CHEMISTRY
A EUROPEAN JOURNAL

Supporting Information

Neutral Nickel Oligo- and Polymerization Catalysts: The Importance of Alkyl Phosphine Intermediates in Chain Termination

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chem_201101152_sm_miscellaneous_information.pdf

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The standard state conversion

The standard state for each species has been taken to be 1 M ideal dilute solution. The thermodynamic functions calculated by Gaussian 03 by default assume ideal gas at 1 atm, implying that the concentration c_0 of solute is

$$c_0 = \frac{P^0}{1000RT}(mol/L), \qquad \text{(S1)}$$

where P_0 is the standard pressure 101325 Pa (1 atm). Conversion of the Gibbs free energy (chemical potential) from gas phase at 1 atm to 1 M ideal dilute solution thus involves correction of the gas phase Gibbs free energy (chemical potential) from that of the concentration of Equation S1 above to 1 mol/L:

$$\mu_i^{0`} = \mu_i^0 + RT\ln(\frac{P_i^{0`}}{P^0}). \qquad \text{(S2)}$$

In Equation S2 μ_i^0 stands for the chemical potential corresponding to the 1 atm standard state, whereas $\mu_i^{0`}$ and $P_i^{0`}$ are the chemical potential and pressure corresponding to the concentration of 1 mol/L, respectively. The latter pressure can be obtained from the Mendeleev-Clapeyron equation:

$$PV = nRT. \qquad \text{(S3)}$$

Thus, taking the concentration of substance *i*, $\frac{n_i}{V}$, to be 1 mol/L, or equivalently, 1000 mol/m^3, the corresponding pressure can be obtained as

$$P_i^{0`} = \frac{n_i}{V}RT = \frac{1000(mol)}{1(m^3)}R(\frac{J}{mol\cdot K})T(K) = 1000RT(Pa). \qquad \text{(S4)}$$

Thus, for a dissociation reaction AB → A + B, the corresponding $\Delta G^{o`}$ becomes

$$\Delta G^{0`} = \Delta G^0 + RT\ln(\frac{P_i^{0`}\cdot P_i^{0`}\cdot P^0}{P^0\cdot P^0\cdot P_i^{0`}}) = \Delta G^0 + RT\ln(\frac{P_i^{0`}}{P^0}), \qquad \text{(S5)}$$

where P_i^0 and $P_i^{0`}$ stand for the pressure of the substance *i* at a standard state of 1 atm and 1 M, respectively. Thus, for all dissociations AB = A + B, $\Delta G^{o`} = \Delta G^o + 2.02$ kcal/mol at 313.15 K and $\Delta G^{o`} = \Delta G^o + 2.36$ kcal/mol at 353.15 K . Analogously, for the corresponding association reactions A + B = AB, $\Delta G^{o`} = \Delta G^o - 2.02$ kcal/mol at 313.15 K and $\Delta G^{o`} = \Delta G^o - 2.36$ kcal/mol at 353.15 K. When modeled in solvent, each ΔG^o also includes the change of solvation Gibbs free energies ($\Delta\Delta G^o$(solv)).

Intrinsic Reaction Coordinate (IRC) calculations

All IRC calculations in the present work were performed using the PRIRODA 08 DFT code, which is the upgraded version of PRIRODA 04.[1] The choice of PRIRODA was motivated by the computational efficiency of this code. IRC calculations are computationally demanding and the PRIRODA code contains fast implementation, including density fitting algorithms,[2] of several GGA functionals as well as efficient routines for geometry optimization and IRC following. Unfortunately, BP86,[3-5] our "workhorse" functional for geometry optimization in this work (using Gaussian 03, see the Computational Details section of the main part of the paper), is not available in PRIRODA. Instead, another GGA functional, PBE,[6, 7] which often performs comparably to BP86 (including for the present systems), has been employed for the IRC calculations.

In general, default program settings were adopted, except for the gradient threshold which was tightened, from 0.0001 a.u. to 0.00001 a.u.. Built-in PRIRODA basis sets,[8] essentially of cc-pVDZ quality (Ni (21s16p11d5f)/[6s5p3d1f], C(10s7p3d)/[3s2p1d], N(10s7p3d)/[3s2p1d], P(15s11p3d)/[4s3p1d], H(6s2p)/[2s1p], O(10s7p3d)/[3s2p1d]), were used in all PRIRODA calculations. The all-electron scalar relativistic Hamiltonian was used as described in refs. [9, 10]. The transition states serving as starting points for the IRC computations were reoptimized in PRIRODA prior to starting the IRC calculations. Only a limited number of geometry optimization cycles were needed in PRIRODA to reoptimize the transition states and the resulting PBE-optimized transition states turned out to be very similar to the corresponding transition states optimized using the BP86 functional in Gaussian 03.[11] The transition states were in all cases, both in the Gaussian 03 and PRIRODA optimizations, confirmed to be first-order saddle points by the presence of a single negative eigenvalue of the Hessian matrix.

In total, three representative IRC calculations were performed to verify the connection of transition states to the respective reactants and products. For the salicylaldiminato catalyst (**III**)

the IRC started in both directions from **2a_3b_TS** lead, as expected, to **2a** and **3b**. Similarly, for the SHOP-type catalyst (**I**) the IRC started from **2a_3b_TS** also lead to **2a** and **3b,** while that from **2a_3a_TS** lead to **3a**. These specific transition states have been selected for IRC calculations due to the fact that, to the best of our knowledge, such chain rearrangement transition states have not previously been described in the literature, in contrast to, e.g., well-established ethylene insertion transition states.

Calculated energies and corrections

SHOP-type catalyst (I)

Table S1. Absolute energies and corrections for stationary points of the SHOP-type catalyst (**I**).

	E_{gas}[a][b] (BP86)	E_{gas}[a][b] (B3LYP)	E_{gas}[a][b] (BLYP)	E_{gas}[a][b] (PBE)	$\Delta H_{353.15}$[b] (BP86)	$\Delta G_{353.15}$[b] (BP86)	ΔE_{Grimme}[b][c] (BP86)	ΔE_{Grimme}[b][c] (B3LYP)	ΔE_{Grimme}[b][c] (BLYP)	ΔE_{Grimme}[b][c] (PBE)	ΔG_{solv}[d][e] (SM8)
1a	-367.7720	-367.0447	-366.1655	-367.0805	0.5483	0.4133	-0.1568	-0.1612	-0.1953	-0.0945	-22.3480
1a_2a_TS	-367.7432	-367.0072	-366.1314	-367.0531	0.5453	0.4103	-0.1603	-0.1640	-0.1986	-0.0965	-20.2640
2a	-367.7486	-367.0127	-366.1356	-367.0592	0.5466	0.4127	-0.1629	-0.1667	-0.2019	-0.0981	-19.7380
2a_3a_TS	-367.7305	-366.9891	-366.1184	-367.0400	0.5428	0.4076	-0.1595	-0.1632	-0.1976	-0.0960	-20.0870
3a	-367.7436	-367.0019	-366.1316	-367.0533	0.5447	0.4107	-0.1627	-0.1664	-0.2015	-0.0979	-20.1130
3a_4a_TS	-367.7347	-367.0046	-366.1297	-367.0433	0.5434	0.4085	-0.1631	-0.1666	-0.2017	-0.0981	-22.3840
4a	-347.0573	-346.3868	-345.6176	-346.4358	0.4575	0.3378	-0.1358	-0.1398	-0.1694	-0.0812	-25.5650
1b	-367.7690	-367.0381	-366.1608	-367.0779	0.5486	0.4150	-0.1580	-0.1624	-0.1968	-0.0952	-24.0140
2a_3b_TS	-367.7383	-366.9994	-366.1258	-367.0480	0.5428	0.4073	-0.1597	-0.1635	-0.1980	-0.0962	-20.4600
3b	-367.7566	-367.0182	-366.1463	-367.0659	0.5448	0.4096	-0.1612	-0.1649	-0.1997	-0.0971	-19.8680
3b_4b_TS	-367.7448	-367.0182	-366.1430	-367.0525	0.5435	0.4076	-0.1584	-0.1622	-0.1964	-0.0954	-21.8940
4b	-347.0662	-346.3985	-345.6285	-346.4437	0.4575	0.3353	-0.1308	-0.1353	-0.1641	-0.0784	-24.3720
1a_1b_TS	-367.7320	-367.0014	-366.1282	-367.0400	0.5463	0.4098	-0.1534	-0.1578	-0.1912	-0.0926	-24.8680
1a_5a_TS	-381.5351	-380.7706	-379.8234	-380.7962	0.6045	0.4576	-0.1757	-0.1793	-0.2170	-0.1062	-20.4850
5a	-381.5515	-380.7729	-379.8294	-380.8149	0.6062	0.4653	-0.1797	-0.1836	-0.2223	-0.1088	-17.4200
5a_7a_TS	-381.5267	-380.7600	-379.8165	-380.7876	0.6045	0.4581	-0.1619	-0.1666	-0.2019	-0.0990	-19.2880
1a_6a_TS	-367.7395	-367.0150	-366.1375	-367.0471	0.5457	0.4076	-0.1458	-0.1502	-0.1821	-0.0885	-21.4930
6a	-338.6440	-337.9978	-337.2757	-338.0541	0.4237	0.3127	-0.1166	-0.1213	-0.1472	-0.0706	-23.8270
6a_7a_TS	-352.4142	-351.7315	-350.9408	-351.7763	0.4798	0.3538	-0.1347	-0.1389	-0.1684	-0.0815	-22.3930
7a	-352.4351	-351.7458	-350.9577	-351.7983	0.4824	0.3625	-0.1333	-0.1382	-0.1676	-0.0811	-21.8700
7a_TS	-352.3982	-351.7060	-350.9167	-351.7622	0.4807	0.3597	-0.1318	-0.1367	-0.1659	-0.0804	-23.2190
7a_7b_TS	-352.4156	-351.7218	-350.9383	-351.7787	0.4806	0.3627	-0.1314	-0.1361	-0.1652	-0.0800	-22.0260
7b	-352.4303	-351.7379	-350.9529	-351.7934	0.4822	0.3612	-0.1308	-0.1359	-0.1649	-0.0797	-22.6480
7b_TS	-352.4149	-351.7232	-350.9331	-351.7790	0.4820	0.3641	-0.1317	-0.1368	-0.1661	-0.0802	-22.9530
1a_PPh	-456.8257	-455.7750	-454.5304	-455.8913	0.7202	0.5526	-0.2361	-0.2411	-0.2918	-0.1424	-34.3950

