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ELECTRONIC SUPPLEMENTARY INFORMATION

High-level *ab initio* mapping of the multiple H-abstraction pathways of the OH + glycine reaction

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Table S1. Harmonic frequencies (in cm^{-1}) of the transition states for H-abstraction from the CH_2 group of glycine obtained at the CCSD(T)-F12b/aug-cc-pVDZ level of theory

$\mathbf{I}_{\mathbf{CH}}^{\mathbf{TS}}$	$\mathbf{II}_{\mathbf{CH}}^{\mathbf{TS}}$	$\mathbf{III}_{\mathbf{CH}}^{\mathbf{TS}}$	$\mathbf{IV}_{\mathbf{CH}}^{\mathbf{TS}}$	$\mathbf{V}_{\mathbf{CH}}^{\mathbf{TS}}$
1089*i*	338*i*	547*i*	859*i*	837*i*
67	58	61	38	51
129	92	107	109	84
162	146	135	130	128
295	226	179	217	182
328	261	277	280	278
425	303	288	360	357
491	465	468	494	474
562	516	514	526	527
655	618	628	601	591
673	628	638	622	657
764	671	675	678	694
823	771	713	727	774
887	856	867	843	860
955	989	963	928	926
968	1136	1110	991	1089
1127	1154	1158	1157	1125
1200	1206	1203	1196	1205
1240	1251	1244	1230	1248
1313	1333	1327	1330	1329
1381	1391	1376	1369	1368
1422	1448	1432	1425	1415
1526	1643	1665	1628	1624
1667	1838	1762	1668	1671
1839	2060	1832	1807	1824
3103	3089	3103	3110	3139
3519	3529	3538	3555	3534
3616	3629	3641	3651	3625
3642	3724	3728	3703	3713
3683	3773	3772	3764	3775

Table S2. Harmonic frequencies (in cm^{-1}) of the product-channel complexes for H-abstraction from the CH_2 group of glycine obtained at the CCSD(T)-F12b/aug-cc-pVDZ level of theory

$\mathbf{I_{CH}^{MIN}}$	$\mathbf{II_{CH}^{MIN}}$
51	52
154	151
177	157
194	193
225	225
295	301
315	310
372	364
499	394
504	511
557	537
634	641
702	690
705	697
766	743
914	918
1145	1148
1168	1173
1318	1315
1357	1333
1564	1563
1656	1657
1711	1706
1736	1747
3243	3211
3443	3433
3620	3630
3719	3717
3798	3832
3904	3905

Table S3. Harmonic frequencies (in cm^{-1}) of the transition states for H-abstraction from the NH_2 group of glycine obtained at the CCSD(T)-F12b/aug-cc-pVDZ level of theory

$\mathbf{I}_{\mathbf{NH}}^{\mathbf{TS}}$	$\mathbf{II}_{\mathbf{NH}}^{\mathbf{TS}}$	$\mathbf{III}_{\mathbf{NH}}^{\mathbf{TS}}$	$\mathbf{IV}_{\mathbf{NH}}^{\mathbf{TS}}$	$\mathbf{V}_{\mathbf{NH}}^{\mathbf{TS}}$
1395*i*	1486*i*	1425*i*	1593*i*	1280*i*
64	41	51	48	48
133	114	101	134	60
195	152	175	165	172
264	255	268	264	212
398	329	380	359	277
442	454	436	452	411
475	477	471	479	438
525	526	477	495	477
640	622	571	571	557
659	642	650	634	634
745	692	747	684	679
863	840	857	850	808
885	900	885	908	868
944	996	944	995	985
1114	1102	1111	1107	1099
1173	1172	1167	1164	1147
1190	1233	1188	1241	1211
1307	1248	1300	1258	1273
1339	1335	1335	1314	1306
1419	1451	1394	1436	1436
1460	1465	1453	1462	1456
1507	1509	1505	1480	1575
1741	1609	1731	1599	1836
1821	1824	1849	1854	1879
3039	3001	3014	2991	3001
3114	3077	3089	3038	3050
3495	3502	3484	3496	3523
3746	3708	3741	3706	3769
3771	3767	3811	3821	3817

Table S4. Harmonic frequencies (in cm^{-1}) of the product-channel complexes for H-abstraction from the NH_2 group of glycine obtained at the CCSD(T)-F12b/aug-cc-pVDZ level of theory

