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Supporting Information

A Computational Exploration of the Oxygen Reduction Reaction over a Carbon Catalyst containing a Phosphinate Functional Group

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Contribution from the

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Computational Methods

All quantum mechanical computations were performed at the density functional theory (DFT) level using the hybrid B3LYP density functional method, which is a combination of exchange from Becke's 3-parameter hybrid exchange functional (B3)[1] with the electron correlation functional of Lee, Yang, and Parr (LYP).[2] All of the structures were fully optimized with the 6-31G(d) basis set. All closed-shell species were treated by a restricted formalism, and all open-shell (doublet, triplet, etc) were treated with an unrestricted formalism. For example, catalyst **1** is closed-shell and was treated as a singlet. Catalyst **2** is formed from protonation and electron injection; thus, **2** is open-shell and was treated as a doublet. Addition of molecular oxygen (triplet) to catalyst **2** then forms structure **2a** which was a doublet.

Vibrational frequency analyses were computed to ensure that the optimized structures corresponded to minima, and these analyses yielded the zero-point vibrational energy (ZPVE) corrections. The ZPVE was scaled by a factor of 0.9806.[3] Transition states were verified to have one imaginary vibrational frequency and were connected to reactant and product by optimizations along the reaction coordinate.

On the basis of the optimized structures, single-point energy calculations at the B3LYP/6-311++G(d,p) level of theory were performed, using the B3LYP/6-31G(d) geometries. The Gaussian 03 suite of programs[4] was used for these calculations. Natural population analysis (NPA)[5] methods were used for each of the stationary points to determine the spin density on each atom of the models. These NPA calculations were performed at the B3LYP/6-311++G(d,p)//B3LYP/6-31G(d) level of theory

The proton affinity (PA), using H_3O^+ as proton source, was determined by the following equation:

$$\text{Model} + H_3O^+ \rightarrow \text{Model-}H^+ + H_2O$$

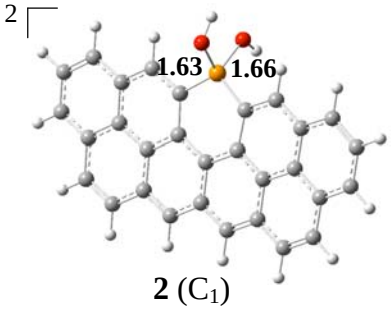
$$PA = E(H_2O) + E(\text{Model-}H^+) - E(H_3O^+) - E(\text{Model})$$

The energies are the bottom-of-the-well energies with ZPVE corrections evaluated at the B3LYP/6-31G(d) and B3LYP/6-311++G(d,p)//B3LYP/6-31G(d) level of theory.

Table S1. Proton affinity (PA) of **1** (using H_3O^+ as proton source, in kcal/mol).

	B3LYP/6-31G(d)	B3LYP/6-311++G(d,p)//B3LYP/6-31G(d)
1	–64.0 [a]	–66.8 [a]

[a] The energies are the bottom-of-the-well energies with ZPVE corrections.



2 (C_1)

Figure S1. The B3LYP/6-31G(d) optimized structure of model **2** with C_1 symmetry. Color representations: grey is for carbon, white is for hydrogen, red is for oxygen, and orange is for phosphorous. Bond lengths are shown in Å. The energy of C_1 symmetry conformer is 0.4 kcal/mol higher than the C_{2v} symmetry conformer. The multiplicity is also shown.

Table S2. The relative energy of the two conformers of **2** (in kcal/mol).

	B3LYP/6-31G(d)		B3LYP/6-311++G(d,p)//B3LYP/6-31G(d)	
	ΔE^a	$\Delta H(0K)^b$	ΔE^a	$\Delta H(0K)^b$
C_{2v} symmetry	0.0	0.0	0.0	0.0
C_1 symmetry	0.4	0.3	0.3	0.1

[a] ΔE is the relative bottom-of-the-well energy. [b] ΔH(0K) is the relative bottom-of-the-well energy after ZPVE correction.

Table S3. The relative energy of O_2 adsorption at the P site of **2** and the subsequent hydrogen transfer reaction (in kcal/mol).

	B3LYP/6-31G(d)		B3LYP/6-311++G(d,p)//B3LYP/6-31G(d)	
	ΔE^a	$\Delta H(0K)^b$	ΔE^a	$\Delta H(0K)^b$
2 + O_2	0.0	0.0	0.0	0.0
2a	–20.1	–15.9	–14.3	–10.1
TS	–19.8	–17.1	–14.8	–12.1
2b	–39.4	–36.1	–37.3	–34.1

[a] ΔE is the relative bottom-of-the-well energy. [b] ΔH(0K) is the relative bottom-of-the-well energy after ZPVE correction.

Table S4. The relative energy of the hydrogen-atom abstraction reaction from the OH group of **2** by hydroperoxyl radical (in kcal/mol).

	B3LYP/6-31G(d)		B3LYP/6-311++G(d,p)//B3LYP/6-31G(d)	
	ΔE^a	$\Delta H(0K)^b$	ΔE^a	$\Delta H(0K)^b$
2 + $HO_2^{\bullet}$	0.0	0.0	0.0	0.0
2d	–14.9	–12.8	–12.3	–10.2
TS	–7.4	–8.5	–5.5	–6.6
2e	–69.1	–64.3	–66.3	–61.6

[a] ΔE is the relative bottom-of-the-well energy. [b] ΔH(0K) is the relative bottom-of-the-well energy after ZPVE correction.

Table S5. The relative energy of the H_2O_2 dissociation over **2** (in kcal/mol).

	B3LYP/6-31G(d)		B3LYP/6-311++G(d,p)//B3LYP/6-31G(d)	
	ΔE^a	$\Delta H(0K)^b$	ΔE^a	$\Delta H(0K)^b$
2 + $HO_2^{\bullet}$	0.0	0.0	0.0	0.0
2f	–12.9	–10.6	–9.8	–7.6
TS	–4.2	–4.1	–3.4	–3.3
2g	–57.3	–55.5	–56.8	–55.1

[a] ΔE is the relative bottom-of-the-well energy. [b] ΔH(0K) is the relative bottom-of-the-well energy after ZPVE correction.

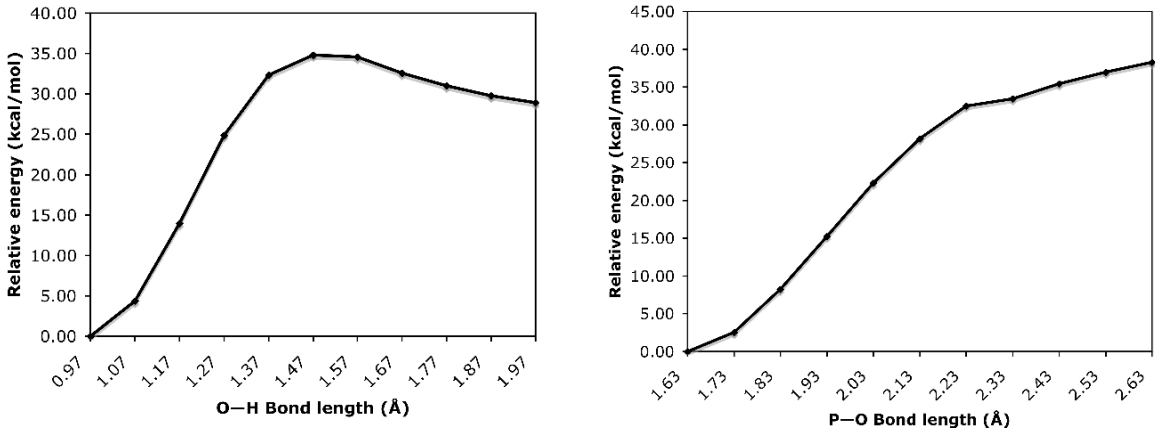


Figure S2. Energy profiles of O–H (left) and P–O (right) bond cleavages of **2** via potential energy surface scan studies. The high reaction energy barriers of breaking these two bonds indicate that **2** is rather stable to undergo the subsequent reactions.

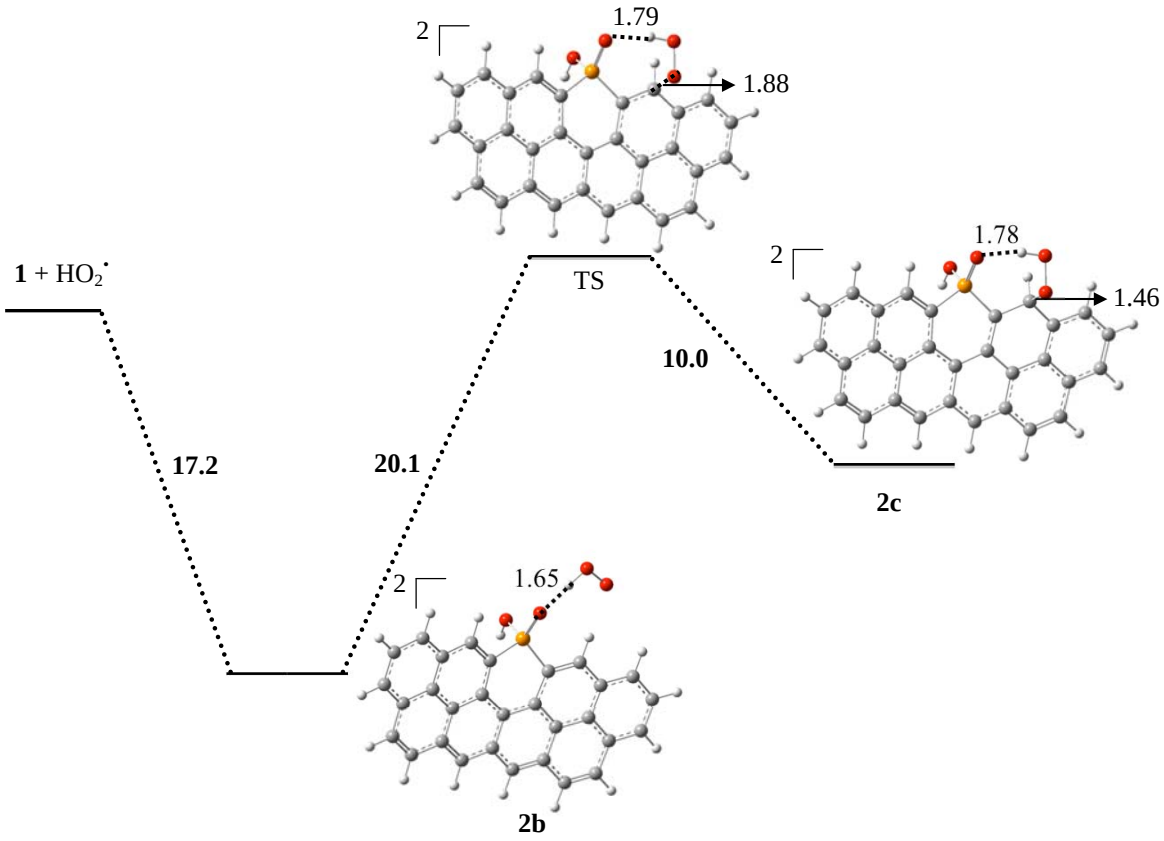


Figure S3. Energy profile (bottom-of-the-well energy) of the hydroperoxyl radical addition to **1** (in kcal/mol). Color representations: grey is for carbon, white is for hydrogen, red is for oxygen, and orange is for phosphorous. Bond lengths are shown in Å. The multiplicity is also shown.

Table S6. The relative energy of the hydroperoxyl radical addition to **1** (in kcal/mol).

	B3LYP/6-31G(d)		B3LYP/6-311++G(d,p)//B3LYP/6-31G(d)	
	ΔE^a	$\Delta H(0K)^b$	ΔE^a	$\Delta H(0K)^b$
1 + $HO_2^{\bullet}$	0.0	0.0	0.0	0.0
2b	–17.2	–15.6	–15.6	–14.0
TS	2.9	4.3	4.9	6.3
2c	–7.1	–4.5	–4.3	–1.7

[a] ΔE is the relative bottom-of-the-well energy. [b] ΔH(0K) is the relative bottom-of-the-well energy after ZPVE correction.