2a_PPh	-456.7999	-455.7389	-454.4976	-455.8680	0.7180	0.5583	-0.2438	-0.2476	-0.2994	-0.1469	-32.9190
2a_3b_TS_PPh	-456.7871	-455.7225	-454.4839	-455.8550	0.7153	0.5520	-0.2471	-0.2506	-0.3031	-0.1488	-31.9610
3b_TS$_{BHE}$	-367.7373	-366.9949	-366.1237	-367.0471	0.5416	0.4099	-0.1599	-0.1638	-0.1983	-0.0964	-20.2920
3b_TS$_{BHE}$_PPh	-456.7918	-455.7263	-454.4891	-455.8597	0.7147	0.5489	-0.2433	-0.2469	-0.2987	-0.1467	-32.5920
1a_1b_TS_PPh	-456.7916	-455.7356	-454.4976	-455.8569	0.7182	0.5480	-0.2333	-0.2382	-0.2883	-0.1407	-35.1940
1b'_3b_TS	-367.7384	-366.9991	-366.1269	-367.0479	0.5428	0.4074	-0.1585	-0.1622	-0.1964	-0.0955	-19.9290
3b_TS$_{phosdiss}$	-367.7264	-367.0000	-366.1270	-367.0340	0.5432	0.4037	-0.1619	-0.1666	-0.2019	-0.0990	-20.4600
5a_TS$_{BHT}$	-381.4850	-380.6972	-379.7622	-380.7480	0.5997	0.4588	-0.1770	-0.1814	-0.2197	-0.1074	-20.2980
5b_TS	-381.5097	-380.7288	-379.7865	-380.7731	0.6045	0.4597	-0.1759	-0.1800	-0.2179	-0.1065	-18.7070

[a] Electronic energy obtained from single point calculations. See the Computational Details section in the main part of the paper. [b] In Hartrees. [c] Grimme empirical dispersion correction.[12-14] See the Computational Details section in the main part of the paper. [d] SM8[15, 16] free energy of solvation, in toluene. See the Computational Details section in the main part of the paper. [e] In kcal/mol.

Table S2. Relative energies and corrections (kcal/mol) for stationary points of the SHOP-type catalyst (**I**).

	E_{gas}[a][b] (BP86)	E_{gas}[a][b] (B3LYP)	E_{gas}[a][b] (BLYP)	E_{gas}[a][b] (PBE)	$\Delta H_{353.15}$[b] (BP86)	$\Delta G_{353.15}$[b] (BP86)	ΔE_{Grimme}[b][c] (BP86)	ΔE_{Grimme}[b][c] (B3LYP)	ΔE_{Grimme}[b][c] (BLYP)	ΔE_{Grimme}[b][c] (PBE)	ΔG_{solv}[b][d] (SM8)
1a	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1a_2a_TS	18.1	23.5	21.4	17.2	-1.9	-1.9	-2.2	-1.8	-2.1	-1.2	2.1
2a	14.7	20.1	18.8	13.4	-1.1	-0.4	-3.8	-3.5	-4.1	-2.2	2.6
2a_3a_TS	26.0	34.9	29.6	25.4	-3.5	-3.6	-1.7	-1.2	-1.4	-0.9	2.3
3a	17.8	26.9	21.3	17.1	-2.3	-1.6	-3.7	-3.3	-3.9	-2.1	2.2
3a_4a_TS	23.4	25.2	22.5	23.3	-3.1	-3.1	-4.0	-3.4	-4.0	-2.2	0.0
4a	20.7	19.8	15.7	23.8	-3.6	-17.4	8.8	8.4	10.1	5.3	-3.2
1b	1.8	4.2	3.0	1.6	0.2	1.0	-0.8	-0.8	-0.9	-0.4	-1.7
2a_3b_TS	21.1	28.4	25.0	20.4	-3.5	-3.8	-1.8	-1.4	-1.7	-1.1	1.9
3b	9.7	16.6	12.1	9.1	-2.2	-2.4	-2.8	-2.3	-2.7	-1.6	2.5
3b_4b_TS	17.0	16.7	14.1	17.6	-3.1	-3.6	-1.0	-0.6	-0.7	-0.6	0.5
4b	15.1	12.5	8.8	18.9	-3.7	-18.9	11.9	11.3	13.4	7.1	-2.0
1a_1b_TS	25.1	27.2	23.4	25.4	-1.3	-2.2	2.1	2.2	2.6	1.2	-1.3
1a_5a_TS	5.3	6.9	7.2	2.8	0.6	12.3	-9.8	-8.9	-10.6	-5.8	3.1
5a	-5.0	5.5	3.5	-8.9	1.6	17.1	-12.3	-11.6	-13.8	-7.5	6.1
5a_7a_TS	10.6	13.5	11.6	8.2	0.6	12.6	-1.2	-0.9	-1.1	-1.3	4.3
1a_6a_TS	20.4	18.7	17.6	20.9	-1.6	-3.6	6.9	6.9	8.3	3.8	0.9

6a	20.9	19.0	17.5	24.1	-0.8	-14.8	15.2	14.1	16.7	8.7	-1.9
6a_7a_TS	21.8	21.0	20.1	22.8	1.4	-4.5	6.0	5.5	6.5	3.3	1.2
7a	8.7	12.0	9.6	9.0	0.3	0.9	6.8	5.9	7.0	3.5	1.7
7a_TS	31.9	36.9	35.3	31.7	0.3	-0.8	7.8	6.9	8.1	4.0	0.3
7a_7b_TS	20.9	27.1	21.7	21.3	0.2	1.0	8.0	7.2	8.5	4.2	1.5
7b	11.7	17.0	12.6	12.1	1.2	0.1	8.4	7.4	8.7	4.4	0.9
7b_TS	21.4	26.2	25.0	21.2	1.1	1.9	7.9	6.8	8.0	4.1	0.6
1a_PPh	4.8	5.0	6.0	3.9	1.5	3.4	-9.3	-8.2	-9.6	-5.6	5.5
2a_PPh	21.0	27.7	26.6	18.5	0.1	7.1	-14.2	-12.3	-14.4	-8.4	6.9
2a_3b_TS_PPh	29.0	38.0	35.2	26.7	-1.6	3.1	-16.2	-14.2	-16.7	-9.6	7.9
3b_TS$_{BHE}$	21.8	31.3	26.2	21.0	-4.3	-2.2	-2.0	-1.6	-1.9	-1.2	3.3
3b_TS$_{BHE}$_PPh	26.0	35.6	31.9	23.7	-2.0	1.2	-13.8	-11.9	-13.9	-8.2	7.3
1a_1b_TS_PPh	26.2	29.8	26.6	25.5	0.2	0.6	-7.5	-6.4	-7.4	-4.5	4.7
1b'_3b_TS	21.1	28.6	24.3	20.4	-3.5	-3.7	-1.1	-0.6	-0.7	-0.6	2.4
3b_TS$_{phosdiss}$	28.6	28.1	24.2	29.2	-3.3	-6.0	-3.2	-3.4	-4.1	-2.8	3.1
5a_TS$_{BHT}$	36.7	52.9	45.6	33.1	-2.4	13.0	-10.6	-10.2	-12.2	-6.6	3.2
5b_TS	21.3	33.2	30.3	17.3	0.6	13.6	-9.9	-9.3	-11.1	-6.0	3.6

[a] Calculated from the electronic energy obtained from single point calculations. See the Computational Details section in the main part of the paper. [b] In kcal/mol. [c] Calculated from the Grimme empirical dispersion correction.[12-14] See the Computational Details section in the main part of the paper. [d] Calculated from the SM8[15, 16] free energy of solvation, in toluene. See the Computational Details section in the main part of the paper.

Table S3. Relative Gibbs free energies (kcal/mol) for stationary points of the SHOP-type catalyst (**I**).

	ΔG_{tot} (BP86)	ΔG_{tot} (B3LYP)	ΔG_{tot} (BLYP)	ΔG_{tot} (PBE)
1a	0.0	0.0	0.0	0.0
1a_2a_TS	16.0	21.5	19.5	16.1
2a	13.1	18.5	16.9	13.4
2a_3a_TS	23.0	31.9	26.8	23.2
3a	14.7	23.7	18.0	15.5
3a_4a_TS	16.3	18.1	15.4	18.0
4a	11.2	10.4	7.5	10.9
1b	0.4	2.8	1.4	0.6
2a_3b_TS	17.4	24.7	21.4	17.4

3b	7.0	14.0	9.5	7.6
3b_4b_TS	12.9	12.5	10.3	13.9
4b	8.4	5.8	3.6	7.3
1a_1b_TS	23.7	25.7	22.5	23.1
1a_5a_TS	8.5	10.1	9.6	10.0
5a	3.5	14.0	10.4	4.4
5a_7a_TS	23.9	26.8	25.0	21.4
1a_6a_TS	24.5	22.8	23.2	22.0
6a	21.9	19.9	19.8	18.4
6a_7a_TS	24.4	23.5	23.3	22.7
7a	18.1	21.4	19.1	15.1
7a_TS	39.1	44.2	42.8	35.1
7a_7b_TS	31.5	37.6	32.8	28.0
7b	21.1	26.4	22.2	17.5
7b_TS	31.7	36.5	35.4	27.7
1a_PPh	4.3	4.6	5.3	7.2
2a_PPh	20.8	27.5	26.1	24.1
2a_3b_TS_PPh	23.8	32.8	29.5	28.1
3b_TS$_{BHE}$	20.9	30.4	25.4	20.9
3b_TS$_{BHE}$_PPh	20.6	30.2	26.4	23.9
1a_1b_TS_PPh	23.8	27.4	24.3	26.2
1b'_3b_TS	18.7	26.2	22.3	18.5
3b_TS$_{phosdiss}$	22.4	21.9	17.2	23.5
5a_TS$_{BHT}$	40.0	56.2	47.2	40.3
5b_TS	26.2	38.1	34.0	26.1

Anilinotropone catalyst (II)

Table S4. Absolute energies and corrections for stationary points of the anilinotropone catalyst (**II**).

