C	0.70971682	-1.30685723	0.00000000	3444.780	3548.146	3689.496
C	-0.20489560	1.41073215	0.00000000			
H	-2.21400622	1.49182199	0.00000000			

I48 Zero-Point Energy = 0.026121 CCSD(T)-F12A Energy = -243.53699879

N	0.01019065	-0.65428846	0.00000000	194.677	249.538	450.582
O	0.04081349	-1.86770590	0.00000000	528.679	925.978	1262.255
H	-0.68599090	2.27090290	0.00000000	1451.372	2574.826	3833.173
O	0.14114373	1.77496486	0.00000000			
C	-0.10578603	0.48731722	0.00000000			

I49 Zero-Point Energy = 0.062214 CCSD(T)-F12A Energy = -317.04412571

H	-1.19700151	2.60978370	-0.26738248	110.626	151.387	387.057
O	-0.00014571	-2.74720803	0.01960547	438.488	452.128	499.848
C	0.10051172	1.05029998	-0.02404650	574.527	618.156	682.256
H	-1.92946278	1.07228757	-0.34202542	728.666	870.782	1100.479
H	1.14525509	2.62878167	0.00193334	1125.224	1341.492	1513.240
N	0.02896457	-1.55262176	0.00866203	1637.937	1746.830	2495.475
N	-1.14764123	1.62988955	-0.04439635	3508.966	3611.886	3726.242
N	1.23401080	1.61431617	0.02090556			
C	0.05460621	-0.40185752	-0.00223089			

I50 Zero-Point Energy = 0.049076 CCSD(T)-F12A Energy = -336.86303991

H	-0.72340031	3.09962072	-0.38218360	148.890	187.528	455.936
O	-1.23283821	-0.77187896	0.05042391	509.578	558.450	589.306
C	0.15487146	1.46953742	0.14415436	793.071	808.569	864.836
O	0.57775460	-1.93115937	-0.10946815	902.644	1023.628	1150.071
H	1.83463300	0.19072132	-0.08099734	1398.860	1452.310	1674.744
N	-0.02639339	-0.88602948	-0.01659379	2194.437	3297.902	3541.408
C	0.77109927	0.31063806	0.01334460			
N	-0.37240618	2.52098977	0.37636978			

I51 Zero-Point Energy = 0.049198 CCSD(T)-F12A Energy = -336.82513802

O	-1.15306992	-1.66249469	0.04501765	146.504	168.220	246.009
C	-0.00000237	0.23412289	0.00509183	345.904	373.190	489.083
O	1.00300412	-1.74443191	-0.08589606	533.315	658.562	790.712
H	-0.73177017	3.27526940	0.24619075	895.464	1151.952	1321.881
N	-0.05365098	-1.15211844	-0.01381751	1484.508	1630.703	1649.063
C	0.05239753	1.43334063	0.01940417	2388.372	3612.814	3719.634
H	0.98418590	3.21570093	0.14767686			
N	0.09971577	2.75135775	0.03392584			

I52 Zero-Point Energy = 0.047225 CCSD(T)-F12A Energy = -336.82849099

O	-0.69541085	-0.77812653	-0.00591160	126.276	139.861	257.221
C	-0.35291946	0.47950937	-0.00423756	335.477	377.056	427.587
O	0.18710279	-2.76691974	0.00332680	486.886	494.317	588.513
H	0.15573643	3.44246434	-0.84202258	719.861	942.682	1201.948
N	0.52761834	-1.68350336	0.00704128	1386.839	1643.677	1931.948
C	-0.03673347	1.63641920	-0.00281091	2423.578	3586.123	3669.386
H	0.13960540	3.44492144	0.83475164			
N	0.36109807	2.92634671	-0.00082220			

I53 Zero-Point Energy = 0.048715 CCSD(T)-F12A Energy = -336.89592039

O	-0.65099187	2.02602163	0.00000000	168.968	218.152	279.637
C	-0.10989296	1.02521585	0.00000000	300.159	392.068	513.465
O	-1.54176751	-1.10512271	0.00000000	620.670	725.642	760.425
H	2.25549944	-0.71041331	0.82766082	826.985	1166.637	1233.396
N	-0.34968312	-1.30754377	0.00000000	1428.357	1618.766	1673.105
C	0.48706425	-0.18402866	0.00000000	2263.354	3561.490	3642.144
H	2.25549944	-0.71041331	-0.82766082			
N	1.88787578	-0.26324189	0.00000000			

I54 Zero-Point Energy = 0.038839 CCSD(T)-F12A Energy = -207.06453082

H	0.47827365	2.52430872	0.00552627	222.514	365.125	418.134
C	0.02964027	-0.73153774	-0.00173851	539.106	570.868	973.364
N	-0.13993787	1.73162321	0.00035909	1171.123	1616.228	1683.923
H	-1.12927820	1.92585014	-0.00114111	2244.252	3573.443	3678.478
O	-0.08055752	-1.90243488	0.00078555			
C	0.34952144	0.50615390	-0.00022522			