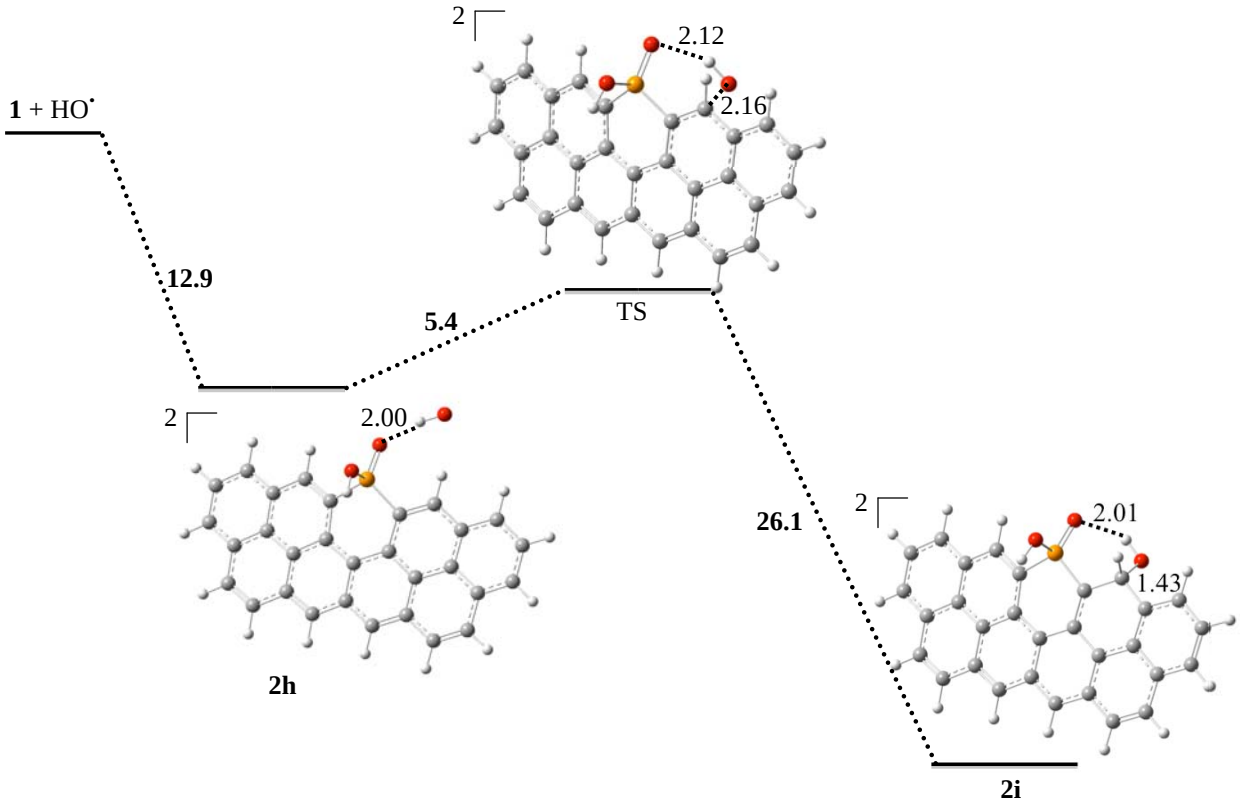


Figure S4. Energy profile (bottom-of-the-well energy) of the hydroxyl radical addition to **1** (in kcal/mol). Color representations: grey is for carbon, white is for hydrogen, red is for oxygen, and orange is for phosphorous. Bond lengths are shown in Å. The multiplicity is also shown.

Table S7. The relative energy of the hydroxyl radical addition to **1** (in kcal/mol).

	B3LYP/6-31G(d)		B3LYP/6-311++G(d,p)//B3LYP/6-31G(d)	
	ΔE^a	$\Delta H(0K)^b$	ΔE^a	$\Delta H(0K)^b$
1 + HO•	0.0	0.0	0.0	0.0
2h	–12.9	–10.8	–10.1	–8.0
TS	–7.5	–5.6	–6.1	–4.2
2i	–33.6	–29.6	–30.1	–26.1

[a] ΔE is the relative bottom-of-the-well energy. [b] ΔH(0K) is the relative bottom-of-the-well energy after ZPVE correction.

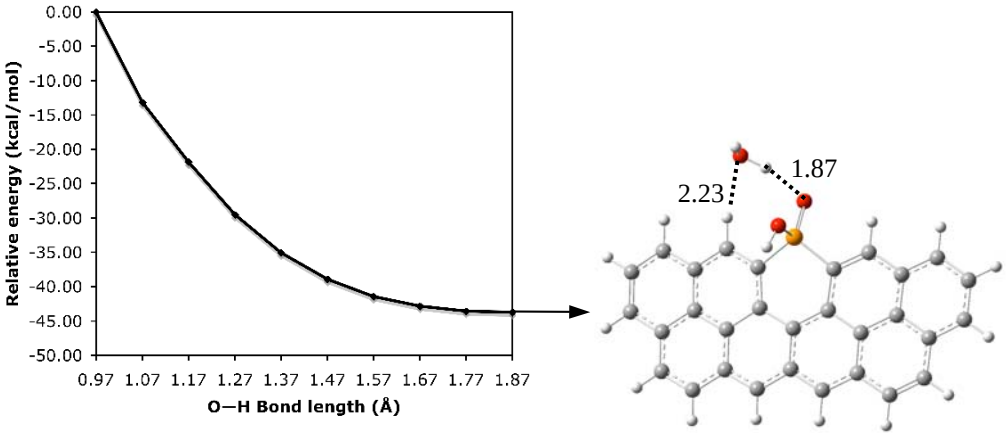


Figure S5. Potential energy surface scan of hydrogen-atom abstraction reaction by hydroxyl radical from OH moiety of **2**.

Table S8. The relative energy of each steps in the ORR catalyzed by **1** (in kcal/mol)

		B3LYP/6-31G(d)		B3LYP/6-311++G(d,p)// B3LYP/6-31G(d)	
	Species	ΔE^a	$\Delta H(0K)^b$	ΔE^a	$\Delta H(0K)^b$
1	O_2 + **1** + $4H_3O^+$ + 4e	0.0	0.0	0.0	0.0
2	O_2 + **1-H**$^+$ + H_2O + $3H_3O^+$ + 4e	–62.8	–64.0	–65.6	–66.8
3	O_2 + **2** + H_2O + $3H_3O^+$ + 3e	–165.4	–168.9	–176.1	–179.5
4	O_2-**2** + H_2O + $3H_3O^+$ + 3e	–185.6	–184.8	–190.4	–189.6
5	O_2-**2** (TS) + H_2O + $3H_3O^+$ + 3e	–185.3	–185.9	–190.9	–191.6
6	$HO_2^{\bullet}$-**1** + H_2O + $3H_3O^+$ + 3e	–204.8	–205.0	–213.4	–213.5
7	$HO_2^{\bullet}$ + **1** + H_2O + $3H_3O^+$ + 3e	–187.6	–189.4	–197.7	–199.5
8	$HO_2^{\bullet}$ + **1-H**$^+$ + $2H_2O$ + $2H_3O^+$ + 3e	–250.5	–253.4	–263.4	–266.3
9	$HO_2^{\bullet}$ + **2** + $2H_2O$ + $2H_3O^+$ + 2e	–353.1	–358.3	–373.8	–379.0
10	$HO_2^{\bullet}$-**2** + $2H_2O$ + $2H_3O^+$ + 2e	–367.9	–371.1	–386.1	–389.2
11	$HO_2^{\bullet}$-**2** (TS) + $2H_2O$ + $2H_3O^+$ + 2e	–360.5	–366.8	–379.3	–385.5
12	H_2O_2-**1** + $2H_2O$ + $2H_3O^+$ + 2e	–422.2	–422.6	–440.2	–440.6
13	H_2O_2 + **1** + $2H_2O$ + $2H_3O^+$ + 2e	–409.7	–412.1	–430.8	–433.2
14	H_2O_2 + **1-H**$^+$ + $3H_2O$ + H_3O^+ + 2e	–472.6	–476.1	–496.5	–499.9
15	H_2O_2 + **2** + $3H_2O$ + H_3O^+ + e	–575.1	–580.9	–606.9	–612.6
16	H_2O_2-**2** + $3H_2O$ + H_3O^+ + e	–588.0	–591.6	–616.7	–620.2
17	H_2O_2-**2** (TS) + $3H_2O$ + H_3O^+ + e	–579.3	–585.1	–610.3	–615.9
18	H_2O-$HO^{\bullet}$-**1** + $3H_2O$ + H_3O^+ + e	–632.5	–636.5	–663.8	–667.7
19	H_2O + $HO^{\bullet}$ + **1** + $3H_2O$ + H_3O^+ + e	–609.9	–618.5	–648.1	–656.5
20	H_2O + $HO^{\bullet}$ + **1-H**$^+$ + $4H_2O$ + e	–672.8	–682.5	–713.7	–723.3
21	H_2O + $HO^{\bullet}$ + **2** + $4H_2O$	–775.4	–787.4	–824.2	–836.0
22	$2H_2O$ + **1** + $4H_2O$	–864.3	–873.1	–913.8	–922.4

[a] ΔE is the relative bottom-of-the-well energy. [b] $\Delta H(0K)$ is the relative bottom-of-the-well energy after ZPVE correction.

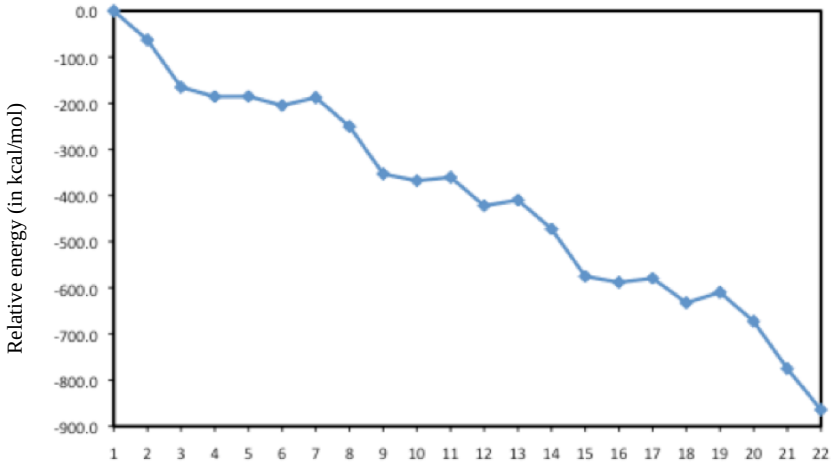


Figure S6. The energy profile of ORR catalyzed by **1** with the supply of four protons (using H_3O^+ as a proton source) and four electrons (in kcal/mol). The species (**1** – **22**) are shown in the Table S8.

Cartesian coordinates and vibrational frequencies of the studied models

1

Cartesian coordinates

1	6	0	-3.748039	0.182177	-0.147015
2	6	0	-2.480766	0.822934	0.020969
3	6	0	-1.277305	0.062037	0.077997
4	6	0	-1.406681	-1.372663	0.016019
5	6	0	-2.620352	-1.983132	-0.177924
6	6	0	-3.826427	-1.235717	-0.276140
7	6	0	-0.000001	0.734854	0.149173
8	6	0	1.406679	-1.372665	0.016003
9	6	0	1.277300	0.062036	0.077995
10	6	0	2.480763	0.822933	0.020969
11	6	0	3.748037	0.182178	-0.147016
12	6	0	3.826428	-1.235715	-0.276145
13	6	0	2.620352	-1.983130	-0.177937
14	1	0	-2.660570	-3.067543	-0.245816
15	1	0	2.660569	-3.067540	-0.245837
16	15	0	0.000002	-2.444680	0.336427
17	6	0	-0.000001	2.169068	0.227845
18	6	0	-2.441883	2.259072	0.128036
19	6	0	-1.218321	2.886732	0.246863
20	6	0	2.441881	2.259070	0.128037
21	6	0	1.218318	2.886731	0.246862
22	6	0	-5.079823	-1.854528	-0.464955
23	6	0	-4.953018	0.952572	-0.200147
24	6	0	-3.675325	3.004659	0.092219
25	6	0	3.675321	3.004660	0.092221
26	6	0	4.953015	0.952575	-0.200144
27	6	0	5.079825	-1.854524	-0.464958
28	6	0	-6.238308	-1.094388	-0.518649
29	1	0	-7.200034	-1.578497	-0.662891
30	6	0	-6.174991	0.297519	-0.384606
31	1	0	-7.087493	0.887341	-0.425373
32	6	0	-4.870952	2.384903	-0.065118
33	1	0	-5.793012	2.959875	-0.097908
34	6	0	4.870949	2.384906	-0.065115
35	1	0	5.793008	2.959879	-0.097905
36	6	0	6.174991	0.297523	-0.384601
37	1	0	7.087490	0.887350	-0.425365
38	6	0	6.238310	-1.094381	-0.518647
39	1	0	7.200035	-1.578491	-0.662887
40	1	0	-5.123362	-2.936008	-0.562656
41	1	0	5.123367	-2.936004	-0.562662
42	1	0	-3.619541	4.086265	0.186179
43	1	0	-1.178058	3.971094	0.320971
44	1	0	1.178058	3.971093	0.320967
45	1	0	3.619535	4.086266	0.186180
46	8	0	0.000005	-3.768975	-0.340388
47	8	0	0.000016	-2.648255	1.970201
48	1	0	-0.000040	-1.806825	2.457570