	E_{gas}[a][b] (BP86)	E_{gas}[a][b] (B3LYP)	E_{gas}[a][b] (BLYP)	E_{gas}[a][b] (PBE)	$\Delta H_{313.15}$[b] (BP86)	$\Delta G_{313.15}$[b] (BP86)	ΔE_{Grimme}[b][c] (BP86)	ΔE_{Grimme}[b][c] (B3LYP)	ΔE_{Grimme}[b][c] (BLYP)	ΔE_{Grimme}[b][c] (PBE)	ΔG_{solv}[d][e] (SM8)
1a	-369.0871	-368.3855	-367.4890	-368.3830	0.6051	0.4950	-0.1602	-0.1651	-0.2002	-0.0993	-14.7090
1a_2a_TS	-369.0384	-368.3332	-367.4375	-368.3358	0.6013	0.4911	-0.1631	-0.1673	-0.2028	-0.1010	-13.1050
2a	-369.0419	-368.3349	-367.4397	-368.3396	0.6023	0.4915	-0.1646	-0.1690	-0.2048	-0.1019	-13.1430
2a_3a_TS	-369.0351	-368.3278	-367.4341	-368.3357	0.5992	0.4884	-0.1673	-0.1716	-0.2080	-0.1037	-12.6970
3a	-369.0481	-368.3342	-367.4458	-368.3453	0.6010	0.4926	-0.1662	-0.1705	-0.2066	-0.1030	-11.9690
3a_4a_TS	-369.0404	-368.3294	-367.4396	-368.3374	0.5999	0.4918	-0.1663	-0.1706	-0.2068	-0.1031	-12.4390
4a	-348.3751	-347.7317	-346.9440	-347.7417	0.5154	0.4159	-0.1420	-0.1459	-0.1769	-0.0874	-16.0050
1b	-369.0836	-368.3792	-367.4832	-368.3795	0.6051	0.4955	-0.1636	-0.1681	-0.2038	-0.1011	-14.5200
1b_2b_TS	-369.0358	-368.3275	-367.4360	-368.3329	0.6004	0.4905	-0.1592	-0.1634	-0.1980	-0.0988	-13.4900
2b	-369.0390	-368.3310	-367.4377	-368.3367	0.6014	0.4898	-0.1617	-0.1660	-0.2011	-0.1004	-12.9320
2b_3b_TS	-369.0364	-368.3262	-367.4349	-368.3338	0.5990	0.4870	-0.1617	-0.1660	-0.2011	-0.1004	-12.9600
3b	-369.0552	-368.3439	-367.4551	-368.3521	0.6011	0.4909	-0.1631	-0.1676	-0.2031	-0.1011	-13.2340
3b_4b_TS	-369.0477	-368.3444	-367.4526	-368.3434	0.5996	0.4876	-0.1616	-0.1661	-0.2014	-0.1001	-14.5910
4b	-348.3829	-347.7413	-346.9541	-347.7476	0.5152	0.4130	-0.1330	-0.1377	-0.1672	-0.0821	-17.9140
1a_1b_TS	-369.0532	-368.3477	-367.4566	-368.3494	0.6029	0.4921	-0.1579	-0.1627	-0.1973	-0.0978	-16.4800
2a_2b_TS	-369.0378	-368.3290	-367.4358	-368.3356	0.6007	0.4920	-0.1626	-0.1669	-0.2023	-0.1009	-13.1970
1a_5a_TS	-382.8416	-382.0991	-381.1344	-382.0913	0.6603	0.5419	-0.1823	-0.1868	-0.2263	-0.1133	-10.8810
5a	-382.8531	-382.1014	-381.1405	-382.1043	0.6612	0.5444	-0.1838	-0.1882	-0.2280	-0.1142	-9.6810
5a_7a_TS	-382.8431	-382.0992	-381.1384	-382.0925	0.6603	0.5424	-0.1722	-0.1768	-0.2142	-0.1074	-10.1080
6a	-339.9560	-339.3371	-338.5969	-339.3536	0.4819	0.3906	-0.1207	-0.1255	-0.1525	-0.0755	-15.4510
6a_7a_TS	-353.7197	-353.0627	-352.2541	-353.0700	0.5372	0.4368	-0.1387	-0.1435	-0.1741	-0.0867	-13.5870
7a	-353.7521	-353.0876	-352.2823	-353.1028	0.5404	0.4422	-0.1381	-0.1433	-0.1739	-0.0867	-13.2730
7a_TS	-353.7164	-353.0523	-352.2437	-353.0683	0.5381	0.4427	-0.1383	-0.1433	-0.1740	-0.0869	-13.7350
7a_7b_TS	-353.7318	-353.0634	-352.2629	-353.0826	0.5384	0.4421	-0.1358	-0.1411	-0.1714	-0.0853	-14.5910
7b	-353.7518	-353.0861	-352.2821	-353.1022	0.5403	0.4423	-0.1357	-0.1412	-0.1715	-0.0852	-13.8560
7b_TS	-353.7256	-353.0611	-352.2533	-353.0766	0.5392	0.4401	-0.1338	-0.1392	-0.1692	-0.0839	-14.7210
7b_TS$_{nonagostic}$	-353.7254	-353.0610	-352.2535	-353.0762	0.5394	0.4400	-0.1332	-0.1388	-0.1687	-0.0836	-14.3820
1a_PPh	-458.1384	-457.1135	-455.8519	-457.1910	0.7742	0.6372	-0.2378	-0.2436	-0.2950	-0.1462	-26.9320
1a_2a_TS_PPh	-458.0929	-457.0648	-455.8029	-457.1482	0.7706	0.6359	-0.2449	-0.2493	-0.3017	-0.1506	-25.1580
2a_PPh	-458.0948	-457.0651	-455.8035	-457.1504	0.7719	0.6366	-0.2471	-0.2516	-0.3044	-0.1519	-24.8010

5a_7a_PPh	-471.8999	-470.8322	-469.5053	-470.9070	0.8294	0.6874	-0.2521	-0.2574	-0.3114	-0.1561	-22.6580
3b_TS$_{BHE}$	-369.0341	-368.3193	-367.4305	-368.3317	0.5990	0.4890	-0.1647	-0.1690	-0.2049	-0.1021	-12.0100
3b_TS$_{BHE}$_PPh	-458.0890	-457.0516	-455.7964	-457.1443	0.7687	0.6354	-0.2472	-0.2517	-0.3046	-0.1521	-22.6620

[a] Electronic energy obtained from single point calculations. See the Computational Details section in the main part of the paper. [b] In Hartrees. [c] Grimme empirical dispersion correction.[12-14] See the Computational Details section in the main part of the paper. [d] SM8[15, 16] free energy of solvation, in toluene. See the Computational Details section in the main part of the paper. [e] In kcal/mol.

Table S5. Relative energies and corrections for stationary points of the anilinotropone catalyst (**II**).

	E_{gas}[a][b] (BP86)	E_{gas}[a][b] (B3LYP)	E_{gas}[a][b] (BLYP)	E_{gas}[a][b] (PBE)	$\Delta H_{313.15}$[b] (BP86)	$\Delta G_{313.15}$[b] (BP86)	ΔE_{Grimme}[b][c] (BP86)	ΔE_{Grimme}[b][c] (B3LYP)	ΔE_{Grimme}[b][c] (BLYP)	ΔE_{Grimme}[b][c] (PBE)	ΔG_{solv}[b][d] (SM8)
1a	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1a_2a_TS	30.6	32.9	32.3	29.6	-2.4	-2.4	-1.8	-1.4	-1.6	-1.1	1.6
2a	28.3	31.8	31.0	27.2	-1.8	-2.2	-2.8	-2.4	-2.9	-1.7	1.6
2a_3a_TS	32.6	36.2	34.4	29.7	-3.7	-4.1	-4.5	-4.1	-4.9	-2.8	2.0
3a	24.5	32.2	27.1	23.7	-2.6	-1.5	-3.8	-3.4	-4.0	-2.4	2.7
3a_4a_TS	29.3	35.2	31.0	28.6	-3.3	-2.0	-3.8	-3.4	-4.1	-2.4	2.3
4a	18.9	17.3	13.8	21.7	-3.6	-17.0	7.1	7.1	8.4	4.4	-4.3
1b	2.2	4.0	3.6	2.2	0.0	0.3	-2.1	-1.9	-2.3	-1.2	0.2
1b_2b_TS	32.2	36.4	33.3	31.4	-2.9	-2.8	0.6	1.1	1.4	0.3	1.2
2b	30.1	34.2	32.2	29.1	-2.3	-3.3	-1.0	-0.5	-0.6	-0.7	1.8
2b_3b_TS	31.8	37.2	34.0	30.9	-3.9	-5.0	-1.0	-0.6	-0.6	-0.7	1.7
3b	20.0	26.1	21.3	19.4	-2.6	-2.5	-1.8	-1.5	-1.8	-1.1	1.5
3b_4b_TS	24.7	25.8	22.8	24.9	-3.4	-4.6	-0.9	-0.6	-0.7	-0.5	0.1
4b	14.1	11.2	7.5	18.0	-3.7	-18.8	12.7	12.2	14.5	7.8	-6.2
1a_1b_TS	21.3	23.7	20.3	21.1	-1.4	-1.8	1.4	1.5	1.8	0.9	-1.8
2a_2b_TS	30.9	35.5	33.4	29.8	-2.8	-1.9	-1.5	-1.1	-1.3	-1.0	1.5
1a_5a_TS	10.7	14.6	15.0	7.5	0.4	11.7	-11.4	-13.6	-13.3	-7.3	5.4
5a	3.5	13.2	11.2	-0.7	1.0	13.3	-12.3	-14.5	-14.3	-7.9	6.6
5a_7a_TS	9.8	14.6	12.5	6.7	0.4	12.1	-5.1	-7.3	-5.7	-3.6	6.2
6a	22.9	19.9	18.9	25.9	-1.0	-13.9	14.8	13.9	16.5	8.6	-1.1
6a_7a_TS	27.9	27.0	26.5	28.3	-0.5	-2.6	5.6	5.0	6.0	2.9	2.3
7a	7.5	11.4	8.8	7.8	1.5	0.8	6.0	5.2	6.1	3.0	2.6
7a_TS	29.9	33.5	33.1	29.4	0.0	1.1	5.8	5.1	6.1	2.9	2.2