I55 Zero-Point Energy = 0.054816 CCSD(T)-F12A Energy = -412.00564029

O	-0.14521845	-2.13256545	-0.00765570	81.973	179.264	252.458
H	0.40251512	2.22097634	1.23784918	273.639	399.666	462.942
O	1.50806060	-0.74608384	0.06060900	556.345	603.460	822.598
C	0.05921076	1.34187607	-0.57377952	841.112	865.517	880.621
N	0.33520444	-1.04014530	-0.01898664	1085.414	1216.783	1474.792
O	-1.79326902	0.00657229	0.12071652	1621.607	1730.882	1741.403
N	0.46806332	2.25987850	0.22388198	1918.680	3472.567	3591.128
H	0.91090306	3.08898672	-0.14961007			
C	-0.64135990	0.18700383	-0.07935798			

I56 Zero-Point Energy = 0.055234 CCSD(T)-F12A Energy = -412.04610159

O	-1.62403752	-0.63818884	0.00000000	121.305	186.459	270.405
C	0.49878989	0.16786970	0.00000000	314.897	366.343	513.663
O	0.01611591	-2.04606248	0.00000000	562.936	593.517	700.498
H	2.23471477	-0.42789644	-0.83035860	750.353	794.314	892.348
N	-0.44111698	-0.92790837	0.00000000	1188.453	1236.026	1423.509
O	-0.51708456	2.42776904	0.00000000	1500.238	1670.846	1683.039
H	2.23471477	-0.42789644	0.83035860	2294.389	3557.164	3636.006
N	1.87475209	0.02153067	0.00000000			
C	-0.08256084	1.37399767	0.00000000			

I57 Zero-Point Energy = 0.044841 CCSD(T)-F12A Energy = -298.80246934

O	-0.13392419	-1.23903562	-0.64909629	155.565	379.795	424.858
C	-0.72384013	0.77032188	0.24336542	620.023	797.175	828.372
O	0.57918259	-0.74429097	1.33379731	845.949	934.342	1214.333
H	-0.25570163	2.59323307	-0.38571776	1455.565	1541.403	1678.690
N	-0.01371091	-0.50726232	0.30653690	1698.535	3477.938	3639.656
N	0.07719775	1.64777842	-0.26878592			
H	1.03133013	1.46461446	-0.57036229			

I58 Zero-Point Energy = 0.026740 CCSD(T)-F12A Energy = -93.81676744

H	0.00000000	0.85674916	0.99535955	765.372	1062.162	1461.534
C	0.00000000	0.00000000	-0.84628182	1629.929	3384.213	3439.957
N	0.00000000	0.00000000	0.44100301			
H	0.00000000	-0.85674916	0.99535955			

TS1 Zero-Point Energy = 0.090210 CCSD(T)-F12A Energy = -597.63770929

O	1.53942042	-1.59441829	0.23127399	-914.457	112.752	152.555
O	-1.09045140	-2.07730628	-0.83329631	156.802	192.164	248.165
O	2.17939628	0.42736367	-0.20223087	274.124	323.724	353.577

N	-1.13175006	-1.06659567	-0.19115183	389.027	431.918	457.193
N	1.31053268	-0.42298270	0.05349302	488.680	549.910	609.359
O	-0.93926248	-1.07550199	1.10435413	664.257	683.739	745.661
N	-1.72782682	1.61961002	0.12832045	794.128	830.820	987.011
N	0.42438440	2.38664649	-0.21084247	1085.656	1097.630	1187.013
C	-0.01686321	0.02868128	0.04726485	1252.053	1343.414	1509.750
C	-0.41739521	1.36198076	-0.01803012	1540.894	1595.171	1639.237
H	-2.35973139	0.84903681	0.26714877	1657.819	1683.327	3534.336
H	-2.10321201	2.49746565	-0.18538668	3613.496	3703.124	3727.838
H	0.13969938	3.31089858	0.06179687			
H	1.40616451	2.14887763	-0.26609382			

TS2 Zero-Point Energy = 0.092065 CCSD(T)-F12A Energy = -597.73711824

O	2.32171992	0.32737472	0.30729324	-83.077	112.806	147.949
O	-0.32214637	-2.54191397	-0.76039709	170.266	201.695	291.380
O	1.18457711	2.02989679	-0.36339503	349.652	361.718	419.060
N	0.61072171	-2.11470098	-0.26682179	439.949	451.684	471.007
N	1.26713900	0.87339586	0.06636460	556.077	593.140	618.764
O	0.20953481	-1.08936336	0.82125173	669.042	705.692	723.178
N	-2.26846693	-0.07313595	0.43477175	773.342	826.787	891.873
N	-1.44106603	1.87011943	-0.48398285	1075.981	1114.880	1207.865
C	0.07531161	0.13786099	0.27296753	1317.831	1372.221	1491.157
C	-1.18648309	0.66373635	0.05414898	1591.058	1642.129	1653.250
H	-2.07386816	-1.01819622	0.72040698	1694.318	1914.648	3545.294
H	-3.12201666	0.06187121	-0.07990188	3615.468	3703.819	3716.333
H	-2.33998840	2.28366822	-0.30859848			
H	-0.63768533	2.46666900	-0.62582071			