Vibrational frequencies

28.10	49.70	67.17
91.66	121.19	134.75
156.01	174.30	189.63
207.85	208.16	223.60
229.90	253.40	271.05
285.16	296.80	312.88
339.87	360.58	374.74
414.16	415.93	422.66
444.86	456.60	486.75
500.58	504.32	513.97
524.40	524.64	538.51
541.68	549.70	550.35
557.66	579.04	605.51
606.84	620.26	637.73
661.58	674.01	690.30
698.54	720.84	725.77
747.11	757.84	774.27
780.47	791.31	794.76
811.55	820.23	828.65
838.84	842.87	844.10
876.34	887.79	907.27
910.67	916.94	919.23
945.74	945.97	949.75
974.65	975.05	985.09
985.56	1012.09	1015.87
1031.83	1049.68	1065.85
1112.42	1116.84	1156.86
1162.77	1181.00	1181.77
1204.39	1208.90	1215.78
1244.63	1258.87	1265.96
1273.91	1274.03	1284.41
1292.16	1305.51	1334.89
1339.96	1373.58	1386.31
1393.48	1402.95	1407.05
1420.28	1430.48	1446.36
1457.36	1459.59	1481.70
1484.39	1494.02	1503.45
1528.02	1529.22	1558.06
1605.03	1624.53	1625.82
1641.84	1643.66	1649.91
1655.62	1679.95	1686.21
3178.30	3180.50	3181.64
3184.03	3184.64	3185.04
3193.22	3193.28	3196.16
3196.47	3200.22	3200.46
3210.49	3210.62	3732.14

2 (C_{2v})

Cartesian coordinates

1	6	0	3.762983	0.217489	-0.000215
2	6	0	2.484816	0.862921	0.000117
3	6	0	1.268898	0.110889	0.000152
4	6	0	1.401085	-1.331864	-0.000009
5	6	0	2.659962	-1.957045	-0.000414
6	6	0	3.851980	-1.214026	-0.000534
7	6	0	0.000000	0.788908	0.000232
8	6	0	-1.401081	-1.331869	0.000175
9	6	0	-1.268894	0.110889	0.000099
10	6	0	-2.484813	0.862920	-0.000025
11	6	0	-3.762985	0.217490	-0.000259
12	6	0	-3.851983	-1.214027	-0.000232
13	6	0	-2.659970	-1.957048	0.000036
14	1	0	2.719843	-3.042423	-0.000395
15	1	0	-2.719852	-3.042426	0.000387
16	15	0	-0.000005	-2.344605	0.000390
17	6	0	0.000001	2.232020	0.000395
18	6	0	2.441692	2.303331	0.000392
19	6	0	1.215067	2.943500	0.000543
20	6	0	-2.441688	2.303329	0.000091
21	6	0	-1.215062	2.943500	0.000344
22	6	0	5.129896	-1.832016	-0.000935
23	6	0	4.968865	0.986276	-0.000268
24	6	0	3.672990	3.047217	0.000420
25	6	0	-3.672984	3.047217	-0.000103
26	6	0	-4.968862	0.986278	-0.000488
27	6	0	-5.129903	-1.832012	-0.000458
28	6	0	6.283328	-1.067610	-0.000998
29	1	0	7.255225	-1.554152	-0.001309
30	6	0	6.209181	0.331247	-0.000663

31	1	0	7.119364	0.925440	-0.000714
32	6	0	4.877263	2.422045	0.000096
33	1	0	5.799862	2.997435	0.000092
34	6	0	-4.877258	2.422046	-0.000409
35	1	0	-5.799857	2.997437	-0.000585
36	6	0	-6.209185	0.331252	-0.000740
37	1	0	-7.119364	0.925450	-0.000940
38	6	0	-6.283334	-1.067602	-0.000722
39	1	0	-7.255231	-1.554144	-0.000913
40	1	0	5.186273	-2.917617	-0.001161
41	1	0	-5.186284	-2.917613	-0.000407
42	1	0	3.611643	4.132781	0.000682
43	1	0	1.180021	4.030622	0.000716
44	1	0	-1.180017	4.030622	0.000456
45	1	0	-3.611636	4.132780	-0.000014
46	8	0	-0.000220	-3.489067	1.173461
47	8	0	0.000251	-3.491208	-1.170636
48	1	0	-0.000257	-3.065393	-2.043892
49	1	0	0.000066	-3.061389	2.045834

Vibrational frequencies

18.97	45.09	57.86
78.90	104.44	122.28
158.63	169.44	185.73
192.26	216.44	227.04
247.27	258.68	266.37
281.02	297.26	301.51
306.57	338.79	376.49
385.43	404.48	417.44
423.52	446.49	455.65
465.02	485.15	503.84
504.92	505.93	520.09
522.48	535.72	544.16
551.36	557.87	562.44
591.64	598.79	619.94
634.86	638.12	661.82
663.09	682.69	711.30
719.20	743.25	748.15
756.79	760.82	761.61
790.29	802.13	805.20
809.77	810.34	826.89
833.25	840.12	843.37
846.47	865.36	878.85
884.47	910.66	910.94
923.19	958.72	963.92
964.00	976.21	976.90
1008.08	1030.76	1044.01
1051.23	1074.58	1097.94
1112.58	1115.73	1147.66
1168.91	1177.50	1181.62
1191.77	1206.89	1212.16
1239.99	1244.05	1266.40
1272.09	1276.02	1288.96
1297.00	1335.24	1341.15
1362.20	1364.64	1373.84
1387.81	1390.58	1407.47
1426.05	1441.37	1444.84
1455.00	1474.26	1480.33
1487.65	1496.10	1503.13
1507.11	1526.39	1570.95
1583.01	1600.46	1612.28
1621.76	1636.40	1641.28
1671.89	1676.60	3176.21
3177.24	3178.73	3179.88
3180.10	3182.94	3186.72
3187.24	3189.51	3189.67
3197.08	3197.36	3204.58
3204.78	3756.41	3757.20

2 (C_1)

Cartesian coordinates

1	6	0	-3.762221	0.220472	-0.027673
2	6	0	-2.484335	0.865482	0.000986
3	6	0	-1.268601	0.113615	0.006040
4	6	0	-1.400422	-1.328971	-0.010506
5	6	0	-2.658341	-1.952583	-0.048221
6	6	0	-3.850683	-1.210553	-0.058411
7	6	0	-0.000010	0.791390	0.018123
8	6	0	1.400435	-1.328977	-0.009855
9	6	0	1.268583	0.113614	0.005857
10	6	0	2.484312	0.865499	0.000522
11	6	0	3.762202	0.220496	-0.027868
12	6	0	3.850693	-1.210541	-0.057528
13	6	0	2.658351	-1.952581	-0.046783
14	1	0	-2.720180	-3.037341	-0.075626
15	1	0	2.720243	-3.037373	-0.073004
16	15	0	-0.000050	-2.333013	0.054988
17	6	0	-0.000015	2.234185	0.038947
18	6	0	-2.441468	2.305583	0.025641
19	6	0	-1.215085	2.945635	0.046495
20	6	0	2.441434	2.305604	0.024708
21	6	0	1.215051	2.945648	0.045890
22	6	0	-5.128015	-1.828236	-0.094561
23	6	0	-4.968108	0.989065	-0.030490
24	6	0	-3.672833	3.049431	0.026205
25	6	0	3.672785	3.049478	0.024601
26	6	0	4.968085	0.989109	-0.031248
27	6	0	5.128027	-1.828243	-0.093193
28	6	0	-6.281705	-1.064152	-0.096740
29	1	0	-7.253249	-1.550644	-0.124326
30	6	0	-6.208070	0.334262	-0.064015
31	1	0	-7.118314	0.928361	-0.066196
32	6	0	-4.876923	2.424556	-0.000281
33	1	0	-5.799567	2.999879	-0.001111
34	6	0	4.876882	2.424618	-0.001873
35	1	0	5.799515	2.999955	-0.003217
36	6	0	6.208044	0.334297	-0.064387
37	1	0	7.118283	0.928401	-0.067049
38	6	0	6.281702	-1.064144	-0.096042
39	1	0	7.253256	-1.550633	-0.123309
40	1	0	-5.184303	-2.913599	-0.120098
41	1	0	5.184324	-2.913625	-0.117877
42	1	0	-3.611571	4.134808	0.046724
43	1	0	-1.180098	4.032626	0.063485
44	1	0	1.180065	4.032641	0.062710
45	1	0	3.611499	4.134863	0.044627
46	8	0	-0.001347	-3.500759	-1.084299
47	8	0	0.001518	-3.419842	1.312881
48	1	0	0.002050	-2.955350	2.166669
49	1	0	-0.001069	-4.391319	-0.691928

Vibrational frequencies

20.76	44.43	59.12
78.89	102.56	122.57
158.81	170.34	185.51
192.63	215.22	227.11
247.60	260.38	260.68
281.70	294.62	295.22
302.39	338.84	365.24
376.81	404.90	414.68
423.73	442.31	447.39
469.28	485.37	503.97
506.27	506.42	521.06
522.66	535.84	544.59
551.60	558.13	565.09
594.35	599.45	620.41
634.76	642.72	664.12

665.01	683.68	712.55
720.08	743.21	749.25
756.88	760.26	761.17
785.16	790.44	803.40
805.27	807.10	810.11
837.61	840.80	843.76
845.79	865.04	878.12
884.06	908.19	910.75
925.37	956.88	963.06
963.14	975.95	976.66
1008.84	1030.50	1044.74
1049.86	1068.01	1094.43
1112.83	1115.75	1148.45
1169.37	1178.91	1182.83
1192.22	1207.06	1212.24
1240.52	1244.31	1266.55
1271.81	1275.78	1289.44
1297.15	1335.79	1341.64
1363.46	1365.62	1374.69
1389.52	1390.70	1407.74
1426.56	1441.62	1444.80
1455.16	1474.72	1480.76
1488.08	1496.23	1503.78
1507.74	1527.31	1572.07
1583.66	1601.11	1612.72
1622.09	1636.88	1641.58
1672.09	1676.76	3176.14
3177.12	3178.48	3179.19
3179.57	3182.89	3185.49
3186.08	3188.80	3188.94
3196.99	3197.27	3204.19
3204.40	3714.46	3748.75

2a

Cartesian coordinates

1	6	0	-3.818400	-0.368339	-0.201575
2	6	0	-2.569914	-1.022448	0.030245
3	6	0	-1.343942	-0.292209	0.031751
4	6	0	-1.414861	1.131334	-0.153597
5	6	0	-2.624464	1.749273	-0.371942
6	6	0	-3.853900	1.036044	-0.427385
7	6	0	-0.090421	-0.987515	0.189482
8	6	0	1.400655	1.072517	-0.092474
9	6	0	1.203543	-0.357719	0.064422
10	6	0	2.376220	-1.175907	0.047749
11	6	0	3.664759	-0.625966	-0.233855
12	6	0	3.795581	0.760027	-0.519401
13	6	0	2.639345	1.577940	-0.418156
14	1	0	-2.674529	2.832867	-0.457975
15	1	0	2.765229	2.643033	-0.559686
16	15	0	0.026220	2.230777	0.184550
17	6	0	-0.137754	-2.407887	0.401920
18	6	0	-2.576976	-2.442604	0.267005
19	6	0	-1.375008	-3.087726	0.467381
20	6	0	2.289810	-2.592855	0.298408
21	6	0	1.051030	-3.162645	0.497546
22	6	0	-5.087391	1.678023	-0.663313
23	6	0	-5.045335	-1.105698	-0.206473
24	6	0	-3.829018	-3.157325	0.273078
25	6	0	3.489571	-3.392503	0.309495
26	6	0	4.834818	-1.450385	-0.254291
27	6	0	5.058970	1.301494	-0.837795
28	6	0	-6.267384	0.949930	-0.675914
29	1	0	-7.213658	1.451446	-0.858206
30	6	0	-6.246296	-0.430989	-0.447595
31	1	0	-7.175783	-0.995036	-0.452425
32	6	0	-5.005292	-2.524022	0.042688
33	1	0	-5.942182	-3.075433	0.043824
34	6	0	4.703812	-2.852780	0.044267
35	1	0	5.599145	-3.469239	0.043557
36	6	0	6.069836	-0.874339	-0.569163
37	1	0	6.954855	-1.505766	-0.585130
38	6	0	6.182186	0.489686	-0.863235
39	1	0	7.153690	0.910974	-1.105347
40	1	0	-5.100737	2.752238	-0.829557
41	1	0	5.138197	2.364148	-1.050658
42	1	0	-3.802614	-4.227678	0.461404
43	1	0	-1.365089	-4.161039	0.642685
44	1	0	0.974287	-4.231604	0.682020
45	1	0	3.388664	-4.453330	0.524407
46	8	0	1.380774	3.734900	0.562636
47	8	0	1.385683	4.117927	1.820359
48	8	0	-0.441129	2.498598	1.690498
49	1	0	0.211810	3.175013	2.105510
50	8	0	-0.233620	3.278475	-1.058541
51	1	0	-0.880937	2.882098	-1.667913