7a_7b_TS	20.3	26.6	21.0	20.5	0.2	0.7	7.4	6.5	7.7	3.8	1.3
7b	7.7	12.3	9.0	8.1	1.4	0.9	7.5	6.5	7.6	3.9	2.0
7b_TS	24.1	28.0	27.0	24.2	0.7	-0.6	8.7	7.7	9.1	4.7	1.2
7b_TS$_{nonagostic}$	24.3	28.1	26.9	24.4	0.9	-0.6	9.0	8.0	9.3	4.9	1.5
1a_PPh	6.3	6.4	7.2	5.6	1.5	2.9	-8.3	-7.3	-8.6	-5.0	5.3
1a_2a_TS_PPh	34.8	37.0	38.0	32.5	-0.7	2.0	-12.7	-10.9	-12.8	-7.7	7.1
2a_PPh	33.6	36.8	37.6	31.1	0.1	2.5	-14.1	-12.4	-14.5	-8.6	7.4
5a_7a_TS_PPh	12.7	17.9	17.2	8.3	1.9	16.7	-15.2	-13.5	-15.8	-9.7	11.1
3b_TS$_{BHE}$	33.2	41.5	36.7	32.2	-3.8	-3.7	-2.8	-2.5	-2.9	-1.8	2.7
3b_TS$_{BHE}$_PPh	37.3	45.3	42.1	35.0	-1.9	1.7	-14.2	-12.4	-14.6	-8.7	9.5

[a] Calculated from the electronic energy obtained from single point calculations. See the Computational Details section in the main part of the paper. [b] In kcal/mol. [c] Calculated from the Grimme empirical dispersion correction.[12-14] See the Computational Details section in the main part of the paper. [d] Calculated from the SM8[15, 16] free energy of solvation, in toluene. See the Computational Details section in the main part of the paper.

Table S6. Relative Gibbs free energies (kcal/mol) for stationary points of the anilinotropone catalyst (**II**).

	ΔG_{tot} (BP86)	ΔG_{tot} (B3LYP)	ΔG_{tot} (BLYP)	ΔG_{tot} (PBE)
1a	0.0	0.0	0.0	0.0
1a_2a_TS	28.0	30.2	29.9	27.7
2a	24.9	28.4	27.5	24.9
2a_3a_TS	26.0	29.6	27.5	24.8
3a	21.9	29.6	24.3	22.5
3a_4a_TS	25.7	31.7	27.2	26.5
4a	6.8	5.1	3.0	6.8
1b	0.6	2.4	1.9	1.6
1b_2b_TS	31.2	35.4	33.1	30.1
2b	27.7	31.8	30.2	26.9
2b_3b_TS	27.5	33.0	30.1	26.9
3b	17.1	23.3	18.4	17.2
3b_4b_TS	19.3	20.5	17.6	19.8
4b	3.8	1.0	-0.9	2.8
1a_1b_TS	19.1	21.5	18.6	18.4
2a_2b_TS	29.0	33.6	31.8	28.4

1a_5a_TS	14.4	18.3	16.9	15.2
5a	9.1	18.8	14.8	9.3
5a_7a_TS	20.9	25.7	23.0	19.3
6a	24.6	21.7	22.3	21.4
6a_7a_TS	33.2	32.3	32.2	31.0
7a	16.9	20.8	18.3	14.2
7a_TS	39.0	42.6	42.4	35.5
7a_7b_TS	29.7	36.0	30.8	26.3
7b	18.1	22.7	19.5	15.0
7b_TS	33.4	37.3	36.7	29.5
7b_TS$_{nonagostic}$	34.2	38.0	37.2	30.2
1a_PPh	6.2	6.3	6.8	8.8
1a_2a_TS_PPh	31.2	33.4	34.3	33.9
2a_PPh	29.4	32.6	33.0	32.4
5a_7a_PPh	23.3	28.5	27.2	24.4
3b_TS$_{BHE}$	29.4	37.7	32.8	29.4
3b_TS$_{BHE}$_PPh	34.4	42.4	38.8	37.6

Salicylaldiminato catalyst (III)

Table S7. Absolute energies and corrections for stationary points of the salicylaldiminato catalyst (**III**).

	E_{gas} [a][b] (BP86)	E_{gas} [a][b] (B3LYP)	E_{gas} [a][b] (BLYP)	E_{gas} [a][b] (PBE)	$\Delta H_{313.15}$ [b] (BP86)	$\Delta G_{313.15}$ [b] (BP86)	ΔE_{Grimme} [b][c] (BP86)	ΔE_{Grimme} [b][c] (B3LYP)	ΔE_{Grimme} [b][c] (BLYP)	ΔE_{Grimme} [b][c] (PBE)	ΔG_{solv} [d][e] (SM8)
1a	-453.7047	-452.7040	-451.4426	-452.7649	0.7880	0.6511	-0.2320	-0.2387	-0.2893	-0.1437	-23.8120
1a_2a_TS	-453.6591	-452.6546	-451.3954	-452.7205	0.7840	0.6487	-0.2304	-0.2368	-0.2868	-0.1429	-22.8440
2a	-453.6622	-452.6561	-451.3969	-452.7240	0.7851	0.6486	-0.2330	-0.2394	-0.2900	-0.1445	-22.4140
2a_3b_TS	-453.6535	-452.6422	-451.3869	-452.7156	0.7816	0.6454	-0.2356	-0.2419	-0.2931	-0.1461	-21.8880
3a	-453.6666	-452.6540	-451.4013	-452.7280	0.7841	0.6498	-0.2350	-0.2413	-0.2924	-0.1457	-21.5550
3a_4a_TS	-453.6570	-452.6487	-451.3941	-452.7175	0.7826	0.6487	-0.2342	-0.2407	-0.2917	-0.1452	-23.1540
4a	-432.9928	-432.0486	-430.8987	-432.1220	0.6981	0.5705	-0.2053	-0.2119	-0.2572	-0.1266	-28.5430
1b	-453.6963	-452.6925	-451.4333	-452.7572	0.7871	0.6546	-0.2322	-0.2388	-0.2895	-0.1437	-25.8860
1b_2b_TS	-453.6565	-452.6487	-451.3941	-452.7175	0.7829	0.6470	-0.2294	-0.2355	-0.2852	-0.1423	-22.6970
2b	-453.6591	-452.6529	-451.3948	-452.7208	0.7840	0.6469	-0.2312	-0.2373	-0.2874	-0.1434	-22.3870
2b_3b_TS	-453.6571	-452.6484	-451.3925	-452.7186	0.7815	0.6451	-0.2313	-0.2375	-0.2876	-0.1435	-22.3160
3b	-453.6770	-452.6673	-451.4136	-452.7381	0.7840	0.6482	-0.2331	-0.2394	-0.2900	-0.1445	-22.3610
3b_4b_TS	-453.6692	-452.6656	-451.4098	-452.7297	0.7828	0.6461	-0.2331	-0.2393	-0.2899	-0.1446	-22.6680
4b	-433.0056	-432.0643	-430.9135	-432.1339	0.6982	0.5686	-0.2008	-0.2076	-0.2519	-0.1241	-27.9810
1a_1b_TS	-453.6717	-452.6665	-451.4124	-452.7314	0.7854	0.6484	-0.2249	-0.2319	-0.2810	-0.1394	-27.1210
1a_5a_TS	-467.4597	-466.4185	-465.0887	-466.4743	0.8428	0.6985	-0.2559	-0.2619	-0.3170	-0.1589	-18.9590
5a	-467.4709	-466.4209	-465.0951	-466.4865	0.8441	0.7029	-0.2548	-0.2610	-0.3160	-0.1583	-18.6700
5a_7a_TS	-467.4585	-466.4174	-465.0928	-466.4716	0.8430	0.6956	-0.2369	-0.2437	-0.2952	-0.1479	-20.8340
6a	-424.5794	-423.6603	-422.5575	-423.7395	0.6647	0.5455	-0.1836	-0.1912	-0.2322	-0.1144	-27.9330
6a_7a_TS	-438.3421	-437.3857	-436.2143	-437.4554	0.7203	0.5933	-0.2058	-0.2130	-0.2584	-0.1282	-25.1860
7a	-438.3676	-437.4044	-436.2356	-437.4813	0.7234	0.5987	-0.2022	-0.2099	-0.2548	-0.1265	-24.9450
7a_TS	-438.3320	-437.3673	-436.1968	-437.4468	0.7216	0.5952	-0.2027	-0.2103	-0.2553	-0.1268	-25.5630
7a_7b_TS	-438.3551	-437.3870	-436.2235	-437.4690	0.7209	0.5980	-0.2013	-0.2088	-0.2534	-0.1258	-25.7450
7b	-438.3674	-437.4020	-436.2350	-437.4816	0.7233	0.5996	-0.2024	-0.2101	-0.2551	-0.1266	-25.3100
7b_TS	-438.3443	-437.3789	-436.2088	-437.4593	0.7215	0.5945	-0.2020	-0.2096	-0.2543	-0.1263	-24.9950
3b_TS$_{BHE}$	-453.6535	-452.6413	-451.3876	-452.7149	0.7821	0.6468	-0.2314	-0.2379	-0.2883	-0.1436	-22.5320

[a] Electronic energy obtained from single point calculations. See the Computational Details section in the main part of the paper. [b] In Hartrees. [c] Grimme empirical dispersion correction.[12-14] See the Computational Details section in the main part of the paper. [d] SM8[15, 16] free energy of solvation, in toluene. See the Computational Details section in the main part of the paper. [e] In kcal/mol.