TS3 Zero-Point Energy = 0.089618 CCSD(T)-F12A Energy = -597.66385227

O	1.07746645	-1.77168069	0.82344989	-1668.412	122.749	129.091

O	-2.04049553	-0.50489825	-0.21366176	157.589	210.362	244.639
O	1.78796463	0.22055022	1.22125257	249.621	404.368	440.089
O	-0.77314132	-1.89658415	-1.25584979	471.197	481.752	550.282
N	1.07772294	-0.58080118	0.64571421	611.920	631.359	705.319
N	-0.95832528	-0.89011897	-0.63392321	748.251	792.557	821.090
N	-0.92863298	1.91685569	0.82413088	884.199	901.272	1009.757
N	0.60208533	2.02891793	-1.00507253	1098.599	1190.255	1203.682
C	0.19061308	-0.01087123	-0.37571043	1224.805	1424.015	1468.512
C	-0.12816850	1.43515090	-0.11379234	1496.006	1624.954	1679.591
H	-1.56302568	1.27781776	1.27591359	1718.232	1754.476	2042.808
H	-1.10735610	2.90319516	0.90153827	3542.953	3603.103	3717.060
H	0.71008976	3.03709518	-1.05546019			
H	0.90167383	0.80758820	-1.33243414			

TS4 Zero-Point Energy = 0.073165 CCSD(T)-F12A Energy = -392.68208216

H	0.80605433	3.09325836	-0.05068835	-1612.868	124.297	186.165
O	-1.05826229	-1.35594180	0.16837305	281.025	406.460	418.880
H	-1.75316313	2.26108506	-0.12926377	503.005	533.799	620.188
O	0.87475011	-2.23576151	-0.21930585	645.577	718.833	751.170
H	1.73203024	1.07890702	0.17164317	834.509	965.362	1008.098
N	0.16798776	-1.28009025	0.01940143	1070.640	1162.545	1197.933
N	-1.32283892	1.35663301	-0.06260099	1369.710	1450.442	1559.405
N	0.95286971	2.09871753	0.06904889	1643.460	1705.401	2096.291
C	0.78664385	-0.01180255	0.15258150	3565.489	3588.933	3723.390
C	-0.00977295	1.20585298	0.04578888			
H	-1.88014320	0.51532326	-0.02081855			

TS11 Zero-Point Energy = 0.082347 CCSD(T)-F12A Energy = -467.91209889

O	0.60141226	-0.95454168	-1.15055200	-156.794	96.235	209.407
H	1.91063508	2.17634980	0.11225511	280.133	332.077	391.533

O	0.20321673	-2.45672708	0.57350297	479.546	483.274	520.692
H	1.96596291	0.46648228	-0.26081863	603.038	618.763	637.213
N	0.43664032	-1.30601155	0.19117090	657.026	755.073	774.515
O	-1.70644878	-0.28664388	0.02601949	839.223	1024.892	1078.209
N	-0.70679649	2.09979705	0.29087685	1123.419	1137.955	1479.191
N	1.45624579	1.28000072	0.06670727	1509.733	1541.728	1647.285
C	-0.49615040	-0.24183753	0.03326493	1759.526	1778.167	3497.366
C	0.15770257	1.13448495	0.12416117	3522.145	3689.580	3696.494
H	-1.67415672	1.78633452	0.31268406			
H	-0.46951133	3.07571844	0.33195173			

TS12 Zero-Point Energy = 0.071559 CCSD(T)-F12A Energy = -338.21879037

H	-2.10085176	1.16971326	0.00000000	-177.791	92.177	113.017
H	1.24110579	2.30506337	0.00000000	200.800	337.619	484.932
O	1.27688210	-1.54844460	0.00000000	529.510	551.907	564.702
H	1.85451784	0.68810837	0.00000000	652.916	705.542	773.768
H	-1.11933442	2.57982484	0.00000000	1059.304	1144.263	1346.375
O	-0.99567375	-1.94304583	0.00000000	1349.807	1511.941	1653.133
N	-1.17890026	1.56748971	0.00000000	1671.438	2306.567	3502.459
N	1.06019836	1.30783580	0.00000000	3513.582	3662.520	3697.358
C	0.10471933	-1.55820912	0.00000000			
C	-0.13642541	0.74861007	0.00000000			

TS13 Zero-Point Energy = 0.046891 CCSD(T)-F12A Energy = -149.70436123

H	1.94099507	-0.44889378	-0.22199893	-1885.704	412.715	657.780
H	-0.50318949	0.01361009	1.41093594	682.209	756.366	951.813
N	-1.09854722	-0.02714907	0.06664570	1027.015	1083.717	1238.732
H	-1.94099507	0.44889378	-0.22199893	1377.747	1432.317	1820.870
H	0.50318949	-0.01361009	1.41093594	1860.772	3637.846	3652.700
C	0.00000000	0.00000000	-0.54356210			

N	1.09854722	0.02714907	0.06664570			

TS14 Zero-Point Energy = 0.029948 CCSD(T)-F12A Energy = -148.44152240

H	0.78453624	1.07022616	-0.50988313	-770.772	690.227	953.888
C	-0.79081572	-0.09021406	0.15787291	976.079	1190.613	1231.208
N	0.19715615	-0.79838931	-0.23695302	1439.421	3282.905	3387.751
H	0.65399215	-1.25134932	0.56690417			
N	-0.09172410	1.10306006	0.03812266			