Vibrational frequencies

21.91	43.61	53.73
75.82	102.63	122.48
131.26	145.84	163.19
183.77	194.89	199.89
215.70	227.18	236.67
257.42	275.91	283.43
300.15	330.79	337.86
356.03	372.13	409.69
416.38	422.18	428.96
448.53	450.18	487.37
492.59	501.94	504.07
514.09	523.56	524.08
538.95	540.37	549.51
552.81	558.67	567.43
586.15	600.52	608.54
625.76	635.80	658.18
676.11	690.32	699.52
713.00	726.98	742.11
757.85	773.61	779.43
791.39	792.44	795.93
811.47	826.16	837.97
843.32	845.63	875.00
886.09	901.41	903.76
909.37	917.39	933.10
942.31	947.35	960.09
972.39	974.34	975.65
983.26	985.15	1013.79
1032.39	1046.63	1064.22
1113.59	1117.45	1131.63
1161.54	1166.31	1180.31
1182.19	1205.06	1210.81
1220.17	1246.26	1256.05
1260.55	1269.33	1281.09
1284.27	1294.34	1313.74
1336.43	1337.75	1376.35
1386.01	1390.16	1400.47
1404.83	1425.52	1431.41
1451.55	1456.96	1458.86
1482.48	1485.08	1487.03
1495.38	1504.55	1525.86
1527.12	1560.64	1603.43
1623.09	1626.58	1639.47
1643.49	1653.22	1658.09
1681.24	1687.69	2718.17
3174.41	3179.19	3181.03
3182.23	3183.87	3185.10
3185.98	3190.60	3195.23
3200.60	3201.08	3209.27
3211.80	3251.22	3713.42

TS connected 2a and 2b

Cartesian coordinates

1	6	0	-3.827345	-0.360712	-0.196470
2	6	0	-2.581995	-1.021465	0.033628
3	6	0	-1.352432	-0.298228	0.029855
4	6	0	-1.419476	1.124445	-0.161382
5	6	0	-2.624674	1.751093	-0.378882
6	6	0	-3.857256	1.043623	-0.427069
7	6	0	-0.101076	-0.997336	0.187832
8	6	0	1.399046	1.056285	-0.098959
9	6	0	1.195638	-0.372746	0.062573
10	6	0	2.365140	-1.194870	0.048467
11	6	0	3.655862	-0.648805	-0.230902
12	6	0	3.792218	0.736810	-0.516981
13	6	0	2.638584	1.559247	-0.422162
14	1	0	-2.666328	2.834514	-0.471664
15	1	0	2.768234	2.623871	-0.563757
16	15	0	0.020937	2.204195	0.167721
17	6	0	-0.154379	-2.417017	0.402721
18	6	0	-2.594847	-2.440954	0.273759
19	6	0	-1.394955	-3.090943	0.471645
20	6	0	2.272784	-2.611332	0.299702
21	6	0	1.031533	-3.176337	0.498460
22	6	0	-5.088490	1.690853	-0.661052
23	6	0	-5.057897	-1.092084	-0.195120
24	6	0	-3.850526	-3.149118	0.285628
25	6	0	3.469703	-3.415180	0.312598
26	6	0	4.822884	-1.477395	-0.248458
27	6	0	5.058454	1.273634	-0.831792
28	6	0	-6.271759	0.968273	-0.666946
29	1	0	-7.216350	1.473551	-0.847333
30	6	0	-6.256243	-0.412071	-0.434205
31	1	0	-7.188476	-0.971553	-0.433985
32	6	0	-5.024180	-2.510013	0.057759
33	1	0	-5.963937	-3.056438	0.063562
34	6	0	4.686212	-2.879364	0.049665
35	1	0	5.579405	-3.498911	0.050686
36	6	0	6.060780	-0.905803	-0.560252
37	1	0	6.943549	-1.540413	-0.573937
38	6	0	6.178842	0.457779	-0.853968
39	1	0	7.152492	0.875607	-1.093343
40	1	0	-5.097286	2.764553	-0.830604
41	1	0	5.141968	2.335960	-1.044387
42	1	0	-3.829291	-4.219105	0.476523
43	1	0	-1.389492	-4.163932	0.649035
44	1	0	0.950711	-4.244780	0.684025
45	1	0	3.364963	-4.475641	0.527375
46	8	0	1.518086	3.802463	0.572601
47	8	0	1.368578	4.196279	1.818641
48	8	0	-0.376836	2.580509	1.643504
49	1	0	0.325882	3.333355	2.006952
50	8	0	-0.181760	3.272644	-1.060785
51	1	0	-0.835553	2.909647	-1.684808

Vibrational frequencies

-237.12	20.75	43.78
52.46	76.84	108.51
124.82	138.46	155.47
164.19	191.56	199.51
212.83	220.49	230.19
251.80	272.99	280.90
289.46	307.42	337.89
352.93	357.42	377.01
411.30	420.92	421.47
442.39	452.43	459.38
487.12	497.83	504.25
510.61	520.58	523.51
534.65	539.78	549.24
550.83	553.77	557.87
583.30	599.63	607.20
625.20	635.01	659.74
675.18	689.45	698.18
714.98	726.76	743.96
757.79	773.70	779.59
792.19	795.41	809.35
811.79	826.24	837.96
843.22	845.57	875.32
888.32	903.89	904.48
909.51	917.39	931.53
942.60	946.97	972.95
974.76	983.76	985.63
1006.32	1016.79	1032.89
1047.29	1064.78	1088.94
1113.61	1117.37	1123.35
1161.64	1166.45	1180.39
1182.47	1205.19	1210.86
1219.95	1246.31	1256.46
1266.17	1269.53	1280.53
1284.40	1294.23	1313.21
1336.42	1338.28	1376.17
1385.78	1390.26	1400.51
1405.03	1425.21	1431.47
1451.14	1457.09	1458.89
1481.82	1484.56	1485.02
1495.10	1505.06	1526.54
1527.44	1560.60	1603.88
1623.72	1626.55	1639.86
1643.76	1652.89	1657.91
1681.15	1687.56	1892.16
3174.81	3179.54	3181.40
3182.56	3184.42	3185.41
3186.30	3191.21	3195.97
3200.98	3201.28	3209.85
3212.26	3251.59	3703.63

2b

Cartesian coordinates

1	6	0	3.935473	-0.145135	-0.128561
2	6	0	2.744481	-0.923058	0.015099
3	6	0	1.464609	-0.299885	0.081674
4	6	0	1.440169	1.141408	0.048914
5	6	0	2.582019	1.885535	-0.119313
6	6	0	3.861564	1.275610	-0.222889
7	6	0	0.268390	-1.108095	0.135016
8	6	0	-1.364932	0.836731	0.055240
9	6	0	-1.074084	-0.577032	0.083519
10	6	0	-2.188914	-1.462678	0.019235
11	6	0	-3.520702	-0.960271	-0.119363
12	6	0	-3.756020	0.442764	-0.205625
13	6	0	-2.642274	1.320249	-0.102090
14	1	0	2.507739	2.968959	-0.166043
15	1	0	-2.817106	2.395179	-0.135143
16	15	0	-0.076008	2.038564	0.360823
17	6	0	0.424245	-2.535184	0.181184
18	6	0	2.861613	-2.357036	0.087495
19	6	0	1.713390	-3.116285	0.185479
20	6	0	-1.993423	-2.888271	0.089073
21	6	0	-0.707996	-3.381720	0.185723
22	6	0	5.041137	2.031855	-0.387260
23	6	0	5.217268	-0.778936	-0.192098
24	6	0	4.168690	-2.963707	0.040794
25	6	0	-3.138791	-3.762750	0.042146
26	6	0	-4.635210	-1.855437	-0.182380
27	6	0	-5.070846	0.929840	-0.361878
28	6	0	6.275023	1.403091	-0.450919

29	1	0	7.179488	1.991420	-0.576152
30	6	0	6.361495	0.009399	-0.351579
31	1	0	7.332673	-0.476850	-0.400528
32	6	0	5.290740	-2.214615	-0.093429
33	1	0	6.269773	-2.685262	-0.134493
34	6	0	-4.396481	-3.273263	-0.088938
35	1	0	-5.250637	-3.944484	-0.130062
36	6	0	-5.923031	-1.330826	-0.335313
37	1	0	-6.766657	-2.015035	-0.384463
38	6	0	-6.139961	0.049210	-0.426719
39	1	0	-7.150608	0.428844	-0.546252
40	1	0	4.967625	3.113739	-0.458576
41	1	0	-5.228071	2.002969	-0.425490
42	1	0	4.229920	-4.046962	0.107807
43	1	0	1.790980	-4.199995	0.233942
44	1	0	-0.549318	-4.456584	0.233220
45	1	0	-2.964362	-4.833802	0.106291
46	8	0	-3.139160	4.624810	-0.100487
47	8	0	-1.993563	5.283887	-0.242552
48	8	0	-0.168133	3.350679	-0.361645
49	1	0	-1.284705	4.568397	-0.282671
50	8	0	-0.121142	2.330660	1.973896
51	1	0	-0.336477	1.541683	2.499157

Vibrational frequencies

21.66	27.33	47.36
54.50	62.29	73.03
89.04	109.97	119.70
132.56	159.82	173.92
181.59	207.28	213.62
225.27	230.04	237.08
268.01	272.61	287.27
307.07	328.06	341.54
371.87	377.35	415.53
418.33	422.62	448.01
456.76	486.89	500.27
504.29	516.04	524.79
526.20	539.66	542.17
548.98	550.62	558.60
576.85	605.79	606.58
620.76	638.98	662.95
673.00	689.69	692.20
698.79	721.92	726.10
748.32	757.74	775.26
782.65	791.31	796.22
812.15	824.38	838.51
840.71	843.78	846.57
877.98	891.65	909.33
917.44	918.94	924.48
943.96	949.59	975.69
977.03	984.78	986.39
1000.12	1011.50	1018.15
1032.43	1050.20	1066.66
1113.24	1117.45	1158.16
1165.54	1180.69	1183.57
1206.16	1209.10	1218.56
1226.81	1231.58	1246.06
1259.61	1270.61	1277.16
1284.91	1294.70	1312.71
1336.69	1340.79	1374.22
1387.01	1394.45	1401.86
1406.95	1424.82	1431.22
1453.25	1458.22	1459.33
1482.21	1484.33	1495.39
1502.90	1527.35	1528.55
1559.75	1580.53	1605.34
1624.65	1626.17	1641.17
1644.14	1650.14	1655.92
1679.73	1685.83	3130.70
3166.41	3179.31	3181.47
3182.70	3185.41	3186.11
3186.42	3194.47	3198.72
3199.46	3201.04	3201.29
3212.06	3214.09	3741.87