Table S8. Relative energies and corrections for stationary points of the salicylaldiminato catalyst (**III**).

	E_{gas}[a][b] (BP86)	E_{gas}[a][b] (B3LYP)	E_{gas}[a][b] (BLYP)	E_{gas}[a][b] (PBE)	$\Delta H_{313.15}$[b] (BP86)	$\Delta G_{313.15}$[b] (BP86)	ΔE_{Grimme}[b][c] (BP86)	ΔE_{Grimme}[b][c] (B3LYP)	ΔE_{Grimme}[b][c] (BLYP)	ΔE_{Grimme}[b][c] (PBE)	ΔG_{solv}[b][d] (SM8)
1a	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1a_2a_TS	28.6	31.0	29.6	27.8	-2.5	-1.5	1.0	1.2	1.6	0.5	1.0
2a	26.7	30.1	28.7	25.6	-1.9	-1.5	-0.6	-0.4	-0.5	-0.5	1.4
2a_3b_TS	32.1	38.8	34.9	30.9	-4.0	-3.5	-2.2	-2.0	-2.4	-1.5	1.9
3a	23.9	31.4	25.9	23.1	-2.5	-0.8	-1.9	-1.6	-1.9	-1.2	2.3
3a_4a_TS	30.0	24.1	20.6	22.1	-3.4	-1.4	-1.4	-1.2	-1.5	-0.9	0.7
4a	18.9	18.2	13.1	22.6	-3.7	-17.9	12.4	11.8	14.0	7.7	-4.7
1b	5.2	7.2	5.8	4.8	-0.6	2.2	-0.1	-0.1	-0.1	0.0	-2.1
1b_2b_TS	30.2	34.7	30.4	29.7	-3.2	-2.5	1.6	2.0	2.6	0.9	1.1
2b	28.6	32.1	30.0	27.7	-2.5	-2.6	0.5	0.9	1.2	0.2	1.4
2b_3b_TS	29.9	34.9	31.5	29.0	-4.1	-3.7	0.4	0.8	1.1	0.1	1.5
3b	17.4	23.0	18.2	16.8	-2.5	-1.8	-0.7	-0.4	-0.5	-0.5	1.5
3b_4b_TS	22.3	24.1	20.6	22.1	-3.3	-3.1	-0.7	-0.4	-0.4	-0.5	1.1
4b	10.9	8.4	3.8	15.1	-3.6	-19.1	15.2	14.5	17.3	9.3	-4.2
1a_1b_TS	20.7	23.5	19.0	21.0	-1.7	-1.7	4.4	4.3	5.2	2.7	-3.3
1a_5a_TS	10.4	14.0	14.6	6.8	0.1	12.1	-12.6	-11.5	-14.3	-8.0	6.4
5a	3.4	12.5	10.6	-0.9	0.9	14.9	-11.9	-10.9	-13.7	-7.7	6.7
5a_7a_TS	11.2	14.7	12.0	8.4	0.3	10.3	-0.6	-0.1	-0.6	-1.2	4.6
6a	19.3	17.0	14.5	23.4	-1.0	-14.7	20.4	18.8	22.3	12.0	-4.5
6a_7a_TS	24.9	24.1	22.4	26.1	-0.4	-2.4	8.5	7.6	9.0	4.9	-0.2
7a	8.8	12.4	9.0	9.8	1.6	1.0	10.8	9.5	11.2	5.9	0.1
7a_TS	31.2	35.7	33.3	31.5	0.4	-1.1	10.5	9.3	10.9	5.7	-0.6
7a_7b_TS	16.7	23.3	16.6	17.6	0.0	0.6	11.4	10.2	12.1	6.3	-0.7
7b	9.0	13.9	9.4	9.6	1.5	1.6	10.7	9.4	11.1	5.8	-0.3
7b_TS	23.5	28.4	25.8	23.7	0.3	-1.6	10.9	9.7	11.5	6.0	0.0
3b_TS$_{BHE}$	32.1	39.4	34.5	31.4	-3.7	-2.6	0.4	0.5	0.7	0.1	1.3

[a] Calculated from the electronic energy obtained from single point calculations. See the Computational Details section in the main part of the paper. [b] In kcal/mol. [c] Calculated from the Grimme empirical dispersion correction.[12-14] See the Computational Details section in the main part of the paper. [d] Calculated from the SM8[15, 16] free energy of solvation, in toluene. See the Computational Details section in the main part of the paper.

Table S9. Relative Gibbs free energies (kcal/mol) for stationary points of the salicylaldiminato catalyst (**III**).

	ΔG_{tot} (BP86)	ΔG_{tot} (B3LYP)	ΔG_{tot} (BLYP)	ΔG_{tot} (PBE)
1a	0.0	0.0	0.0	0.0
1a_2a_TS	29.1	31.5	30.7	27.9
2a	25.9	29.3	28.1	25.0
2a_3b_TS	28.3	34.9	31.0	27.8
3a	23.5	31.0	25.5	23.4
3a_4a_TS	27.8	21.9	18.3	20.3
4a	10.7	10.0	6.5	9.7
1b	5.3	7.3	5.9	5.0
1b_2b_TS	30.5	34.9	31.6	29.2
2b	27.9	31.4	30.0	26.6
2b_3b_TS	28.1	33.1	30.3	27.0
3b	16.4	22.0	17.4	16.0
3b_4b_TS	19.6	21.4	18.3	19.6
4b	4.8	2.3	-0.2	3.2
1a_1b_TS	20.1	23.0	19.2	18.7
1a_5a_TS	14.4	18.0	16.8	15.2
5a	11.1	20.2	16.5	11.0
5a_7a_TS	23.3	26.9	24.2	20.1
6a	22.5	20.2	19.6	18.3
6a_7a_TS	30.8	30.1	28.8	28.4
7a	20.7	24.3	21.3	16.9
7a_TS	40.0	44.5	42.6	35.6
7a_7b_TS	28.0	34.6	28.6	23.8
7b	20.9	25.9	21.8	16.8
7b_TS	32.8	37.7	35.7	28.1
3b_TS$_{BHE}$	31.1	38.4	33.8	30.1

Pyrazolonato-phosphane catalyst (IV)

Table S10. Absolute energies and corrections for stationary points of the pyrazolonato-phosphane catalyst (**IV**).

	E_{gas}[a][b] (BP86)	E_{gas}[a][b] (B3LYP)	E_{gas}[a][b] (BLYP)	E_{gas}[a][b] (PBE)	$\Delta H_{353.15}$[b] (BP86)	$\Delta G_{353.15}$[b] (BP86)	ΔE_{Grimme}[b][c] (BP86)	ΔE_{Grimme}[b][c] (B3LYP)	ΔE_{Grimme}[b][c] (BLYP)	ΔE_{Grimme}[b][c] (PBE)	ΔG_{solv}[d][e] (SM8)
1a	-400.3158	-399.4949	-398.5121	-399.5489	0.5977	0.4536	-0.1759	-0.1804	-0.2185	-0.1064	-22.9530
1a_2a_TS	-400.2896	-399.4603	-398.4811	-399.5237	0.5948	0.4529	-0.1787	-0.1824	-0.2208	-0.1080	-21.0120
2a	-400.2978	-399.4681	-398.4874	-399.5329	0.5961	0.4527	-0.1831	-0.1870	-0.2264	-0.1106	-20.0050
2a_3b_TS	-400.2854	-399.4497	-398.4734	-399.5204	0.5920	0.4481	-0.1827	-0.1865	-0.2258	-0.1104	-19.9060
3b	-400.3011	-399.4688	-398.4932	-399.5350	0.5941	0.4501	-0.1808	-0.1845	-0.2234	-0.1093	-19.9120
7a	-384.9785	-384.1951	-383.3038	-384.2661	0.5317	0.4019	-0.1518	-0.1567	-0.1901	-0.0926	-22.5420
7a_7b_TS	-384.9615	-384.1744	-383.2872	-384.2485	0.5296	0.3991	-0.1482	-0.1531	-0.1857	-0.0905	-22.9290
7b_TS	-384.9576	-384.1722	-383.2787	-384.2461	0.5312	0.4028	-0.1503	-0.1555	-0.1886	-0.0918	-23.6260
3b_TS$_{BHE}$	-400.2813	-399.4453	-398.4704	-399.5159	0.5920	0.4484	-0.1796	-0.1836	-0.2223	-0.1087	-20.2910

[a] Electronic energy obtained from single point calculations. See the Computational Details section in the main part of the paper. [b] In Hartrees. [c] Grimme empirical dispersion correction.[12-14] See the Computational Details section in the main part of the paper. [d] SM8[15, 16] free energy of solvation, in toluene. See the Computational Details section in the main part of the paper. [e] In kcal/mol.

Table S11. Relative energies and corrections for stationary points of the pyrazolonato-phosphane catalyst (**IV**).