TS15 Zero-Point Energy = 0.070831 CCSD(T)-F12A Energy = -338.23201057

O	1.23593716	-1.31155247	0.00000000	-1124.140	170.156	304.843
H	1.06525614	2.44486398	0.00000000	409.696	479.886	599.029
H	-1.67572657	1.91922603	0.00000000	643.076	660.207	713.982
H	1.92265892	0.91932816	0.00000000	745.352	841.748	869.853
H	-1.66153673	-0.17188357	0.00000000	1076.315	1191.152	1213.061
O	-1.04445324	-1.34891816	0.00000000	1372.813	1443.617	1609.770
N	-1.29276666	0.98774602	0.00000000	1793.184	1893.312	2142.329
N	1.05620428	1.44082989	0.00000000	3564.605	3648.856	3719.313
C	0.11715028	-0.84625660	0.00000000			
C	-0.03808964	0.70818754	0.00000000			

TS16 Zero-Point Energy = 0.043097 CCSD(T)-F12A Energy = -149.14817123

H	0.54419942	1.81770518	-0.63637104	-703.045	431.563	484.500
H	1.10938972	-1.27224215	0.03687085	577.904	722.300	1116.142
N	0.10964523	-1.13751610	-0.05895559	1228.748	1629.365	1789.822
H	-0.48064173	-1.94848420	-0.05396911	3509.195	3714.572	3722.483
N	0.10236011	1.19862682	0.01701839			
C	-0.42739654	0.08035941	-0.08922119			

TS17 Zero-Point Energy = 0.039686 CCSD(T)-F12A Energy = -149.10755657

H	0.54420892	2.10185125	0.46720392	-336.365	209.809	266.855
H	0.81967082	-1.80812348	-0.53325175	380.688	600.331	728.589
N	0.32281828	-1.48601111	0.30224361	827.940	1547.369	2106.107
H	-0.59901706	-1.91653790	0.19354246	3423.791	3509.246	3827.524
N	0.18074654	1.34420308	-0.07013295			
C	-0.20925114	0.33476710	-0.50500022			

TS21 Zero-Point Energy = 0.079606 CCSD(T)-F12A Energy = -467.94301232

O	-0.61226503	-2.29951137	0.00000000	-1154.757	111.801	149.408
H	2.00311845	2.22927531	0.00000000	292.917	335.745	385.425
O	1.34333793	-1.34356512	0.00000000	387.084	476.931	604.034
H	2.07662837	0.47147034	0.00000000	613.887	654.292	723.169
N	0.09861977	-1.31553766	0.00000000	725.764	747.902	775.225
O	-1.76781273	0.10156080	0.00000000	875.431	1083.452	1172.151
N	-0.68078061	2.16649125	0.00000000	1195.773	1230.420	1336.427
N	1.54976777	1.33381301	0.00000000	1478.489	1570.934	1625.007
C	-0.50581767	-0.05403069	0.00000000	1663.673	1756.247	2066.628
C	0.22378667	1.23909039	0.00000000	3547.461	3650.539	3723.253
H	-1.69479168	1.29163782	0.00000000			
H	-0.42155310	3.13982482	0.00000000			

TS22 Zero-Point Energy = 0.082433 CCSD(T)-F12A Energy = -467.89920816

O	0.86199032	-1.03507780	-1.01190428	-380.732	133.111	191.773
H	1.96277041	2.18432369	0.27902210	284.071	312.059	410.252
O	-0.11070707	-2.38805765	0.60613463	449.782	467.976	525.290
H	2.03523097	0.50028147	-0.09946556	583.934	614.825	638.809
N	0.24675491	-1.29183508	0.17086916	746.008	816.443	855.460
O	-1.72197223	-0.15208905	-0.14016330	877.256	1095.431	1119.179
N	-0.70703758	2.14455263	0.15407299	1141.176	1218.036	1418.618
N	1.51620835	1.28416997	0.27025732	1443.762	1526.944	1622.518

C	-0.44807820	-0.13892999	0.00300936	1711.766	1777.679	3375.873
C	0.17782069	1.22930878	0.13486980	3561.084	3572.932	3709.290
H	-1.98599967	0.80332925	-0.16365912			
H	-0.34234771	3.08700342	0.23627785			

TS23 Zero-Point Energy = 0.073011 CCSD(T)-F12A Energy = -338.22521704

O	1.24316185	-1.16762255	0.25822837	-575.031	112.540	295.862
H	0.99872985	2.45911823	-0.05353881	383.765	435.640	461.775
H	-1.39381937	2.16087371	0.08724124	521.677	589.612	630.484
H	1.88511525	0.98390675	-0.05777361	792.245	840.436	905.596
H	-1.33930133	-1.81269448	0.70418401	1104.114	1126.456	1148.243
O	-0.93627788	-1.53580099	-0.12425105	1270.954	1452.168	1626.948
N	-1.32835286	1.14441922	0.11102536	1766.444	1877.415	3500.692
N	1.01324067	1.46595424	-0.20190883	3611.038	3733.582	3875.872
C	0.14184577	-0.74790869	0.06920537			
C	-0.13043513	0.74806237	-0.01380999			