2d

Cartesian coordinates

1	6	0	-3.751424	-0.657465	-0.094804
2	6	0	-2.471573	-1.290281	0.012948
3	6	0	-1.260314	-0.533531	-0.024115
4	6	0	-1.399196	0.902918	-0.158060
5	6	0	-2.657261	1.513893	-0.279943
6	6	0	-3.845765	0.764516	-0.255652
7	6	0	0.011953	-1.200410	0.049038
8	6	0	1.401253	0.917746	-0.157983
9	6	0	1.277162	-0.520142	-0.023370
10	6	0	2.496201	-1.264203	0.014480
11	6	0	3.769403	-0.618106	-0.092504
12	6	0	3.848989	0.804704	-0.253632
13	6	0	2.652888	1.541766	-0.279300
14	1	0	-2.720688	2.591255	-0.407723
15	1	0	2.704681	2.619536	-0.407911
16	15	0	-0.004031	1.910459	-0.086553
17	6	0	0.019377	-2.636222	0.190911
18	6	0	-2.421812	-2.722548	0.162632
19	6	0	-1.192473	-3.350839	0.253105
20	6	0	2.461313	-2.696998	0.164155
21	6	0	1.238679	-3.338134	0.253836
22	6	0	-5.124288	1.367650	-0.376413
23	6	0	-4.953036	-1.431231	-0.052686
24	6	0	-3.649723	-3.470811	0.210356
25	6	0	3.696988	-3.432386	0.212721
26	6	0	4.979068	-1.379272	-0.049442
27	6	0	5.121243	1.421238	-0.373525
28	6	0	-6.274267	0.598700	-0.333412
29	1	0	-7.247091	1.074236	-0.426350
30	6	0	-6.194840	-0.790166	-0.171014
31	1	0	-7.102114	-1.387832	-0.138147
32	6	0	-4.855812	-2.857860	0.108199
33	1	0	-5.775680	-3.436498	0.142645
34	6	0	4.896642	-2.806871	0.111456
35	1	0	5.822484	-3.375864	0.146622
36	6	0	6.214073	-0.725247	-0.166891
37	1	0	7.127571	-1.313326	-0.133215
38	6	0	6.279129	0.664444	-0.329436
39	1	0	7.247042	1.150029	-0.421647
40	1	0	-5.185217	2.445685	-0.502069
41	1	0	5.170798	2.499824	-0.499362
42	1	0	-3.584041	-4.549735	0.327525
43	1	0	-1.152272	-4.432172	0.363096
44	1	0	1.209724	-4.419830	0.363807
45	1	0	3.642484	-4.511933	0.329880
46	8	0	-0.014889	2.940419	1.287885
47	8	0	-0.002525	3.109841	-1.147167
48	1	0	-0.043829	4.032592	-0.778606
49	8	0	-0.110524	5.659972	-0.097712
50	8	0	-0.101465	5.622741	1.227875
51	1	0	-0.064892	4.643747	1.445643
52	1	0	-0.028729	2.400480	2.097135

Vibrational frequencies

7.95	23.79	47.37
47.87	57.87	91.60
113.91	119.14	138.30
151.72	176.94	182.35
184.54	195.63	228.20

244.67	257.92	263.53
272.33	282.41	283.32
320.32	324.25	332.44
339.06	374.00	403.90
419.32	421.77	446.25
460.74	476.40	485.21
503.54	505.32	506.17
521.04	523.34	535.91
544.94	551.70	555.60
566.79	595.55	597.07
606.46	619.56	630.86
641.71	663.02	667.00
668.68	686.20	689.14
714.21	721.01	755.23
756.85	761.42	763.52
764.81	790.29	804.01
808.04	810.92	813.04
843.63	844.42	847.57
866.26	875.45	880.89
886.04	910.48	926.46
928.52	964.96	965.05
968.13	976.71	977.35
1009.57	1031.30	1045.37
1073.56	1097.62	1112.56
1115.80	1147.12	1169.96
1175.12	1181.08	1192.70
1206.72	1212.37	1230.03
1241.14	1243.15	1247.99
1266.89	1271.18	1274.73
1289.38	1296.68	1335.98
1340.94	1364.57	1365.77
1374.70	1390.08	1390.86
1407.83	1426.21	1441.31
1443.82	1455.31	1474.36
1480.75	1488.19	1495.07
1503.55	1508.17	1528.03
1573.00	1583.02	1601.30
1610.85	1613.28	1621.34
1637.22	1641.87	1672.36
1676.83	3176.86	3177.94
3179.40	3180.49	3180.74
3183.39	3187.60	3188.71
3189.01	3190.15	3191.03
3197.69	3197.97	3205.15
3205.37	3324.20	3734.40

TS connected 2d and 2e

Cartesian coordinates

1	6	0	-3.640131	-0.836889	-0.111667
2	6	0	-2.325665	-1.396565	0.004335
3	6	0	-1.157729	-0.560602	-0.007586
4	6	0	-1.377034	0.850339	-0.116143
5	6	0	-2.676158	1.395590	-0.263235
6	6	0	-3.815222	0.580980	-0.262072
7	6	0	0.157495	-1.162636	0.066814
8	6	0	1.416443	1.029839	-0.101899
9	6	0	1.375223	-0.413306	0.003572
10	6	0	2.639563	-1.087743	0.018923
11	6	0	3.864267	-0.369489	-0.093005
12	6	0	3.858612	1.056701	-0.233968
13	6	0	2.618362	1.722099	-0.228719
14	1	0	-2.793822	2.469054	-0.388976
15	1	0	2.601887	2.803633	-0.332771
16	15	0	-0.053579	1.965153	-0.000468
17	6	0	0.243459	-2.596868	0.188161
18	6	0	-2.193970	-2.818706	0.139833
19	6	0	-0.916617	-3.381607	0.235410
20	6	0	2.688973	-2.522512	0.149058
21	6	0	1.506031	-3.230527	0.239265
22	6	0	-5.130020	1.105689	-0.397493
23	6	0	-4.790723	-1.680724	-0.091965
24	6	0	-3.364266	-3.634824	0.166960
25	6	0	3.965775	-3.186935	0.174928
26	6	0	5.120926	-1.059149	-0.075341
27	6	0	5.087590	1.751222	-0.360306
28	6	0	-6.237980	0.265385	-0.375498
29	1	0	-7.234346	0.687291	-0.478199
30	6	0	-6.082935	-1.109539	-0.222386
31	1	0	-6.950052	-1.764008	-0.205243
32	6	0	-4.612756	-3.088934	0.054705
33	1	0	-5.494145	-3.725243	0.071898
34	6	0	5.125849	-2.491269	0.067731
35	1	0	6.083623	-3.005271	0.084550
36	6	0	6.307901	-0.329485	-0.198976
37	1	0	7.256536	-0.860015	-0.185109
38	6	0	6.288941	1.066084	-0.342222
39	1	0	7.225086	1.608862	-0.438877
40	1	0	-5.254683	2.178879	-0.513646
41	1	0	5.069656	2.832426	-0.469659
42	1	0	-3.240165	-4.709539	0.274587
43	1	0	-0.817080	-4.460113	0.331007
44	1	0	1.537575	-4.313488	0.335766
45	1	0	3.975466	-4.269087	0.278302
46	8	0	-0.139375	2.787842	1.476402
47	8	0	-0.076166	3.197589	-0.943726
48	1	0	-0.715943	4.118359	-0.635412
49	8	0	-1.415284	5.106273	-0.283051
50	8	0	-1.243109	5.294228	1.065586
51	1	0	-0.790252	4.467817	1.380424
52	1	0	-0.329407	2.181998	2.213403

Vibrational frequencies

-1712.14	22.76	26.87
47.95	49.25	73.92
94.12	115.04	135.21
147.91	160.91	178.04
183.14	198.09	219.58
227.75	236.87	248.58
261.95	277.71	281.55
299.75	327.65	336.43
340.13	377.53	403.34
417.21	423.34	445.53
470.16	477.07	483.29
503.04	504.67	511.79
520.57	521.91	530.74
542.56	549.65	552.51
568.01	572.35	586.57
597.64	604.78	618.68
640.13	647.20	662.57
668.87	684.67	705.03
713.37	717.82	746.86
754.58	759.83	763.35
773.96	789.74	802.09
809.39	810.28	831.74
842.02	842.48	856.43
867.56	883.01	885.45
902.28	912.82	924.35
945.89	960.13	968.98
971.03	981.02	1007.30
1028.07	1041.34	1046.01
1069.18	1095.86	1108.98
1111.68	1117.15	1126.30
1151.69	1157.65	1178.45
1182.58	1197.37	1209.43
1211.33	1234.26	1246.15
1256.68	1266.76	1270.65
1277.19	1308.69	1317.59

1334.47	1345.51	1372.74
1381.95	1385.97	1392.25
1407.60	1415.85	1443.14
1444.37	1453.26	1463.18
1476.16	1479.72	1491.65
1497.36	1512.26	1527.02
1553.08	1554.86	1568.77
1576.87	1580.22	1608.01
1613.28	1616.29	1634.48
1650.72	1671.45	3178.67
3179.94	3181.94	3182.50
3184.52	3184.96	3186.10
3192.48	3194.13	3197.31
3198.13	3200.59	3207.01
3209.69	3330.31	3735.55

2e

Cartesian coordinates

1	6	0	-3.575759	-0.917296	-0.136227
2	6	0	-2.249810	-1.437637	-0.008923
3	6	0	-1.114888	-0.573205	-0.022047
4	6	0	-1.377800	0.840547	-0.146638
5	6	0	-2.654106	1.339390	-0.272120
6	6	0	-3.788531	0.484499	-0.278769
7	6	0	0.216297	-1.128225	0.071390
8	6	0	1.442892	1.085383	-0.127918
9	6	0	1.431705	-0.349871	0.004865
10	6	0	2.700326	-1.001102	0.032928
11	6	0	3.914813	-0.257400	-0.094631
12	6	0	3.879077	1.157062	-0.269253
13	6	0	2.610219	1.794842	-0.278349
14	1	0	-2.808545	2.414873	-0.342355
15	1	0	2.564075	2.873082	-0.408853
16	15	0	-0.060825	2.051395	-0.048503
17	6	0	0.340986	-2.552755	0.207910
18	6	0	-2.082831	-2.861208	0.136901
19	6	0	-0.807577	-3.375154	0.250434
20	6	0	2.783130	-2.430910	0.187672
21	6	0	1.615657	-3.159867	0.280534
22	6	0	-5.099422	0.990962	-0.406120
23	6	0	-4.709184	-1.791292	-0.121306
24	6	0	-3.244605	-3.714715	0.154939
25	6	0	4.076426	-3.066405	0.231586
26	6	0	5.183843	-0.919068	-0.060840
27	6	0	5.082119	1.880440	-0.411727
28	6	0	-6.186429	0.130822	-0.394140
29	1	0	-7.193548	0.525430	-0.493029
30	6	0	-5.991544	-1.248292	-0.252283
31	1	0	-6.848741	-1.917075	-0.241843
32	6	0	-4.495692	-3.207837	0.030215
33	1	0	-5.363255	-3.862750	0.042210
34	6	0	5.220435	-2.348780	0.113727
35	1	0	6.189311	-2.840760	0.144014
36	6	0	6.352053	-0.163187	-0.201760
37	1	0	7.313059	-0.670952	-0.175586
38	6	0	6.302867	1.224951	-0.377428
39	1	0	7.225754	1.787288	-0.486398
40	1	0	-5.240342	2.063204	-0.510776
41	1	0	5.036169	2.957850	-0.545780
42	1	0	-3.087944	-4.784448	0.267966
43	1	0	-0.670324	-4.448570	0.358361
44	1	0	1.666801	-4.240434	0.392252
45	1	0	4.109003	-4.145707	0.356839
46	8	0	-0.159225	2.639204	1.499539
47	8	0	-0.109877	3.215895	-0.985464
48	1	0	-1.490288	4.454350	-0.626949
49	8	0	-2.279265	4.690761	-0.087188
50	8	0	-1.643786	5.225200	1.106088
51	1	0	-1.300457	4.406957	1.516924
52	1	0	-0.299148	1.940106	2.161005

