Table 1S: Experimental and calculated vibrational frequencies and intensities for the lowest energy conformer of DMMP, TMP and TEP

Mode	DMMP			TMP			TEP		
	ν^{exp} (cm^{-1})	ν^{calc} * (cm^{-1})	I^{calc}* (km/mol)	ν^{exp} * (cm^{-1})	ν^{calc} * (cm^{-1})	I^{calc}* (km/mol)	ν^{exp} ** (cm^{-1})	ν^{calc} ** (cm^{-1})	I^{calc}** (km/mol)
1	55.6	57.05	3.42	54.7	62.02	4.36	--	28.10	0.52
2	83.6	82.18	5.32	54.7	62.02	4.36	--	29.39	0.76
3	--	90.65	1.22	93.5	97.69	7.22	--	37.62	0.38
4	--	93.86	1.76	--	109.90	0.04	--	51.86	1.50
5	--	172.27	0.14	--	109.90	0.04	--	54.43	1.44
6	194.1	179.45	11.53	--	117.29	1.70	80.0	76.18	7.12
7	237.0	225.43	7.93	208.0	196.80	8.76	187.3	144.90	4.55
8	--	260.04	0.68	208.0	196.80	8.76	192.1	145.50	4.54
9	301.6	295.99	12.09	--	231.28	0.60	--	171.17	0.01
10	398.7	395.55	23.99	361.3	357.88	19.32	242.8	253.48	0.63
11	479.5	470.87	9.39	361.3	357.88	19.32	242.8	254.98	0.67
12	500.4	492.85	34.54	450.1	446.46	9.22	--	259.47	0.34
13	715.2	701.51	25.58	513.5	510.55	28.47	--	310.30	1.08
14	790.7	784.01	72.53	513.5	510.55	28.47	328.8	315.91	12.10
15	818.2	809.14	84.38	758.6	748.09	53.26	328.8	316.31	12.00
16	895.5	911.75	33.88	854.1	852.41	110.48	357.5	356.25	12.20
17	919.2	929.00	109.62	854.1	852.42	110.48	368.3	357.41	12.32
18	1049.8	1058.43	403.48	1060.2	1068.85	494.11	469.3	458.63	10.73
19	1076.1	1084.62	205.00	1060.2	1068.86	494.06	538.0	535.27	34.83
20	--	1173.92	0.60	--	1107.44	4.28	538.0	536.14	35.01
21	--	1175.87	0.95	--	1175.36	0.02	748.5	758.22	31.29
22	1188.4	1196.45	23.85	--	1175.36	0.02	793.0	819.76	33.29
23	1188.4	1198.99	23.48	--	1176.60	1.51	793.0	819.83	34.58
24	1275.7	1279.38	196.32	1192.8	1201.82	43.71	--	824.10	1.69
25	1312.6	1339.93	44.75	1192.8	1201.82	43.71	818.6	825.04	30.21
26	1424.4	1457.11	4.09	--	1202.43	0.17	818.6	825.26	28.56
27	1424.4	1461.96	5.06	1291.6	1292.75	203.59	919.2	960.34	1.17
28	--	1471.45	0.67	--	1473.83	2.03	972.5	979.97	272.74
29	--	1475.34	0.66	--	1473.83	2.03	972.5	981.07	267.46
30	1471.9	1494.64	6.34	--	1478.76	1.33	1050.1	1061.77	463.71
31	1471.9	1498.00	7.00	1466.6	1495.52	5.18	1050.1	1062.86	472.97
32	1521.1	1504.06	10.65	1466.6	1495.52	5.17	--	1100.07	0.79
33	1521.1	1506.08	10.33	1466.6	1496.48	8.14	1100.4	1128.50	12.28
34	2858.7	3033.94	56.42	1472.4	1504.76	11.85	1100.4	1128.59	12.15
35	2864.0	3039.81	39.98	1472.4	1505.83	11.64	--	1130.49	3.21
36	--	3049.62	1.00	1472.4	1505.83	11.64	1173.5	1185.75	2.68
37	2962.6	3109.78	22.77	2863.3	3040.75	63.19	1173.5	1186.22	3.25
38	2968.4	3114.34	17.60	2863.3	3040.75	63.17	1173.5	1187.32	3.64
39	--	3129.80	3.19	--	3041.86	0.91	1280.0	1282.86	157.76
40	--	3138.02	9.00	2964.3	3117.32	13.91	--	1308.61	0.18
41	3008.2	3139.19	3.38	2964.3	3117.42	17.68	--	1309.57	0.85
42	3014.7	3141.04	15.29	2964.3	3117.42	17.69	1307.3	1312.98	13.78
43				3001.2	3143.02	14.24	1374.8	1405.76	4.10
44				3001.2	3143.02	14.24	1374.8	1406.22	3.75
45				3001.2	3143.16	13.45	1378.4	1409.24	3.39
46							1397.7	1436.01	21.76
47							1397.7	1436.18	14.77
48							1399.3	1436.80	8.36
49							1450.2	1497.92	3.94
50							1450.2	1497.96	5.73
51							1457.0	1498.21	5.32
52							--	1515.02	0.83
53							1498.7	1515.73	2.27
54							1498.7	1515.85	2.28
55							1521.3	1536.43	1.23
56							1521.3	1536.63	1.13
57							--	1537.40	1.07
58							2879.9	3050.11	29.42
59							2879.9	3050.66	28.83
60							2879.9	3051.04	18.56
61							2884.0	3054.86	20.73
62							2884.0	3054.95	18.36
63							2884.0	3055.14	6.93
64							2916.3	3101.07	6.22
65							2916.3	3101.38	7.06
66							2916.3	3101.83	7.87
67							2949.3	3129.54	22.63
68							2949.3	3129.85	22.18
69							2949.3	3129.92	25.35
70							2988.9	3140.09	26.01
71							2988.9	3140.14	30.76
72							2988.9	3140.26	31.33

* Frequencies and intensities calculated with the B3LYP method and the 6-311++G(d,p) basis set for O, C , H atoms and the 6-311++G(3df,2p) basis set for P atom.

** Frequencies and intensities calculated with the B3LYP method and the 6-31+G(d,p) basis set for all atoms