	E_{gas}[a][b] (BP86)	E_{gas}[a][b] (B3LYP)	E_{gas}[a][b] (BLYP)	E_{gas}[a][b] (PBE)	$\Delta H_{353.15}$[b] (BP86)	$\Delta G_{353.15}$[b] (BP86)	ΔE_{Grimme}[b][c] (BP86)	ΔE_{Grimme}[b][c] (B3LYP)	ΔE_{Grimme}[b][c] (BLYP)	ΔE_{Grimme}[b][c] (PBE)	ΔG_{solv}[b][d] (SM8)
1a	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1a_2a_TS	16.5	21.7	19.4	15.8	-1.9	-0.4	-1.8	-1.3	-1.4	-1.0	1.9
2a	11.3	16.8	15.5	10.0	-1.0	-0.6	-4.5	-4.1	-4.9	-2.6	2.9
2a_3b_TS	19.1	28.4	24.3	17.9	-3.6	-3.5	-4.3	-3.8	-4.6	-2.5	3.0
3b	9.2	16.4	11.9	8.7	-2.3	-2.2	-3.1	-2.6	-3.0	-1.8	3.0
7a	9.0	12.5	9.8	9.3	1.3	0.4	7.2	6.3	7.4	3.8	1.6
7a_7b_TS	19.7	25.5	20.2	20.4	0.0	-1.4	9.5	8.6	10.2	5.1	1.2
7b_TS	22.1	26.9	25.6	21.9	1.0	0.9	8.2	7.1	8.3	4.3	0.5
3b_TS$_{BHE}$	21.6	31.1	26.2	20.7	-3.6	-3.2	-2.3	-2.0	-2.4	-1.4	2.7

[a] Calculated from the electronic energy obtained from single point calculations. See the Computational Details section in the main part of the paper. [b] In kcal/mol. [c] Calculated from the Grimme empirical dispersion correction.[12-14] See the Computational Details section in the main part of the paper. [d] Calculated from the SM8[15, 16] free energy of solvation, in toluene. See the Computational Details section in the main part of the paper.

Table S12. Relative Gibbs free energies (kcal/mol) for stationary points of the pyrazolonato-phosphane catalyst (**IV**).

	ΔG_{tot} (BP86)	ΔG_{tot} (B3LYP)	ΔG_{tot} (BLYP)	ΔG_{tot} (PBE)
1a	0.0	0.0	0.0	0.0
1a_2a_TS	16.2	21.5	19.5	16.4
2a	9.2	14.7	12.9	9.8
2a_3b_TS	14.4	23.7	19.3	15.0
3b	7.0	14.1	9.6	7.7
7a	18.2	21.8	19.3	15.1
7a_7b_TS	28.9	34.8	30.2	25.3
7b_TS	31.7	36.5	35.4	27.6
3b_TS$_{BHE}$	18.8	28.2	23.2	18.7

Ligands

Table S13. Absolute energies and corrections for the ligands.

	E_{gas}[a][b] (BP86)	E_{gas}[a][b] (B3LYP)	E_{gas}[a][b] (BLYP)	E_{gas}[a][b] (PBE)	$\Delta H_{313.15}$[b] (BP86)	$\Delta G_{313.15}$[b] (BP86)	$\Delta H_{353.15}$[b] (BP86)	$\Delta G_{353.15}$[b] (BP86)	ΔE_{Grimme}[b][c] (BP86)	ΔE_{Grimme}[b][c] (B3LYP)	ΔE_{Grimme}[b][c] (BLYP)	ΔE_{Grimme}[b][c] (PBE)	ΔG_{solv}[d][e] (SM8)
PMe_3	-29.0946	-29.0167	-28.8620	-28.9880	0.1217	0.0822	0.1234	0.0770	-0.0159	-0.0175	-0.0215	-0.0102	-0.3870
Ethylene	-13.7716	-13.7369	-13.6693	-13.7202	0.0546	0.0282	0.0553	0.0247	-0.0033	-0.0039	-0.0049	-0.0023	-1.5820
PPh_3	-118.1559	-117.7549	-117.2364	-117.8050	0.2883	0.2198	0.2929	0.2108	-0.0804	-0.0843	-0.1026	-0.0492	-17.8890
Propene	-20.6818	-20.6263	-20.5230	-20.6068	0.0840	0.0520	0.0850	0.0478	-0.0069	-0.0080	-0.0099	-0.0048	-2.9640

[a] Electronic energy obtained from single point calculations. See the Computational Details section in the main part of the paper. [b] In Hartrees. [c] Grimme empirical dispersion correction.[12-14] See the Computational Details section in the main part of the paper. [d] SM8[15, 16] free energy of solvation, in toluene. See the Computational Details section in the main part of the paper. [e] In kcal/mol.

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List of xyz coordinates of the stationary points

SHOP-type catalyst (I)

SHOP_1a_1b_TS

62

Ni	0.32858	-1.65119	-0.13058
P	0.31068	0.92051	0.12446
O	-1.55035	-1.39845	-0.20467
C	-1.49527	0.99904	-0.04331
C	-2.18720	-0.19150	-0.14807
C	-3.67608	-0.26847	-0.23328
C	-4.27671	-1.45757	-0.71025
C	-5.67292	-1.56093	-0.81781
C	-6.49525	-0.48347	-0.44089
C	-5.90843	0.69870	0.05037
C	-4.51287	0.80582	0.15525
C	0.90787	2.19052	-1.09616
C	0.15940	2.47738	-2.26385
C	0.67004	3.34195	-3.24941
C	1.93517	3.93526	-3.08785
C	2.69140	3.65399	-1.93311
C	2.18779	2.78526	-0.95058
C	0.60125	1.78585	1.75941
C	0.47382	3.18517	1.93279
C	0.65037	3.76836	3.19979
C	0.95136	2.96471	4.31606
C	1.07906	1.57329	4.15810
C	0.91021	0.99125	2.88854
C	1.12302	-1.80509	-1.89123
C	2.52272	-1.27251	-2.17933
C	2.81001	-1.20766	-3.70320
H	-4.07150	1.71911	0.56323
H	-2.01554	1.96103	-0.03250
H	-3.62297	-2.28691	-0.98677
H	-6.12086	-2.48554	-1.19385
H	-7.58308	-0.56510	-0.52045
H	-6.54092	1.53546	0.36107
H	-0.82847	2.02419	-2.38982
H	0.07399	3.55596	-4.14161
H	2.32912	4.61053	-3.85246
H	3.67557	4.11244	-1.79761
H	2.78543	2.57577	-0.05805
H	0.24088	3.81867	1.07301
H	0.54847	4.85132	3.31676
H	1.08608	3.42068	5.30085
H	1.31335	0.94232	5.02064
H	1.01167	-0.09232	2.76641
H	0.34529	-1.19235	-2.39192
H	1.00459	-2.86510	-2.18748
H	2.63426	-0.26134	-1.74826
H	3.29115	-1.91101	-1.70112
H	2.09478	-0.53334	-4.20440
H	2.72112	-2.20522	-4.16880
H	3.82842	-0.82737	-3.89592
P	1.75521	-2.92810	0.79512
C	1.02942	-3.62527	2.37035
C	3.37357	-2.22480	1.40923
C	2.31995	-4.47761	-0.07443
H	1.76252	-4.25481	2.90450
H	0.14021	-4.22499	2.11972
H	3.96986	-1.86991	0.55412
H	3.95297	-2.97839	1.97073
H	3.16481	-1.36136	2.06088
H	2.86198	-4.21175	-0.99577
H	1.43717	-5.07616	-0.35005
H	2.98274	-5.07755	0.57216
H	0.71094	-2.80204	3.03000

SHOP_1a_2a_TS

62

P	-0.84411	0.51890	-0.15744
O	1.84173	-0.24505	0.72879
C	0.68478	1.10426	-0.87460
C	1.85972	0.59826	-0.30844
C	3.21247	0.99048	-0.82058
C	4.34650	0.76326	-0.00603
C	5.63043	1.11832	-0.44935
C	5.80666	1.70017	-1.71887
C	4.68690	1.92047	-2.54288
C	3.40195	1.56768	-2.09925
C	-1.83949	2.05201	0.22619
C	-1.14250	3.19549	0.68515
C	-1.83917	4.36608	1.03272
C	-3.24219	4.41058	0.93179
C	-3.94373	3.27868	0.47857
C	-3.24882	2.10668	0.12785
C	-1.90739	-0.29345	-1.45700
C	-1.70826	-0.04229	-2.83324
C	-2.52297	-0.66609	-3.79631
C	-3.54884	-1.54250	-3.39628
C	-3.75382	-1.80070	-2.02790
C	-2.93360	-1.18471	-1.06438
Ni	-0.10023	-0.80372	1.35000
C	-1.12170	0.03123	2.78246
C	-0.10684	-0.74307	3.56675
P	0.25918	-2.86940	0.40924
C	0.76113	-2.85151	-1.38565
C	-1.01485	-4.24182	0.40419
C	1.72612	-3.75203	1.16010
C	0.94702	0.08672	4.32197
H	2.54278	1.71921	-2.75824
H	0.69346	1.89470	-1.63001
H	4.18964	0.30448	0.97256
H	6.49645	0.94099	0.19538
H	6.80707	1.97431	-2.06601
H	4.81643	2.36043	-3.53619
H	-0.05086	3.16227	0.75285
H	-1.28534	5.24349	1.37905
H	-3.78406	5.32156	1.20088
H	-5.03372	3.30801	0.39090
H	-3.80667	1.24076	-0.23797
H	-0.90418	0.62774	-3.14830
H	-2.35499	-0.46825	-4.85884
H	-4.18083	-2.02594	-4.14635
H	-4.54673	-2.48480	-1.71143
H	-3.07041	-1.40630	-0.00114
H	-2.16595	-0.30873	2.82982
H	-1.03403	1.12537	2.82713
H	0.50771	-1.44876	2.83251
H	1.07699	-3.85414	-1.72319
H	1.59404	-2.14194	-1.51016
H	-0.08410	-2.50689	-2.00205
H	-1.33056	-4.45504	1.43894
H	-0.61785	-5.16658	-0.05090
H	-1.89702	-3.91063	-0.16749
H	1.51500	-3.99591	2.21515
H	2.58590	-3.06408	1.12520
H	1.97186	-4.68244	0.61866
H	1.42291	0.80813	3.63843
H	1.73949	-0.55270	4.74592
H	0.47237	0.64306	5.14793
H	-0.57521	-1.51252	4.20764