$\mathbf{I}_{\mathbf{NH}}^{\mathbf{MIN}}$	$\mathbf{II}_{\mathbf{NH}}^{\mathbf{MIN}}$	$\mathbf{III}_{\mathbf{NH}}^{\mathbf{MIN}}$	$\mathbf{IV}_{\mathbf{NH}}^{\mathbf{MIN}}$	$\mathbf{V}_{\mathbf{NH}}^{\mathbf{MIN}}$	$\mathbf{VI}_{\mathbf{NH}}^{\mathbf{MIN}}$	$\mathbf{VII}_{\mathbf{NH}}^{\mathbf{MIN}}$	$\mathbf{VIII}_{\mathbf{NH}}^{\mathbf{MIN}}$	$\mathbf{IX}_{\mathbf{NH}}^{\mathbf{MIN}}$	$\mathbf{X}_{\mathbf{NH}}^{\mathbf{MIN}}$
46	29	71	11	76	52	38	71	15	21
73	76	131	48	103	80	71	99	82	68
144	162	138	72	191	162	116	189	132	98
197	188	182	101	219	194	149	218	175	116
256	266	217	155	253	254	173	241	244	142
303	286	336	306	293	294	267	257	285	206
309	303	423	312	306	314	300	301	314	321
366	363	441	385	411	415	380	408	400	351
502	445	532	481	464	467	469	441	506	371
530	589	539	483	584	549	507	595	523	514
623	629	592	566	661	608	532	674	539	535
662	721	652	647	724	697	644	722	666	645
871	872	759	649	838	850	665	840	817	749
880	881	864	864	886	863	860	893	861	855
892	906	879	926	981	902	923	979	886	880
1084	1062	1076	1075	1057	1092	1087	1060	1095	1063
1181	1165	1153	1175	1127	1167	1176	1128	1178	1130
1190	1191	1195	1200	1256	1187	1193	1252	1194	1174
1267	1322	1285	1259	1294	1297	1293	1294	1271	1261
1398	1401	1385	1333	1355	1368	1348	1357	1358	1389
1413	1420	1403	1404	1445	1404	1429	1413	1392	1392
1478	1483	1437	1446	1508	1414	1439	1505	1424	1418
1646	1646	1673	1666	1651	1632	1647	1639	1635	1650
1816	1788	1836	1825	1841	1830	1813	1839	1831	1859
2979	2971	3005	3011	3044	2942	2957	3041	2967	2995
3011	3042	3033	3036	3121	3069	3083	3117	3025	3040
3413	3411	3468	3413	3436	3448	3400	3445	3437	3460
3453	3447	3615	3708	3449	3497	3766	3454	3547	3613
3687	3689	3701	3771	3618	3688	3770	3627	3736	3814
3904	3902	3915	3915	3901	3899	3917	3907	3908	3923

Table S4 continues

XI_{NH}^{MIN}	XII_{NH}^{MIN}	$XIII_{NH}^{MIN}$	XIV_{NH}^{MIN}	XV_{NH}^{MIN}	XVI_{NH}^{MIN}	$XVII_{NH}^{MIN}$	$XVIII_{NH}^{MIN}$	XIX_{NH}^{MIN}
21	7	33	25	34	20	30	22	38
47	60	50	60	65	63	60	77	78
62	70	85	68	105	83	73	107	102
85	141	119	110	132	120	128	155	146
158	224	151	154	227	131	158	188	234
290	238	265	260	282	195	311	251	258
327	308	276	309	344	275	326	273	313
381	326	337	364	365	320	385	353	340
468	483	444	469	422	435	456	440	444
532	486	521	531	443	470	484	478	487
562	578	546	585	570	552	532	526	537
605	639	643	613	612	596	570	554	577
671	640	689	677	746	695	662	658	653
842	851	859	847	858	847	871	857	855
916	886	886	883	960	881	926	893	894
1080	1086	1073	1081	1051	1065	1074	1081	1086
1156	1149	1156	1166	1110	1144	1174	1143	1142
1196	1189	1198	1195	1218	1195	1212	1200	1200
1272	1224	1230	1239	1282	1243	1262	1227	1223
1367	1334	1345	1365	1366	1355	1315	1310	1310
1395	1399	1403	1406	1385	1407	1412	1406	1413
1431	1455	1461	1440	1490	1438	1423	1434	1434
1666	1680	1660	1673	1671	1651	1663	1655	1679
1838	1850	1827	1829	1823	1835	1855	1873	1879
2954	2983	2989	2974	3018	2977	2992	2967	2964
3110	3016	3035	3037	3147	3050	3018	3010	2999
3450	3436	3418	3436	3411	3417	3404	3428	3432
3713	3759	3755	3726	3765	3771	3718	3767	3771
3773	3775	3767	3765	3782	3800	3809	3819	3816
3915	3902	3910	3913	3882	3918	3915	3900	3903

Table S5. Harmonic frequencies (in cm^{-1}) of the transition states for H-abstraction from the COOH group of glycine obtained at the CCSD(T)-F12b/aug-cc-pVDZ level of theory

$\mathbf{I}_{\mathbf{COOH}}^{\mathbf{TS}}$	$\mathbf{II}_{\mathbf{COOH}}^{\mathbf{TS}}$	$\mathbf{III}_{\mathbf{COOH}}^{\mathbf{TS}}$	$\mathbf{IV}_{\mathbf{COOH}}^{\mathbf{TS}}$	$\mathbf{V}_{\mathbf{COOH}}^{\mathbf{TS}}$
1086*i*	1585*i*	1124*i*	1591*i*	1589*i*
99	41	100	72	63
208	122	203	137	133
267	200	259	216	213
340	246	340	271	264
396	394	396	338	341
456	437	465	476	477
534	497	547	513	496
563	567	562	547	545
586	624	577	625	633
631	672	609	690	680
670	730	665	770	767
745	882	755	849	843
834	913	830	932	931
937	953	954	1029	1029
1055	1156	1051	1104	1105
1090	1189	1077	1190	1190
1269	1341	1300	1290	1288
1322	1389	1319	1388	1388
1343	1407	1369	1470	1469
1415	1468	1439	1477	1476
1561	1490	1512	1500	1499
1604	1668	1583	1634	1633
1649	1677	1623	1686	1685
1779	1715	1795	1733	1729
2303	3059	2243	2978	2975
3093	3105	3092	3112	3112
3496	3516	3509	3514	3515
3688	3595	3689	3605	3605
3823	3784	3833	3783	3784