TS24 Zero-Point Energy = 0.081809 CCSD(T)-F12A Energy = -467.92726047

O	-0.38987806	-2.26217198	0.37663845	-529.227	109.075	128.674
H	1.88299525	2.32261754	-0.00455780	286.745	296.179	362.235
O	1.47929467	-1.24364420	0.02070112	406.047	443.782	454.115
H	2.05074090	0.61835220	-0.22262324	535.788	612.113	659.543
N	0.25726566	-1.27212338	0.11773365	683.114	753.429	863.622
O	-1.77090805	-0.18880475	-0.21809002	880.896	1104.518	1130.903
N	-0.72240790	2.22375709	0.21013327	1155.566	1169.625	1380.992
N	1.46929004	1.43906698	-0.24418314	1399.805	1534.794	1593.734
C	-0.47342698	-0.04685737	-0.07863863	1663.455	1685.446	3510.323
C	0.13129135	1.29682961	-0.02377553	3599.656	3726.046	3796.898
H	-2.26009075	-0.22258757	0.61400043			
H	-0.27241926	3.13631458	0.24797039			

TS25 Zero-Point Energy = 0.082605 CCSD(T)-F12A Energy = -467.89444367

O	1.09018504	-1.04265864	-0.81994852	-299.892	111.660	207.225
H	1.83134985	2.32814978	0.31217532	289.694	326.572	406.096
O	-0.30164072	-2.30803962	0.49546407	446.837	457.844	544.522
H	2.01128482	0.66289389	-0.10730539	579.173	628.261	669.999
N	0.29390213	-1.23565342	0.24641848	748.440	826.988	851.318
O	-1.63912574	-0.27642445	-0.40874735	908.289	1109.513	1120.087
N	-0.81069776	2.18542249	0.11264469	1158.568	1196.420	1397.408
N	1.43899696	1.40410756	0.26836590	1442.865	1545.787	1573.330
C	-0.42147705	-0.09935965	-0.07343408	1627.720	1772.056	3514.374
C	0.09700201	1.30054738	0.08104556	3525.494	3577.372	3712.750
H	-1.82558187	-1.23446261	-0.27874915			
H	-0.42533154	3.11729695	0.25207616			

TS26 Zero-Point Energy = 0.063784 CCSD(T)-F12A Energy = -262.96488454

C	0.04278134	-0.47918513	0.00000000	-1057.159	236.124	356.427
H	-0.04199939	-2.54253278	0.00000000	403.730	584.840	626.707
H	2.05881973	-0.70933053	0.00000000	643.124	722.397	725.274
H	-1.54626054	-1.67134493	0.00000000	841.796	1064.918	1178.079
H	0.94090833	1.16955655	0.00000000	1268.426	1374.726	1599.760
O	-0.13531023	1.76345364	0.00000000	1633.742	1818.438	1995.043
N	1.25928935	-0.09754826	0.00000000	3578.936	3650.189	3708.787
N	-0.53689108	-1.66806478	0.00000000			
C	-0.94040240	0.81338866	0.00000000			

TS27 Zero-Point Energy = 0.019635 CCSD(T)-F12A Energy = -188.91084139

O	-0.15007894	-1.18140664	-0.03202569	-528.073	669.857	1041.502
H	-0.38431601	1.41187425	0.78844218	1136.204	1963.753	3811.410
O	-0.10017935	1.09889906	-0.08089911			

C	0.40309831	-0.15336272	0.01609022			

TS28 Zero-Point Energy = 0.065575 CCSD(T)-F12A Energy = -262.97862678

C	0.05361136	0.45766610	-0.27947955	-455.230	136.667	316.159
H	1.40248198	1.68206520	0.69732736	375.129	451.857	479.707
H	-0.91150701	2.05830686	0.60327100	529.558	562.115	598.905
H	2.05609696	0.31138264	-0.06817333	669.814	1082.857	1084.609
H	-1.90121533	0.95957184	-0.23594148	1352.528	1460.435	1647.535
O	-0.34606852	-2.05224917	-0.61856809	1677.867	1943.872	3527.243
N	-0.97158098	1.30431421	-0.06924792	3535.444	3680.222	3685.370
N	1.27412550	0.93642873	0.02510521			
C	-0.22704405	-1.15305439	0.11263651			

TS31 Zero-Point Energy = 0.079320 CCSD(T)-F12A Energy = -467.96075022

O	-0.52786463	-2.32631716	0.00000000	-774.023	124.439	152.553
H	2.08631385	1.93806569	0.00000000	355.421	363.268	396.394
O	1.39913370	-1.28991138	0.00000000	406.192	490.612	537.503
H	1.75208155	-0.06758939	0.00000000	598.754	629.839	658.318
N	0.09416394	-1.28380638	0.00000000	700.589	751.484	755.262
O	-1.81938459	0.00931967	0.00000000	874.531	1086.684	1146.397
N	-0.50501430	2.29922379	0.00000000	1153.554	1191.509	1338.119
N	1.52055969	1.10297082	0.00000000	1477.184	1584.323	1626.816
C	-0.59872889	-0.05556714	0.00000000	1707.520	1757.004	2024.670
C	0.22762814	1.18962444	0.00000000	3587.634	3624.548	3732.786
H	-1.50748184	2.18047784	0.00000000			
H	-0.09536448	3.21515464	0.00000000			