SHOP_1a_5a_TS

68

Ni	-0.03024	1.23495	-0.39158
P	0.83071	-0.73870	0.15877
O	-1.78535	0.34823	-0.26032
C	-0.68668	-1.69137	0.30869
C	-1.84184	-0.96432	0.07168
C	-3.21003	-1.55866	0.12178
C	-4.28541	-0.89602	-0.51543
C	-5.57887	-1.44183	-0.49390
C	-5.82446	-2.65715	0.17115
C	-4.76429	-3.32072	0.81737
C	-3.47030	-2.77707	0.79495
C	1.62463	-0.66336	1.84415
C	1.06356	-1.36685	2.93454
C	1.64119	-1.28347	4.21462
C	2.78836	-0.49718	4.42440
C	3.35197	0.21313	3.34771
C	2.77241	0.13609	2.06878
C	1.96859	-1.86979	-0.79675
C	1.48695	-2.38568	-2.02516
C	2.28986	-3.22528	-2.81472
C	3.59001	-3.56264	-2.39271
C	4.07608	-3.05985	-1.17325
C	3.27288	-2.21936	-0.37935
C	-0.54857	0.57031	-3.35450
C	-0.93116	1.85794	-3.46679
C	1.61877	2.24786	-0.69811
C	2.70126	1.58524	-1.56891
C	3.82392	2.57210	-1.97236
H	-2.65967	-3.28965	1.31961
H	-0.68569	-2.77107	0.47242
H	-4.08249	0.04575	-1.02901
H	-6.39712	-0.91919	-0.99800
H	-6.83215	-3.08167	0.19049
H	-4.94805	-4.26064	1.34585
H	0.16372	-1.96659	2.77523
H	1.19360	-1.83369	5.04740
H	3.23754	-0.43360	5.41942
H	4.23984	0.83289	3.50377
H	3.20868	0.70892	1.24608
H	0.47194	-2.14037	-2.35059
H	1.89920	-3.61835	-3.75781
H	4.21567	-4.21553	-3.00757
H	5.08087	-3.32528	-0.83187
H	3.66074	-1.85091	0.57351
H	-0.27771	2.62161	-3.90026
H	-1.91701	2.18947	-3.12925
H	-1.20813	-0.18336	-2.91656
H	0.43094	0.22667	-3.70044
H	2.03393	2.54354	0.28892
H	1.28155	3.17640	-1.20478
H	2.24267	1.16674	-2.48455
H	3.15282	0.72111	-1.04656

H	4.32387	2.98888	-1.07903
H	3.41410	3.42005	-2.55063
H	4.59244	2.07732	-2.59332
P	-1.09968	2.99555	0.41376
C	-1.51699	2.68129	2.20032
C	-0.32150	4.68669	0.48816
C	-2.77372	3.35916	-0.30954
H	-3.31186	2.40156	-0.36922
H	-2.65744	3.76812	-1.32606
H	-3.33937	4.07632	0.30964
H	-2.11652	1.75975	2.25481
H	-0.58866	2.52796	2.77300
H	-2.08592	3.52099	2.63688
H	-0.16664	5.07193	-0.53260
H	0.65972	4.62251	0.98456
H	-0.96494	5.38905	1.04446

SHOP_1a_6a_TS

62

Ni	0.03775	-0.33238	1.41489
P	-1.17442	0.32387	-0.19580
O	1.34966	0.96849	0.91579
C	-0.10458	1.59384	-0.87443
C	1.07877	1.74677	-0.15871
C	2.12400	2.75674	-0.49080
C	3.17392	2.98719	0.42946
C	4.17262	3.93410	0.15256
C	4.14415	4.66424	-1.04972
C	3.10784	4.43769	-1.97559
C	2.10761	3.49226	-1.70045
C	-2.81621	1.09672	0.19544
C	-3.01157	1.63834	1.48747
C	-4.20309	2.31214	1.80501
C	-5.21560	2.44900	0.83696
C	-5.03073	1.91117	-0.44977
C	-3.83809	1.23818	-0.77189
C	-1.56574	-0.90462	-1.52747
C	-0.79998	-0.93024	-2.71492
C	-1.05059	-1.90097	-3.70234
C	-2.06604	-2.85579	-3.51369
C	-2.83219	-2.83833	-2.33187
C	-2.58413	-1.87097	-1.34330
C	-0.98980	-1.69581	2.25694
C	0.18900	-1.63758	3.20372
C	-0.11975	-1.20197	4.64863
H	1.31828	3.31586	-2.43588
H	-0.40858	2.25137	-1.69106
H	3.18114	2.40934	1.35542
H	4.97525	4.10339	0.87633
H	4.92286	5.40109	-1.26623
H	3.08200	4.99604	-2.91582
H	-2.22116	1.52974	2.23668
H	-4.34203	2.72667	2.80740
H	-6.14413	2.97064	1.08475
H	-5.81452	2.01534	-1.20542
H	-3.70495	0.82162	-1.77364
H	-0.00967	-0.18699	-2.85507
H	-0.45366	-1.90850	-4.61870
H	-2.26110	-3.60919	-4.28178
H	-3.62289	-3.57845	-2.18002
H	-3.18490	-1.86204	-0.42960
H	-1.07817	-2.60631	1.64672
H	-1.95641	-1.37499	2.67587
H	0.98317	-0.86727	2.80755
H	-0.72079	-1.97727	5.15309
H	-0.69686	-0.26170	4.66163
H	0.80207	-1.04448	5.23393
H	0.79117	-2.56118	3.15982
P	2.47789	-3.08065	0.31311
C	4.13139	-3.89936	0.69147
C	1.80842	-4.32966	-0.92399
C	3.06780	-1.76239	-0.88512
H	4.74664	-3.21300	1.29777
H	4.68725	-4.15945	-0.22746
H	3.96330	-4.81729	1.28020
H	0.88911	-3.92623	-1.38083
H	1.54869	-5.26571	-0.40064
H	2.19116	-1.29371	-1.36223
H	3.59648	-0.97237	-0.32771
H	3.73313	-2.17249	-1.66673
H	2.53718	-4.55632	-1.72303

SHOP_1a_PPh

83

Ni	-0.23880	-0.43735	0.03363
P	2.01303	-0.46952	0.09598
P	-2.40310	-0.11794	0.09449
O	-0.10385	1.51599	-0.11951
H	-3.01902	4.30286	0.41089
C	-2.48782	1.66284	-0.08327
H	-3.42690	2.21730	-0.13189
C	-1.23842	2.26064	-0.14520
C	-1.03098	3.73205	-0.26735
C	0.22408	4.22133	-0.70033
H	1.01039	3.49902	-0.92762
C	0.44408	5.60167	-0.83425
H	1.41849	5.96402	-1.17463
C	-0.58078	6.51682	-0.53098
H	-0.40766	7.59208	-0.63195
C	-1.82969	6.04019	-0.08862
H	-2.62762	6.74540	0.16153
C	-2.05367	4.66083	0.04333
C	-3.27470	-0.59627	1.66373
C	-2.50501	-0.98356	2.78447
H	-1.41759	-1.05768	2.68493
C	-3.12840	-1.26905	4.01272
H	-2.52204	-1.56876	4.87209
C	-4.52633	-1.17278	4.13344
H	-5.01128	-1.39637	5.08777
C	-5.30107	-0.78986	3.02193
H	-6.38854	-0.71418	3.11158
C	-4.68108	-0.50336	1.79350
H	-5.29060	-0.21103	0.93394
C	-3.46545	-0.85635	-1.23370
C	-3.61752	-0.16358	-2.45822
H	-3.16185	0.82452	-2.57216
C	-4.35276	-0.73284	-3.51251
H	-4.46820	-0.18326	-4.45108
C	-4.94023	-2.00282	-3.36087
H	-5.51255	-2.44465	-4.18123
C	-4.78962	-2.70134	-2.14891
H	-5.24434	-3.68819	-2.02443
C	-4.05724	-2.13430	-1.09068
H	-3.95533	-2.68151	-0.15000
C	2.77194	0.47064	-1.31783
C	2.01216	0.63379	-2.49833
H	0.98993	0.24708	-2.53554
C	2.55394	1.31455	-3.60392
H	1.95474	1.43973	-4.50990
C	3.85488	1.84516	-3.53728
H	4.27314	2.38000	-4.39455
C	4.61370	1.69550	-2.36111
H	5.62208	2.11462	-2.30124
C	4.07618	1.01233	-1.25594
H	4.66664	0.91310	-0.34137
C	2.73072	0.34577	1.61208
C	1.99588	1.39088	2.22274
H	1.04219	1.69500	1.78222
C	2.50453	2.04194	3.36068
H	1.92748	2.84857	3.82127
C	3.74483	1.66024	3.90397
H	4.13494	2.16557	4.79199
C	4.48211	0.62537	3.30072
H	5.44801	0.32387	3.71623
C	3.98092	-0.02891	2.16051
H	4.55872	-0.83810	1.70748
C	2.92284	-2.09162	0.05174
C	3.62572	-2.52817	-1.09458
H	3.69909	-1.87702	-1.96878
C	4.23936	-3.79435	-1.11775
H	4.78168	-4.11476	-2.01168
C	4.15916	-4.64189	0.00105
H	4.63780	-5.62477	-0.01829
C	3.45838	-4.21977	1.14631
H	3.38962	-4.87307	2.02056
C	2.84003	-2.95797	1.17063
H	2.30587	-2.63644	2.06922
C	-0.46420	-2.38632	0.02516
H	-1.45568	-2.68607	0.42038
H	0.29397	-2.82741	0.70180
C	-0.29403	-2.92458	-1.40907
H	-1.03471	-2.44770	-2.07950
H	0.70433	-2.65133	-1.80223
C	-0.45749	-4.46248	-1.49140
H	-1.46044	-4.76791	-1.14358
H	0.29091	-4.96915	-0.85702
H	-0.33110	-4.82564	-2.52740