Vibrational frequencies

18.86	41.40	46.24
50.00	82.26	100.55
114.13	122.35	133.15
148.74	159.44	167.72
177.19	197.06	215.41
228.24	232.45	245.91
260.13	268.81	286.08
303.80	316.33	339.98
364.32	375.26	405.82
416.86	422.24	429.69
454.64	473.19	486.92
499.01	504.10	517.36
523.43	524.81	537.91
541.57	548.75	550.23
558.31	575.44	603.88
606.73	620.76	636.24
663.16	669.86	686.68
695.59	715.24	724.53
725.11	745.84	757.74
774.05	781.49	790.88
792.14	803.42	810.66
821.72	839.18	843.94
844.54	877.19	888.42
907.68	915.32	918.49
922.37	936.72	947.76
956.57	972.69	975.67
979.61	986.34	991.22
1017.17	1028.98	1032.88
1050.06	1066.93	1113.57
1117.83	1159.44	1165.57
1180.99	1183.86	1206.20
1209.68	1218.85	1242.34
1247.08	1259.69	1271.00
1278.31	1285.00	1294.42
1311.53	1336.77	1340.59
1375.03	1387.14	1393.77
1400.43	1405.54	1425.17
1431.36	1452.51	1455.60
1457.74	1459.15	1482.90
1484.08	1496.62	1498.35
1503.39	1526.67	1528.04
1560.11	1604.97	1623.92
1626.54	1640.41	1643.62
1650.91	1656.39	1680.36
1686.46	3174.63	3179.19
3181.69	3182.84	3185.56
3186.29	3186.60	3194.73
3197.48	3198.40	3201.12
3201.59	3212.50	3213.56
3528.65	3644.12	3732.96

2f

Cartesian coordinates

1	6	0	3.909329	-0.297497	-0.012235
2	6	0	2.691570	-1.050676	0.011445
3	6	0	1.414979	-0.407727	-0.013000
4	6	0	1.423294	1.040878	-0.065536
5	6	0	2.623548	1.771788	-0.103084
6	6	0	3.874539	1.135227	-0.074705
7	6	0	0.210368	-1.193352	-0.003261
8	6	0	-1.372593	0.794247	-0.051590
9	6	0	-1.113587	-0.630208	-0.027239
10	6	0	-2.259062	-1.485382	-0.021323

11	6	0	-3.588108	-0.954104	-0.042202
12	6	0	-3.802115	0.463499	-0.062494
13	6	0	-2.679278	1.308540	-0.060937
14	1	0	2.588379	2.855846	-0.165009
15	1	0	-2.842036	2.384029	-0.060394
16	15	0	-0.057500	1.915165	-0.053849
17	6	0	0.335614	-2.630269	0.036457
18	6	0	2.773373	-2.488444	0.059460
19	6	0	1.607241	-3.232972	0.069893
20	1	0	1.666778	-4.318533	0.102040
21	6	0	-2.090252	-2.916093	0.009916
22	6	0	-0.812675	-3.445437	0.039991
23	1	0	-0.682334	-4.524981	0.066036
24	8	0	-0.227893	3.000420	1.237443
25	8	0	-0.058099	3.049288	-1.193799
26	1	0	-0.566438	3.873950	-0.985639
27	1	0	-0.275682	2.497071	2.069099
28	8	0	-1.534849	5.273104	-0.505090
29	1	0	-1.073511	6.113951	-0.332869
30	8	0	-2.135004	4.999349	0.788718
31	1	0	-1.496016	4.332799	1.136185
32	6	0	-5.128324	0.968201	-0.079469
33	6	0	-4.722505	-1.825433	-0.038931
34	6	0	-3.251785	-3.764899	0.011084
35	6	0	5.094674	1.860129	-0.105538
36	6	0	5.176874	-0.958455	0.018760
37	6	0	4.064160	-3.122374	0.092972
38	6	0	-6.210612	0.106042	-0.078323
39	1	0	-7.221216	0.505667	-0.093305
40	6	0	-6.014540	-1.280931	-0.058116
41	1	0	-6.869499	-1.952185	-0.056707
42	6	0	-4.505852	-3.247710	-0.013524
43	1	0	-5.374663	-3.901537	-0.012876
44	6	0	6.309831	1.198980	-0.072192
45	1	0	7.236198	1.767030	-0.095671
46	6	0	6.356459	-0.199489	-0.009624
47	1	0	7.314317	-0.712647	0.014888
48	6	0	5.209812	-2.395636	0.075309
49	1	0	6.178633	-2.888688	0.100199
50	1	0	5.057321	2.945419	-0.155754
51	1	0	-5.278205	2.044661	-0.095854
52	1	0	-3.095792	-4.840758	0.031910
53	1	0	4.096771	-4.208512	0.131489

Vibrational frequencies

17.48	35.81	44.92
46.47	62.37	85.70
109.17	124.53	132.51
159.79	163.96	183.44
196.16	204.54	216.27
227.46	250.58	256.55
264.85	273.09	282.73
309.18	320.70	338.38
343.54	369.89	403.81
411.26	418.88	430.36
446.73	463.34	470.48
484.78	503.83	505.88
508.33	520.97	522.39
535.95	544.67	551.06
556.47	565.25	593.67
595.81	613.26	620.32
633.00	642.38	663.31
665.71	683.68	699.98
713.48	719.53	728.09
749.42	756.56	761.55
765.20	765.82	789.85
803.94	807.73	811.34
820.32	843.49	844.34
851.35	866.06	871.69
878.86	885.77	910.43
921.00	925.09	956.73
962.73	963.43	965.15
975.63	976.86	1008.59
1030.89	1044.51	1073.69
1092.31	1112.24	1115.40
1148.81	1168.31	1175.66
1180.74	1192.20	1206.39
1212.48	1230.73	1239.63
1244.03	1265.60	1272.26
1276.46	1288.60	1297.41
1335.37	1342.32	1362.70
1365.29	1365.47	1374.21
1388.41	1391.05	1407.95
1425.70	1441.02	1445.91
1454.51	1474.71	1479.86
1487.85	1496.11	1503.34
1507.94	1526.40	1547.85
1572.06	1583.68	1600.86
1612.66	1622.21	1636.67
1641.49	1672.01	1676.69
3175.73	3176.79	3178.28
3178.67	3179.39	3181.25
3182.87	3188.31	3190.15
3193.27	3196.68	3196.97
3204.15	3205.33	3376.48
3500.56	3699.55	3729.03

TS connected 2f and 2g

Cartesian coordinates

1	6	0	3.930984	-0.237671	0.026254
2	6	0	2.721543	-1.001903	-0.005941
3	6	0	1.440685	-0.368544	-0.008264
4	6	0	1.438167	1.077707	0.011781
5	6	0	2.622150	1.817791	0.036036
6	6	0	3.883475	1.193649	0.049765
7	6	0	0.240921	-1.164996	-0.034455
8	6	0	-1.365375	0.803335	0.032105
9	6	0	-1.090270	-0.615572	-0.013934
10	6	0	-2.224859	-1.483297	-0.020600
11	6	0	-3.557465	-0.965256	0.023012
12	6	0	-3.784025	0.446704	0.084345
13	6	0	-2.667019	1.305303	0.090039
14	1	0	2.576666	2.903466	0.036826
15	1	0	-2.839342	2.378741	0.146510
16	15	0	-0.059012	1.958899	-0.024987
17	6	0	0.380006	-2.598452	-0.070355
18	6	0	2.817430	-2.439429	-0.038585
19	6	0	1.658249	-3.191819	-0.074087
20	1	0	1.726028	-4.276956	-0.100861
21	6	0	-2.042995	-2.912189	-0.069302
22	6	0	-0.760601	-3.426771	-0.094754
23	1	0	-0.617575	-4.504424	-0.127825
24	8	0	-0.220086	3.012738	1.251543
25	8	0	-0.063057	3.007745	-1.207289
26	1	0	-0.754676	3.783146	-1.144274
27	1	0	-0.342642	2.523321	2.083463
28	8	0	-1.828104	4.826202	-0.994011
29	1	0	-1.494529	5.739816	-0.983329
30	8	0	-2.435106	4.820486	0.560212
31	1	0	-1.654773	4.394813	0.971755
32	6	0	-5.110510	0.943367	0.135405
33	6	0	-4.684334	-1.846844	0.012364
34	6	0	-3.197430	-3.771880	-0.085206
35	6	0	5.092380	1.933596	0.080815
36	6	0	5.205530	-0.887434	0.032650
37	6	0	4.114747	-3.062376	-0.032755
38	6	0	-6.186274	0.072857	0.123208

39	1	0	-7.199889	0.462644	0.159869
40	6	0	-5.977937	-1.311512	0.061887
41	1	0	-6.828299	-1.988681	0.052371
42	6	0	-4.455793	-3.266862	-0.046968
43	1	0	-5.318720	-3.928173	-0.058400
44	6	0	6.314518	1.284543	0.089434
45	1	0	7.234968	1.861660	0.113297
46	6	0	6.374420	-0.114867	0.065487
47	1	0	7.338039	-0.617756	0.070587
48	6	0	5.253112	-2.325531	0.002771
49	1	0	6.226570	-2.809688	0.007519
50	1	0	5.042512	3.019271	0.096151
51	1	0	-5.264913	2.018077	0.178901
52	1	0	-3.031651	-4.845552	-0.127181
53	1	0	4.157640	-4.148461	-0.057119

Vibrational frequencies

-897.81	19.37	43.30
44.59	52.60	72.55
88.51	110.59	125.59
128.38	158.56	169.53
178.61	198.55	203.56
218.55	228.11	243.42
264.03	277.15	280.83
286.91	321.00	338.70
350.67	366.52	390.94
401.85	416.63	420.92
427.95	449.62	470.30
480.81	485.55	503.90
513.16	516.09	521.21
523.55	537.92	545.52
547.72	551.16	558.82
566.81	595.28	602.42
620.67	635.79	649.08
663.85	671.10	687.00
716.22	720.09	745.47
756.40	756.83	768.57
775.44	790.01	790.87
805.92	811.86	824.74
837.15	843.79	855.69
869.55	888.90	890.85
893.07	912.44	922.99
923.82	941.96	950.57
967.17	971.35	978.34
980.80	986.84	1011.44
1032.06	1047.84	1051.27
1071.35	1077.72	1112.74
1116.15	1161.76	1171.21
1171.70	1180.59	1197.06
1207.61	1209.45	1215.33
1245.24	1249.35	1266.89
1275.34	1281.64	1293.92
1304.00	1338.03	1340.44
1354.87	1366.85	1374.66
1376.82	1392.00	1393.59
1409.44	1426.77	1446.16
1450.71	1455.82	1478.32
1480.63	1492.59	1496.57
1510.42	1513.04	1528.00
1582.06	1588.43	1609.15
1618.64	1625.93	1639.88
1645.13	1673.14	1679.58
2286.80	3171.88	3177.47
3178.73	3180.16	3182.34
3183.75	3184.53	3190.41
3193.77	3194.66	3198.45
3198.72	3206.85	3209.29
3624.04	3734.10	3744.82

2g

Cartesian coordinates

1	6	0	3.941304	-0.194267	-0.147970
2	6	0	2.742135	-0.949759	0.040435
3	6	0	1.464710	-0.318085	0.016165
4	6	0	1.451762	1.112929	-0.157469
5	6	0	2.602203	1.833340	-0.368741
6	6	0	3.879637	1.211504	-0.379692
7	6	0	0.261459	-1.110545	0.120361
8	6	0	-1.358807	0.827848	-0.176182
9	6	0	-1.076170	-0.578548	-0.004758
10	6	0	-2.195689	-1.461434	0.005429
11	6	0	-3.523953	-0.968402	-0.189763
12	6	0	-3.750349	0.421274	-0.406369
13	6	0	-2.634402	1.301186	-0.382291
14	1	0	2.534316	2.906846	-0.526048
15	1	0	-2.809816	2.371508	-0.512917
16	15	0	-0.064406	2.049309	-0.003448
17	6	0	0.407320	-2.527564	0.306501
18	6	0	2.847984	-2.370810	0.251552
19	6	0	1.692411	-3.111475	0.393938
20	1	0	1.761293	-4.185982	0.547247
21	6	0	-2.010306	-2.875232	0.211639
22	6	0	-0.729651	-3.364653	0.371462
23	1	0	-0.578436	-4.430989	0.522491
24	8	0	-0.130947	2.501881	1.602781
25	8	0	-0.145942	3.297349	-0.818310
26	1	0	-1.865672	4.299369	-0.964737
27	1	0	-0.194478	1.746117	2.212148
28	8	0	-2.768895	4.503431	-0.655638
29	1	0	-2.615754	4.768618	0.270896
30	8	0	-1.842412	4.753761	2.148461
31	1	0	-1.163298	4.052432	1.975695
32	6	0	-5.060978	0.901009	-0.613626
33	6	0	-4.643545	-1.859054	-0.177383
34	6	0	-3.160297	-3.744737	0.233945
35	6	0	5.067857	1.943495	-0.587012
36	6	0	5.220087	-0.836823	-0.119784
37	6	0	4.151703	-2.984908	0.294221
38	6	0	-6.135369	0.024362	-0.603340
39	1	0	-7.143090	0.396974	-0.763075
40	6	0	-5.927260	-1.342855	-0.385077
41	1	0	-6.774859	-2.023911	-0.376335
42	6	0	-4.414145	-3.263404	0.047308
43	1	0	-5.271665	-3.931480	0.060565
44	6	0	6.298464	1.306077	-0.560049
45	1	0	7.209692	1.875447	-0.719179
46	6	0	6.372915	-0.072258	-0.325974
47	1	0	7.341681	-0.565291	-0.304670
48	6	0	5.281619	-2.256962	0.116648
49	1	0	6.258148	-2.733732	0.144398
50	1	0	5.003186	3.013725	-0.764152
51	1	0	-5.207257	1.965087	-0.777228
52	1	0	-2.992322	-4.806099	0.398220
53	1	0	4.204099	-4.057129	0.465307