TS32 Zero-Point Energy = 0.050939 CCSD(T)-F12A Energy = -262.35754197

C	-0.64306170	1.33458386	0.02776472	-236.040	98.392	216.307
H	-0.87481049	-2.59987321	-0.01564685	255.796	321.045	347.920

H	1.68251542	0.09834508	-0.07958424	443.774	463.135	687.420
H	1.72974538	-1.62505111	-0.15771174	867.795	1115.028	1207.070
C	-0.13701186	-0.79536237	-0.00515917	1612.514	1925.100	2109.288
O	0.31705488	1.94424543	-0.02232501	3452.599	3566.516	3680.545
N	1.20304700	-0.78160750	0.01338316			
N	-1.06569050	-1.59785284	-0.01742119			

TS41 Zero-Point Energy = 0.077049 CCSD(T)-F12A Energy = -392.71639870

H	0.63908995	3.01326898	0.46464154	-510.633	109.150	218.563
O	-0.25860390	-0.99401225	-1.10808051	296.722	404.623	450.489
H	-1.63958619	2.17675929	0.31399146	487.047	502.189	571.695
O	-0.11266167	-2.13826426	1.03663873	665.273	728.763	897.429
H	1.69565098	-0.13904151	-0.69916213	902.800	959.225	1102.993
N	0.14486927	-1.26066306	0.23484211	1133.137	1168.235	1178.581
N	-1.19947906	1.28253059	0.18901867	1341.712	1457.864	1637.740
N	1.03654084	2.12040790	0.17903723	1785.913	1803.801	3185.151
C	0.66268391	-0.13257696	-0.36608751	3515.914	3606.328	3725.417
C	0.15040347	1.22731134	0.01859592			
H	-1.75690474	0.54992137	-0.22003105			

TS42 Zero-Point Energy = 0.062520 CCSD(T)-F12A Energy = -262.95562181

H	0.66594785	2.38529309	-0.02555099	-1341.319	111.880	211.016
H	-1.91134314	-0.38017820	-0.01081438	416.837	491.343	535.823
H	-2.00231903	1.34611990	-0.01127407	617.226	679.195	732.359
O	0.46596778	-1.93252348	-0.01577654	843.428	1058.923	1134.127
H	1.68507352	0.50549525	-0.02616899	1151.523	1344.539	1626.160
C	-0.12008686	0.48513580	-0.02059988	1725.101	1878.651	2032.229
N	-1.43859481	0.51169079	-0.01734328	3559.389	3635.154	3671.151
N	0.79455640	1.38493848	-0.02550312			
C	0.89747577	-0.82960963	-0.02092054			

TS43 Zero-Point Energy = 0.076084 CCSD(T)-F12A Energy = -392.66838472

H	-1.50461476	2.33784991	-0.27932315	-490.349	131.925	168.258
O	-1.04203968	-2.21324277	-0.29935434	229.270	381.059	392.251
H	1.95969793	1.70942088	-0.36203900	420.085	436.431	495.061
O	0.99654664	-1.48550011	0.56572576	536.305	676.852	690.168
H	1.01262252	2.75538106	0.54971279	736.600	830.142	1062.625
N	-0.15618304	-1.40809624	-0.14902475	1109.868	1148.119	1277.121
N	-1.19451067	1.55325094	0.27837961	1427.069	1601.843	1633.573
N	1.03218387	2.06513893	-0.18806483	1665.479	1901.759	3556.196
C	0.31093080	-0.22241248	-0.34030396	3565.847	3666.446	3672.450
C	0.06733093	1.08140386	-0.04394482			
H	-1.90380802	0.84411555	0.37806015			

TS44 Zero-Point Energy = 0.074604 CCSD(T)-F12A Energy = -392.82496654

H	-2.44437693	0.79793043	0.00000000	-467.800	129.806	287.510
O	-0.61654692	-1.96785152	0.00000000	368.325	399.460	447.750
H	0.87082345	2.24063184	0.00000000	461.540	559.939	640.436
O	1.87764285	0.34082361	0.00000000	653.894	713.480	765.426
H	-0.80588125	2.76455796	0.00000000	788.181	870.133	1081.039
N	0.60139659	-1.54786238	0.00000000	1191.409	1205.392	1290.982
N	-1.61569789	0.22114503	0.00000000	1387.744	1482.258	1600.633
N	-0.11887201	2.03194613	0.00000000	1683.106	1770.234	2097.068
C	0.77110942	-0.18950426	0.00000000	3562.913	3607.104	3717.324
C	-0.43113691	0.74663894	0.00000000			
H	-1.44370083	-0.92354402	0.00000000			

TS45 Zero-Point Energy = 0.072629 CCSD(T)-F12A Energy = -392.75869335

H	-2.55397554	1.12623785	0.00000000	-222.813	76.769	98.549
O	-0.88940802	-1.96707191	0.00000000	253.666	259.935	273.396

H	1.12769257	2.02897103	0.00000000	322.688	426.696	470.945
O	1.98320976	0.13615938	0.00000000	476.457	546.195	586.363
H	-0.33336764	2.99647628	0.00000000	646.109	675.907	920.558
N	0.41737459	-1.62236936	0.00000000	951.487	1119.663	1241.028
N	-1.72157522	0.54103433	0.00000000	1428.957	1577.553	1602.712
N	0.11920058	2.09535394	0.00000000	1919.724	2182.703	3151.258
C	1.00953905	-0.54648371	0.00000000	3481.878	3541.523	3662.815
C	-0.56214187	0.96584964	0.00000000			
H	-1.41463141	-1.12121875	0.00000000			

TS46 Zero-Point Energy = 0.074422 CCSD(T)-F12A Energy = -392.80807202

H	-2.52475540	0.90405918	0.00000000	-1158.419	150.114	284.292
O	-0.43789243	-2.03683686	0.00000000	311.675	378.199	415.030
H	1.19668667	1.59115959	0.00000000	491.623	609.431	651.788
O	1.78473481	0.51311257	0.00000000	726.442	748.728	755.099
H	-0.65378549	2.74807785	0.00000000	784.915	789.140	1088.951
N	0.72603749	-1.52400051	0.00000000	1190.505	1220.984	1321.933
N	-1.73542050	0.28165271	0.00000000	1356.781	1471.624	1572.383
N	-0.04313414	1.94688927	0.00000000	1650.764	1793.978	2074.775
C	0.72662938	-0.18415026	0.00000000	3501.032	3650.255	3692.768
C	-0.49435009	0.73928992	0.00000000			
H	-1.83780597	-0.72679973	0.00000000			

TS47 Zero-Point Energy = 0.071724 CCSD(T)-F12A Energy = -392.71890858

H	-2.03613964	2.49374477	0.00000000	-271.587	77.800	91.469
O	-1.11892768	-2.37411532	0.00000000	156.938	203.513	297.229
H	1.75416589	0.64587225	0.00000000	304.739	326.195	414.191
O	1.92465354	-0.36002829	0.00000000	449.150	469.650	495.189
H	0.76702440	2.95591929	0.00000000	680.415	858.337	913.833
N	-0.09838921	-1.69236067	0.00000000	994.025	1116.812	1231.728

N	-1.65250667	1.55850113	0.00000000	1440.607	1522.787	1621.514
N	0.73338518	1.93701430	0.00000000	1857.553	2486.161	2798.070
C	0.76274908	-0.92385200	0.00000000	3456.303	3545.219	3688.688
C	-0.35088219	1.32327167	0.00000000			
H	-2.29169094	0.78158445	0.00000000			

TS48 Zero-Point Energy = 0.073556 CCSD(T)-F12A Energy = -392.67119075

H	0.87959814	3.02477504	-0.26763093	-463.716	138.646	174.443
O	-1.25248529	-0.93003099	0.50114111	241.675	334.132	344.625
H	-1.46726477	2.52597379	-0.12200749	405.957	513.907	548.711
O	0.21615752	-2.29751005	-0.26597742	609.476	741.033	788.865
H	1.82608820	-0.50782406	-0.28386053	826.226	855.876	896.609
N	-0.14130279	-1.18692553	0.06302433	988.165	1016.030	1170.946
N	-1.27433706	1.60405191	-0.52409894	1396.156	1438.721	1525.312
N	1.02455112	2.26560617	0.39456929	1664.484	1950.521	3284.910
C	0.83685909	-0.15817091	-0.04625048	3415.127	3510.508	3521.908
C	0.60733480	1.15235165	0.07519403			
H	-1.82002467	0.94172730	0.03425478			

TS50 Zero-Point Energy = 0.073294 CCSD(T)-F12A Energy = -392.64780425

H	-0.64634674	3.09857448	0.26220092	-509.162	89.029	118.489
H	1.78779144	1.42058052	0.87198916	151.832	208.837	227.160
H	-2.19462989	2.29204652	0.15849355	304.465	344.816	510.324
H	1.73307697	1.37792122	-0.72670999	526.506	568.265	654.401
N	-1.19700564	2.25674920	0.27512221	744.998	806.130	862.664
N	1.37034606	1.90360446	0.07278901	921.729	1138.683	1301.876
N	0.11555411	-1.31074177	-0.29776027	1469.071	1551.116	1598.547
O	-0.64540098	-2.21621219	-0.56671302	1644.997	2153.918	3436.801
C	-0.55874211	1.11064118	0.15570410	3520.039	3606.414	3726.671
C	-0.43568821	-0.11527880	0.13764687			

O	1.33116353	-1.36520260	-0.37321423

TS51 Zero-Point Energy = 0.061243 CCSD(T)-F12A Energy = -541.70664592

O	-1.33178895	-1.27963097	0.96399591	-310.949	117.931	145.531
O	-0.29872504	2.26516691	0.10877559	148.752	173.655	203.154
O	-0.32389734	-2.38808786	-0.58979176	320.898	376.857	393.524
O	-1.91118176	1.06751534	-0.69130334	455.832	483.491	546.438
N	-0.49970169	-1.41059648	0.09833454	612.627	641.957	775.470
N	-0.84928554	1.25773652	-0.20535267	795.364	906.569	1144.654
N	2.72406729	0.55189270	0.14112547	1303.205	1394.398	1460.888
H	3.51229319	0.30844157	-0.43624006	1635.991	1687.486	1779.280
C	0.36271826	-0.29094396	-0.12968891	2137.680	3575.515	3678.242
C	1.56835869	-0.02596303	-0.01771937			
H	2.82832756	1.31137155	0.79719949			