Vibrational frequencies

21.69	30.77	41.74
53.53	74.80	88.04
101.47	117.98	129.03
138.98	158.52	162.67
178.77	183.31	198.81
223.11	230.32	235.59
251.71	256.75	271.10
288.00	301.47	316.17
340.43	360.99	374.90
398.31	414.90	420.14

423.03	434.24	447.15
456.16	486.91	499.28
504.04	504.98	517.43
524.82	528.93	541.19
543.29	549.08	550.54
558.14	576.49	603.34
605.38	617.33	629.16
637.46	660.70	672.16
687.40	690.16	699.32
723.65	726.08	745.90
757.82	774.90	782.35
785.23	791.45	799.39
811.93	825.64	840.45
844.45	847.75	876.95
887.33	908.98	917.21
919.35	927.11	942.20
947.79	975.53	977.95
986.21	989.77	1017.10
1032.26	1041.53	1048.53
1050.58	1066.25	1113.07
1117.26	1158.88	1166.68
1180.82	1183.77	1206.04
1209.68	1219.33	1245.32
1252.76	1259.47	1271.61
1277.89	1286.66	1295.41
1317.21	1337.05	1341.02
1374.57	1387.20	1394.40
1400.92	1406.76	1426.00
1431.63	1455.09	1458.74
1460.88	1482.58	1484.37
1496.33	1503.05	1526.52
1528.31	1560.65	1605.33
1624.34	1626.26	1640.72
1644.16	1650.19	1656.06
1679.82	1685.86	1759.84
3116.75	3178.92	3181.30
3182.63	3185.13	3185.83
3186.40	3194.52	3197.68
3199.89	3201.01	3201.43
3212.25	3214.34	3511.05
3638.41	3712.01	3730.29

TS connected 2b and 2c

Cartesian coordinates

1	6	0	-3.946317	0.181973	-0.055473
2	6	0	-2.714469	0.905000	-0.007475
3	6	0	-1.464400	0.224788	0.113180
4	6	0	-1.514906	-1.212090	0.212947
5	6	0	-2.698647	-1.905415	0.138228
6	6	0	-3.948157	-1.242657	0.001492
7	6	0	-0.230546	0.967854	0.101362
8	6	0	1.304542	-1.036892	0.278890
9	6	0	1.090534	0.361946	0.142507
10	6	0	2.256284	1.200847	0.059010
11	6	0	3.576153	0.637601	0.074939
12	6	0	3.763091	-0.766919	0.143657
13	6	0	2.594470	-1.623998	0.137491
14	1	0	-2.683472	-2.991502	0.185370
15	1	0	2.736395	-2.632283	0.512255
16	15	0	-0.041440	-2.188424	0.502180
17	6	0	-0.314610	2.397497	0.003480
18	6	0	-2.757707	2.341218	-0.085745
19	6	0	-1.569301	3.043704	-0.068820
20	6	0	2.124613	2.624816	-0.019861
21	6	0	0.856830	3.185314	-0.040260
22	6	0	-5.167563	-1.947989	-0.063566
23	6	0	-5.194802	0.872802	-0.170736
24	6	0	-4.030441	3.009374	-0.188319
25	6	0	3.302324	3.452049	-0.072665
26	6	0	4.727551	1.486178	0.038357
27	6	0	5.054291	-1.304859	0.181421
28	6	0	-6.369047	-1.264585	-0.176270
29	1	0	-7.304782	-1.814077	-0.224852
30	6	0	-6.381555	0.133815	-0.227631
31	1	0	-7.326924	0.663456	-0.316015
32	6	0	-5.192631	2.311809	-0.228995
33	1	0	-6.146221	2.827150	-0.311336
34	6	0	4.545485	2.910023	-0.040709
35	1	0	5.428176	3.543562	-0.076560
36	6	0	6.006648	0.910840	0.078577
37	1	0	6.876609	1.562358	0.049991
38	6	0	6.170178	-0.470461	0.152693
39	1	0	7.168322	-0.897891	0.182397
40	1	0	-5.151085	-3.033795	-0.021647
41	1	0	5.174699	-2.383842	0.218515
42	1	0	-4.033043	4.095269	-0.238095
43	1	0	-1.588054	4.129252	-0.131743
44	1	0	0.751958	4.265765	-0.103977
45	1	0	3.166602	4.528761	-0.134463
46	8	0	0.024919	-3.468616	-0.276194
47	8	0	-0.043785	-2.573554	2.099814
48	1	0	-0.055430	-1.788131	2.672941
49	8	0	2.494684	-2.275948	-1.624461
50	8	0	2.388596	-3.653852	-1.563647
51	1	0	1.425195	-3.773417	-1.349808

Vibrational frequencies

-580.04	16.42	41.67
60.28	64.69	93.23
119.54	135.30	158.41
160.17	180.46	185.09
192.86	213.39	231.23
240.06	247.22	262.61
267.97	278.82	292.14
304.25	320.99	338.13
352.81	379.49	415.29
418.27	425.24	451.32
457.96	486.82	497.52
504.99	516.92	524.97
526.47	534.72	541.35
546.70	549.97	560.87
576.17	602.99	606.13
624.69	638.64	656.63
670.64	686.91	695.25
721.03	722.12	742.55
746.18	757.52	769.65
780.99	789.15	792.03
809.05	818.06	828.53
838.14	842.64	847.14
871.79	891.50	905.62
913.22	915.36	920.76
935.52	945.23	972.48
975.39	983.05	985.95
989.08	1017.42	1018.08
1032.50	1042.77	1062.10
1070.40	1114.19	1118.36
1158.36	1163.90	1180.43
1184.76	1203.82	1208.26
1217.03	1223.34	1235.19
1248.02	1267.25	1273.53
1278.12	1282.56	1298.25
1315.76	1334.20	1351.14
1369.99	1389.53	1392.44
1403.91	1412.93	1426.02
1448.99	1450.68	1458.50
1478.34	1483.20	1491.35
1494.87	1506.01	1527.78

1538.17	1539.31	1577.85
1597.68	1619.89	1628.12
1640.61	1648.58	1652.69
1673.78	1681.07	3179.98
3181.60	3182.92	3185.38
3185.91	3186.96	3193.70
3196.07	3197.27	3199.61
3201.00	3201.58	3211.86
3213.66	3349.23	3734.08

2c

Cartesian coordinates

1	6	0	-3.969012	0.165399	-0.075929
2	6	0	-2.742745	0.895076	-0.012503
3	6	0	-1.486225	0.218746	0.094358
4	6	0	-1.530069	-1.219565	0.174415
5	6	0	-2.708123	-1.918683	0.085449
6	6	0	-3.961989	-1.260332	-0.045629
7	6	0	-0.259063	0.961231	0.091081
8	6	0	1.286525	-1.031262	0.172848
9	6	0	1.076061	0.348182	0.097593
10	6	0	2.244555	1.213744	0.036904
11	6	0	3.575881	0.664778	0.025282
12	6	0	3.794715	-0.731047	0.029841
13	6	0	2.634734	-1.685150	-0.013830
14	1	0	-2.684662	-3.005140	0.116447
15	1	0	2.783556	-2.484131	0.720421
16	15	0	-0.046318	-2.177517	0.459169
17	6	0	-0.350345	2.390789	0.034519
18	6	0	-2.793578	2.329739	-0.059454
19	6	0	-1.605288	3.035788	-0.021301
20	6	0	2.097052	2.628098	0.014464
21	6	0	0.817282	3.185092	0.015329
22	6	0	-5.175980	-1.970681	-0.127622
23	6	0	-5.220830	0.851258	-0.180923
24	6	0	-4.068207	2.993899	-0.151482
25	6	0	3.256076	3.478311	-0.006038
26	6	0	4.711467	1.536375	0.010224
27	6	0	5.085621	-1.241117	0.013900
28	6	0	-6.382465	-1.292116	-0.231516
29	1	0	-7.314271	-1.846810	-0.293547
30	6	0	-6.403782	0.105834	-0.255975
31	1	0	-7.352036	0.631401	-0.337144
32	6	0	-5.226887	2.290158	-0.210275
33	1	0	-6.182978	2.801964	-0.285099
34	6	0	4.509341	2.955454	-0.003397
35	1	0	5.381666	3.604077	-0.015325
36	6	0	6.008399	0.986765	0.003193
37	1	0	6.862236	1.659762	-0.007711
38	6	0	6.196514	-0.385097	0.005410
39	1	0	7.200326	-0.800046	-0.003673
40	1	0	-5.153620	-3.056941	-0.105733
41	1	0	5.225583	-2.318236	-0.007080
42	1	0	-4.076910	4.080513	-0.178667
43	1	0	-1.626650	4.122473	-0.056534
44	1	0	0.708918	4.266500	-0.011575
45	1	0	3.101187	4.554009	-0.020623
46	8	0	-0.002793	-3.484023	-0.274352
47	8	0	0.007592	-2.503397	2.071818
48	1	0	0.003352	-1.697364	2.615812
49	8	0	2.658594	-2.351987	-1.314154
50	8	0	2.559169	-3.782264	-1.118936
51	1	0	1.580768	-3.873912	-0.986155

Vibrational frequencies

17.63	35.39	47.77
66.90	97.16	119.23
144.27	157.78	166.22
174.80	192.22	196.81
226.51	232.03	244.16
257.00	268.29	283.43
284.16	294.01	319.61
336.28	347.35	361.01
380.83	412.74	417.48
431.62	448.67	456.54
486.08	494.82	505.84
518.52	522.32	528.04
529.00	543.88	544.70
552.79	568.94	581.67
599.84	607.75	634.77
637.66	652.59	671.57
691.95	699.37	711.76
718.31	729.05	749.64
757.56	766.15	780.78
787.24	792.35	799.83
814.62	824.12	832.47
841.96	845.25	862.68
888.82	902.95	906.75
912.83	913.59	935.73
938.46	941.85	951.41
971.85	975.81	982.99
986.68	1012.80	1017.02
1020.82	1036.51	1055.12
1114.47	1116.84	1146.09
1160.48	1164.83	1180.69
1193.15	1205.06	1211.25
1219.90	1227.50	1229.15
1255.01	1268.38	1277.73
1280.88	1289.94	1307.46
1312.31	1324.52	1340.59
1363.72	1387.13	1390.94
1396.99	1408.63	1421.46
1437.59	1448.26	1454.49
1463.62	1477.01	1482.78
1491.67	1504.05	1527.49
1528.88	1533.98	1569.48
1589.41	1613.68	1625.50
1637.55	1649.11	1656.59
1666.65	1677.93	3065.74
3181.41	3182.25	3183.91
3185.50	3186.66	3189.13
3194.92	3197.62	3200.01
3201.73	3202.14	3212.58
3213.90	3400.83	3732.57

2h

Cartesian coordinates

1	6	0	3.642770	-0.575867	-0.120634
2	6	0	2.341944	-1.151729	0.024625
3	6	0	1.179568	-0.329552	0.090746
4	6	0	1.388650	1.098597	0.060182
5	6	0	2.636178	1.651313	-0.107465
6	6	0	3.797448	0.837715	-0.214602
7	6	0	-0.131162	-0.936314	0.142400
8	6	0	-1.427627	1.242885	0.056582
9	6	0	-1.371448	-0.197404	0.085836
10	6	0	-2.613508	-0.891866	0.012312
11	6	0	-3.845547	-0.181915	-0.137475
12	6	0	-3.850811	1.240929	-0.230797
13	6	0	-2.608066	1.921899	-0.117959
14	1	0	2.750538	2.733533	-0.149931
15	1	0	-2.593259	3.007997	-0.160685
16	15	0	0.033444	2.224198	0.388527
17	6	0	-0.206390	-2.369992	0.188659
18	6	0	2.227347	-2.585898	0.098567