TS52 Zero-Point Energy = 0.045383 CCSD(T)-F12A Energy = -336.72386726

O	-1.11846122	-1.08308055	0.22043253	-719.555	122.101	186.490
C	-0.16908354	0.14568395	0.27337088	325.982	361.003	387.722
O	0.77964255	-2.02347003	-0.50970781	462.062	510.049	620.719
H	-0.50506199	3.20004818	-0.51687841	744.620	1069.797	1158.332
N	0.23423924	-1.22616412	0.17563818	1294.173	1642.901	1659.430
C	0.02124822	1.35003022	0.11639219	2105.110	3598.643	3681.143
H	1.00821358	3.11122155	0.29226072			
N	0.18893306	2.63883612	-0.05161272			

TS53 Zero-Point Energy = 0.045645 CCSD(T)-F12A Energy = -336.82014549

O	-1.29723501	-0.94166285	-0.23925633	-104.397	181.364	205.896
C	-0.91002501	0.23549357	-0.18621208	285.514	305.897	353.979
O	0.95755768	-1.63669402	0.81852413	398.623	443.370	532.757
H	0.44690699	2.90502552	0.83732843	563.376	900.027	1165.121

N	0.61974842	-1.24175142	-0.16332848	1506.774	1646.769	2015.050
C	-0.23739905	1.26638719	-0.14084314	2236.886	3607.090	3696.821
H	0.41765018	3.04265813	-0.86470354			
N	0.36193747	2.44915112	-0.05485061			

TS54 Zero-Point Energy = 0.035524 CCSD(T)-F12A Energy = -207.01393120

H	0.24151479	2.79124791	0.02201401	-275.557	130.553	314.626
C	-0.44065097	-0.67791677	-0.03517281	469.730	640.239	827.394
N	-0.05984804	1.82392400	-0.00963130	1103.348	1464.365	1632.930
H	-1.05908311	1.65786021	-0.14833318	2082.985	3383.034	3551.278
O	-0.01608547	-1.73605962	0.03792212			
C	0.78498975	0.86138148	0.11955368			

TS55 Zero-Point Energy = 0.061287 CCSD(T)-F12A Energy = -541.65887329

O	-0.35231257	-2.03034222	0.12267286	-929.528	15.078	129.411
O	-2.13117901	0.10811976	-0.77688419	168.774	204.464	276.593
O	1.73384363	-1.51474236	-0.08016686	332.524	427.776	483.369
N	-1.20547458	0.51784557	-0.11525663	586.652	609.787	671.909
N	0.55491882	-1.25362961	-0.00704545	776.602	797.517	816.035
O	-1.05608555	0.38553410	1.17560996	880.829	980.513	1139.398
N	1.15575940	2.29903258	0.05179390	1204.041	1300.401	1423.009
H	1.75727858	3.02133241	-0.31680669	1571.671	1615.046	1705.802
C	0.22637041	0.17233553	-0.12946529	1719.440	3458.445	3619.705
C	1.17035331	1.10833469	-0.44124487			
H	0.56534266	2.54686574	0.84370731			

TS56 Zero-Point Energy = 0.052728 CCSD(T)-F12A Energy = -411.98816240

O	1.42797332	-1.21598349	-0.55820912	-287.537	121.914	214.076
H	-0.84265955	1.95980992	1.19190419	221.760	277.234	424.347
O	1.53891446	0.59370901	0.60129298	439.078	587.141	638.368

C	-0.94263122	0.72829743	-0.43309592	658.691	720.052	853.641
N	0.96548400	-0.24927238	-0.03402788	959.964	1191.480	1405.120
O	-1.33293503	-1.62593928	0.19385382	1617.870	1697.471	1731.986
N	-0.88441487	1.86737659	0.18658800	2181.759	3555.489	3658.428
H	-0.70922833	2.70484485	-0.34575702			
C	-1.02284214	-0.52277108	0.05036686			

TS57 Zero-Point Energy = 0.051971 CCSD(T)-F12A Energy = -411.99025791

O	-1.55458270	-0.69242840	0.03686540	-360.604	110.634	146.036
C	0.59761573	0.10390670	0.45949636	304.143	378.172	406.194
O	0.06725731	-2.07772999	-0.20623191	429.904	565.325	611.508
H	1.95692321	-1.04812524	-0.53126753	634.149	753.522	796.809
N	-0.38424117	-0.97432845	0.02273518	907.033	1185.213	1425.683
O	-0.54146374	2.59895760	-0.13980134	1457.601	1638.171	1695.036
H	2.59437466	0.24758615	0.43577503	2190.948	3507.709	3679.925
N	1.79757625	-0.24710686	0.07149551			
C	-0.22050517	1.56461376	-0.45700602			