19	6	0	0.971939	-3.151134	0.196384
20	1	0	0.874163	-4.233200	0.245384
21	6	0	-2.649669	-2.330180	0.084069
22	6	0	-1.460699	-3.023144	0.188245
23	1	0	-1.477064	-4.109526	0.236672
24	8	0	0.057926	2.463297	2.013048
25	1	0	0.208571	1.645351	2.516558
26	8	0	2.416800	5.016903	-0.397205
27	8	0	0.063712	3.557310	-0.292335
28	1	0	1.500656	4.622961	-0.378526
29	6	0	-5.070190	1.929424	-0.401395
30	6	0	-6.266465	1.232235	-0.471994
31	1	0	-7.201861	1.768955	-0.601992
32	6	0	-6.275139	-0.164146	-0.373450
33	6	0	5.082050	1.396704	-0.380693
34	6	0	6.199162	0.577768	-0.446146
35	1	0	7.186058	1.013502	-0.573011
36	6	0	6.061386	-0.811765	-0.346130
37	1	0	6.942036	-1.447589	-0.395728
38	6	0	4.805812	-1.406999	-0.184647
39	6	0	3.420129	-3.394567	0.052617
40	6	0	4.647864	-2.835542	-0.083788
41	1	0	5.538484	-3.457592	-0.124625
42	6	0	-5.089165	-0.886864	-0.208017
43	6	0	-5.081909	-2.324504	-0.109863
44	6	0	-3.920233	-3.009404	0.030328
45	1	0	-5.057232	3.013788	-0.471771
46	1	0	-7.217155	-0.704306	-0.427683
47	1	0	-6.032571	-2.849735	-0.156329
48	1	0	-3.920788	-4.094430	0.096831
49	1	0	3.306510	-4.473508	0.121145
50	1	0	5.178437	2.476646	-0.451260

Vibrational frequencies

26.93	33.85	50.53
66.04	83.54	94.30
120.10	122.46	150.39
163.19	174.66	188.28
208.04	219.81	230.21
245.94	264.43	271.83
288.82	304.63	318.16
340.41	365.91	375.17
415.98	417.36	423.11
445.15	456.77	486.83
500.47	504.45	514.90
522.94	524.78	526.72
540.44	543.43	549.31
550.42	558.43	577.90
605.88	606.42	620.50
637.66	661.57	673.78
690.88	699.08	716.37
726.21	730.40	748.06
757.79	775.43	782.59
791.38	796.48	812.61
824.25	835.52	840.74
844.03	846.87	877.74
890.48	909.26	916.87
918.54	923.61	945.38
949.28	975.50	976.62
984.89	986.12	1001.38
1014.50	1017.77	1032.30
1049.95	1066.24	1112.87
1117.14	1158.09	1165.58
1180.88	1183.15	1205.76
1209.23	1218.27	1241.33
1246.48	1259.29	1270.89
1276.72	1284.55	1294.20
1311.56	1336.35	1340.54
1374.21	1386.90	1394.11
1401.99	1407.00	1424.18
1431.17	1452.30	1458.04
1459.42	1482.19	1484.41
1495.07	1503.14	1527.25
1528.73	1559.35	1605.23
1624.57	1626.10	1641.26
1643.92	1650.11	1655.88
1679.91	1686.03	3169.30
3178.83	3181.14	3182.24
3184.91	3185.50	3185.94
3194.29	3198.05	3198.60
3200.55	3201.11	3211.74
3212.73	3397.61	3737.69

TS connected 2h and 2i

Cartesian coordinates

1	6	0	-3.673185	0.355895	-0.017015
2	6	0	-2.384789	0.977054	0.072269
3	6	0	-1.194496	0.192617	0.148329
4	6	0	-1.353709	-1.230714	0.190666
5	6	0	-2.595462	-1.842656	0.033187
6	6	0	-3.792386	-1.060605	-0.045846
7	6	0	0.098970	0.840033	0.161001
8	6	0	1.462953	-1.299792	0.136261
9	6	0	1.360824	0.138668	0.122519
10	6	0	2.581370	0.869382	0.026455
11	6	0	3.836004	0.194559	-0.098053
12	6	0	3.887028	-1.229695	-0.144451
13	6	0	2.665384	-1.945180	-0.015618
14	1	0	-2.689412	-2.910684	0.192552
15	1	0	2.686234	-3.032213	-0.031033
16	15	0	0.033099	-2.330085	0.467408
17	6	0	0.130176	2.275852	0.155371
18	6	0	-2.312949	2.411944	0.088612
19	6	0	-1.071474	3.019035	0.144775
20	1	0	-1.007632	4.104704	0.152006
21	6	0	2.573040	2.309730	0.048231
22	6	0	1.362837	2.968276	0.126986
23	1	0	1.344808	4.055661	0.136739
24	8	0	0.068772	-2.613018	2.086451
25	1	0	0.206622	-1.804214	2.608360
26	8	0	-2.078128	-2.322688	-2.008663
27	8	0	-0.048071	-3.632462	-0.258998
28	1	0	-1.438479	-3.018719	-1.733176
29	6	0	5.127806	-1.884480	-0.290041
30	6	0	6.301761	-1.152371	-0.380985
31	1	0	7.253992	-1.663184	-0.491889
32	6	0	6.265964	0.245918	-0.328788
33	1	0	7.190460	0.813732	-0.399477
34	6	0	5.057068	0.935790	-0.190063
35	6	0	3.821413	3.026757	-0.027288
36	6	0	5.004675	2.374855	-0.141314
37	1	0	5.938473	2.927805	-0.204475
38	6	0	-5.059305	-1.658625	-0.136659
39	6	0	-6.206043	-0.874865	-0.195222
40	1	0	-7.182510	-1.345078	-0.267826
41	6	0	-6.105728	0.517275	-0.162915
42	6	0	-4.859621	1.151875	-0.074493
43	6	0	-3.527609	3.185635	0.036500
44	6	0	-4.741764	2.586393	-0.041096
45	1	0	5.149217	-2.970417	-0.325954
46	1	0	3.787112	4.112899	0.001317
47	1	0	-3.443333	4.269209	0.056060
48	1	0	-5.651269	3.180334	-0.083532
49	1	0	-5.129518	-2.742223	-0.170067
50	1	0	-7.004348	1.127661	-0.208938

Vibrational frequencies

-245.42	24.49	45.44
64.75	68.20	92.02
120.38	137.92	145.52
158.29	173.88	189.95
210.54	214.96	227.61
230.97	251.12	267.68
285.70	297.11	306.47
338.94	352.14	375.38
414.27	416.21	421.41
447.18	455.70	486.81
499.66	503.36	514.25
522.69	525.08	532.70
538.04	547.57	549.87
553.88	559.48	576.16
605.41	605.48	619.45
637.58	657.34	666.65
683.19	695.46	720.87
722.74	746.72	757.69
772.77	780.19	790.83
792.91	808.18	818.36
821.56	836.22	839.41
843.92	855.12	876.57
886.85	901.54	907.77
915.79	918.68	925.94
938.93	948.08	973.27
975.50	983.89	985.95
1013.94	1017.66	1033.06
1048.98	1065.42	1113.52
1117.94	1157.94	1164.22
1181.35	1183.92	1205.40
1209.36	1216.60	1242.53
1249.35	1258.50	1270.31
1275.55	1282.18	1288.16
1301.72	1327.25	1337.72
1368.48	1381.81	1389.99
1394.61	1405.04	1416.39
1428.33	1447.86	1455.34
1459.24	1482.75	1484.39
1494.79	1498.64	1521.09
1528.25	1551.65	1592.70
1607.77	1624.12	1633.04
1642.55	1649.55	1654.27
1677.94	1683.43	3179.42
3181.49	3182.61	3185.06
3185.58	3186.16	3193.05
3195.43	3197.47	3201.04
3201.37	3211.38	3212.72
3222.68	3580.47	3733.76

2i

Cartesian coordinates

1	6	0	-3.673351	0.396677	-0.035251
2	6	0	-2.368313	1.003018	0.040234
3	6	0	-1.168130	0.185437	0.099205
4	6	0	-1.324912	-1.196538	0.137923
5	6	0	-2.637412	-1.920339	-0.084301
6	6	0	-3.834418	-1.007863	-0.087121
7	6	0	0.143997	0.841820	0.121468
8	6	0	1.487862	-1.302732	0.094038
9	6	0	1.394189	0.137974	0.086467
10	6	0	2.625849	0.861555	0.009088
11	6	0	3.875986	0.178790	-0.099553
12	6	0	3.918108	-1.246201	-0.145954
13	6	0	2.688734	-1.953898	-0.039363
14	1	0	-2.767519	-2.659113	0.725144
15	1	0	2.704704	-3.041089	-0.059037
16	15	0	0.034743	-2.315483	0.365395
17	6	0	0.182551	2.274327	0.128912
18	6	0	-2.274279	2.421268	0.076750
19	6	0	-1.015564	3.024381	0.130487
20	1	0	-0.947724	4.109279	0.151275
21	6	0	2.626481	2.298422	0.035820
22	6	0	1.415603	2.962596	0.108463
23	1	0	1.401821	4.049935	0.124184
24	8	0	0.051221	-2.705780	1.965558
25	1	0	0.150985	-1.925601	2.537409
26	8	0	-2.609285	-2.611859	-1.340540
27	8	0	-0.069217	-3.580526	-0.429651
28	1	0	-1.852911	-3.233518	-1.282904
29	6	0	5.155364	-1.908430	-0.272870
30	6	0	6.336954	-1.183945	-0.346703
31	1	0	7.286815	-1.701889	-0.443522
32	6	0	6.310175	0.213324	-0.295553
33	1	0	7.239271	0.775068	-0.353010
34	6	0	5.103005	0.912056	-0.174161
35	6	0	3.877850	3.009207	-0.025341
36	6	0	5.059483	2.349948	-0.125939
37	1	0	5.997086	2.897634	-0.177341
38	6	0	-5.102166	-1.563191	-0.177657
39	6	0	-6.245719	-0.750633	-0.209109
40	1	0	-7.230598	-1.203733	-0.279435
41	6	0	-6.113966	0.625997	-0.150112
42	6	0	-4.841180	1.223693	-0.064382
43	6	0	-3.466940	3.223778	0.054317
44	6	0	-4.695942	2.649551	-0.011659
45	1	0	5.170571	-2.994493	-0.308787
46	1	0	3.849560	4.095462	0.004400
47	1	0	-3.358338	4.304737	0.089005
48	1	0	-5.593771	3.262354	-0.030309
49	1	0	-5.199314	-2.643362	-0.237179
50	1	0	-6.992941	1.265615	-0.172607

Vibrational frequencies

20.30	46.12	61.74
69.53	101.60	119.93
147.20	159.70	177.46
192.30	199.87	217.35
231.36	239.74	244.42
270.61	274.79	291.61
299.11	327.01	337.58
357.13	381.05	413.85
415.87	426.22	444.97
452.69	483.96	493.73
497.90	513.95	522.51
528.26	529.62	545.04
545.15	550.95	572.35
581.97	596.56	606.52
618.34	622.85	641.42
654.43	672.02	692.52
710.55	717.95	727.64
748.22	757.06	766.01
780.55	787.59	791.38
803.70	815.45	819.30
833.43	840.53	848.53
862.02	884.77	902.01
903.27	912.14	924.56
936.49	939.68	970.30
975.09	981.09	985.78
992.06	1014.53	1016.45
1035.17	1039.11	1054.10
1113.77	1116.05	1141.52
1160.11	1163.21	1180.76
1192.70	1203.32	1210.52
1219.59	1227.41	1231.68
1255.10	1268.36	1277.21
1279.58	1288.59	1307.84

1309.61	1326.25	1341.14
1363.77	1377.33	1388.76
1395.98	1407.92	1418.82
1429.63	1445.49	1455.35
1462.52	1474.27	1482.80
1486.07	1493.87	1512.20
1528.97	1534.24	1569.18
1588.81	1614.58	1625.29
1637.94	1648.91	1656.77
1667.52	1678.16	2962.89
3180.37	3181.32	3183.19
3183.98	3185.94	3188.05
3191.96	3195.14	3198.97
3200.60	3201.69	3211.84
3212.95	3576.41	3732.37

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