SHOP_1a

62

Ni	-0.03513	1.24447	0.16700
P	-1.18762	3.10846	0.44340
P	0.79223	-0.78380	0.04563
O	-1.79185	0.39369	-0.07054
C	-0.70985	-1.73689	-0.17657
C	-1.85674	-0.95776	-0.17546
C	-3.22948	-1.52653	-0.30862
C	-4.29074	-0.69954	-0.74527
C	-5.58945	-1.21384	-0.88639
C	-5.85462	-2.56229	-0.58424
C	-4.80860	-3.39177	-0.13739
C	-3.50853	-2.88010	-0.00047
C	1.67510	-1.43259	1.54564
C	1.62876	-0.67714	2.73988
C	2.20792	-1.17411	3.92138
C	2.84262	-2.42927	3.92154
C	2.89788	-3.18673	2.73588
C	2.31913	-2.69287	1.55383
C	1.93855	-1.20998	-1.34858
C	1.39691	-1.59937	-2.59652
C	2.24058	-1.84262	-3.69443

C	3.63410	-1.69535	-3.56296
C	4.18124	-1.30315	-2.32730
C	3.34107	-1.06013	-1.22601
C	-2.22572	3.54464	-1.03716
C	-2.45940	2.91110	1.78391
C	-0.39884	4.73837	0.87647
C	1.72161	2.11245	0.26464
C	2.10204	2.68491	-1.11725
C	3.49260	3.36657	-1.12430
H	-2.70899	-3.52572	0.37217
H	-0.72073	-2.82222	-0.29293
H	-4.07263	0.34549	-0.97317
H	-6.39717	-0.56202	-1.23223
H	-6.86697	-2.96237	-0.69001
H	-5.00821	-4.43769	0.11299
H	1.13520	0.29984	2.73135
H	2.16637	-0.57974	4.83854
H	3.29435	-2.81556	4.83949
H	3.39152	-4.16279	2.73161
H	2.37055	-3.28574	0.63640
H	0.31335	-1.71327	-2.69579
H	1.80914	-2.14877	-4.65173
H	4.28956	-1.88583	-4.41731
H	5.26345	-1.18770	-2.21860
H	3.77651	-0.76376	-0.26805
H	2.49971	1.39466	0.59397
H	1.69547	2.91788	1.02733
H	2.09514	1.87509	-1.87142
H	1.34083	3.41759	-1.45445
H	4.27992	2.64550	-0.84175
H	3.52804	4.20143	-0.40103
H	3.74226	3.76809	-2.12315
H	0.33133	5.01963	0.10114
H	0.13441	4.64900	1.83659
H	-1.16047	5.53172	0.96025
H	-1.57114	3.84014	-1.87289
H	-2.78240	2.64197	-1.33163
H	-2.92969	4.36531	-0.81564
H	-1.95264	2.79644	2.75588
H	-3.02032	1.98827	1.57193
H	-3.14530	3.77465	1.82966

SHOP_1b'_3b_TS

62

P	-1.06150	-0.29723	0.13912
O	1.74185	-0.02188	-0.58989
C	0.28003	-1.26687	0.84800
C	1.54511	-0.95335	0.37816
C	2.79170	-1.61146	0.87177
C	3.97729	-1.52632	0.10372
C	5.16084	-2.14190	0.54177
C	5.18541	-2.84868	1.75813
C	4.01469	-2.93048	2.53565
C	2.82997	-2.31673	2.09921
C	-2.26486	-1.52976	-0.57772
C	-1.80163	-2.78743	-1.03162
C	-2.67937	-3.68992	-1.65899
C	-4.03068	-3.34695	-1.85117
C	-4.50068	-2.09557	-1.40907
C	-3.62652	-1.19373	-0.77724
C	-2.06909	0.36775	1.56554
C	-2.63773	-0.48596	2.54088
C	-3.35508	0.04779	3.62502
C	-3.52431	1.44121	3.74511
C	-2.97381	2.29799	2.77593
C	-2.24911	1.76233	1.69403
Ni	0.19222	0.98637	-1.18255
C	-0.62850	1.26856	-3.16284
C	0.64019	0.62406	-3.20504
P	1.14250	2.89126	-0.36791
C	1.62190	2.78607	1.43081
C	0.34846	4.58586	-0.43545
C	2.80457	3.25393	-1.14356
C	0.80875	-0.85400	-3.46350
H	1.93491	-2.36659	2.72479
H	0.11094	-2.05266	1.58804
H	3.94640	-0.97086	-0.83547
H	6.06675	-2.07026	-0.06745
H	6.10768	-3.32676	2.10021
H	4.02675	-3.46737	3.48867
H	-0.75053	-3.05323	-0.88274
H	-2.30752	-4.66256	-1.99468
H	-4.71263	-4.04885	-2.33927
H	-5.55076	-1.82326	-1.55127
H	-4.00631	-0.22980	-0.42532
H	-2.52551	-1.56974	2.44695
H	-3.78582	-0.62223	4.37482
H	-4.08520	1.85408	4.58831
H	-3.10948	3.38038	2.85985
H	-1.81709	2.42103	0.93365
H	-0.69921	2.30814	-3.50742
H	-1.52092	0.66410	-3.37094
H	-1.03002	1.67137	-1.73593
H	2.24373	3.64253	1.74559
H	2.18086	1.84870	1.57930
H	0.71254	2.74480	2.05162
H	0.11856	4.84272	-1.48320
H	1.00394	5.36619	-0.01072
H	-0.59909	4.56892	0.12819
H	2.66745	3.51999	-2.20524
H	3.40967	2.33522	-1.08854
H	3.33322	4.07712	-0.63150
H	-0.11836	-1.40946	-3.24333
H	1.61746	-1.26950	-2.83956
H	1.07505	-1.03846	-4.52449
H	1.52550	1.24404	-3.39582

SHOP_1b

62

Ni	-0.08060	1.35380	-0.26923
P	1.73502	2.47183	-0.43898
P	0.63260	-0.78311	0.05739
O	-1.85007	0.58187	-0.27982
C	-0.95681	-1.61221	0.03564
C	-2.03095	-0.75039	-0.11005
C	-3.45423	-1.19859	-0.11687
C	-4.45706	-0.31631	-0.58270
C	-5.80347	-0.71371	-0.60781
C	-6.17351	-1.99579	-0.16204
C	-5.18434	-2.87779	0.31327
C	-3.83750	-2.48365	0.33712
C	1.43693	-1.25150	1.67058
C	1.46143	-0.29135	2.70970
C	1.96341	-0.62274	3.98129
C	2.45086	-1.91828	4.23044
C	2.42786	-2.88305	3.20533
C	1.92325	-2.55451	1.93483
C	1.66657	-1.65042	-1.22803
C	1.03826	-2.01633	-2.44365
C	1.77877	-2.60205	-3.48464
C	3.15871	-2.83419	-3.33009
C	3.79344	-2.47580	-2.12718
C	3.05545	-1.88482	-1.08431
C	3.36059	1.60440	-0.16521
C	2.00498	3.18545	-2.13921
C	1.95134	3.95295	0.67311
C	-1.04349	3.06653	-0.50165
C	-1.74197	3.43888	0.81598
C	-2.72306	4.62778	0.65276
H	-3.08272	-3.16945	0.73065
H	-1.05882	-2.69311	0.14675
H	-4.15333	0.67722	-0.91717
H	-6.56652	-0.02054	-0.97391
H	-7.22282	-2.30399	-0.17838
H	-5.46430	-3.87204	0.67338
H	1.06257	0.71072	2.51887
H	1.96988	0.12859	4.77616
H	2.84180	-2.17718	5.21828
H	2.79852	-3.89424	3.39649
H	1.90429	-3.31357	1.14818
H	-0.03689	-1.84976	-2.55916
H	1.27599	-2.88223	-4.41467
H	3.73292	-3.29521	-4.13844
H	4.86355	-2.66073	-1.99515
H	3.56035	-1.62324	-0.15045
H	-1.77283	2.74671	-1.26945
H	-0.47469	3.93183	-0.89902
H	-2.29345	2.55874	1.18956
H	-0.99418	3.70020	1.59199
H	-3.51194	4.38295	-0.08008
H	-2.19917	5.53241	0.29280
H	-3.21369	4.87735	1.61105
H	1.98348	3.61703	1.72205
H	1.10254	4.64176	0.55379
H	2.89007	4.48154	0.43536
H	3.38447	1.17170	0.84759
H	3.46486	0.78716	-0.89567
H	4.20469	2.30574	-0.28241
H	1.16097	3.83815	-2.40878
H	2.04892	2.35771	-2.86518
H	2.94560	3.76069	-2.18385

SHOP_2a_3a_TS

62

Ni	0.00135	1.02730	-1.14931
P	0.50823	2.87567	0.10648
P	-0.81500	-0.55995	0.18387
O	1.79354	0.24251	-0.74160
C	0.71547	-1.31688	0.72248
C	1.85738	-0.76219	0.15605
C	3.23757	-1.24094	0.47364
C	4.30194	-0.90588	-0.39626
C	5.60835	-1.34648	-0.13097
C	5.87684	-2.12435	1.01055
C	4.82688	-2.45494	1.88807
C	3.51942	-2.01634	1.62405
C	-1.83343	-1.91587	-0.59552
C	-1.16614	-2.88668	-1.38124
C	-1.89339	-3.88414	-2.05336
C	-3.29752	-3.92279	-1.95798

C	-3.97029	-2.95965	-1.18452
C	-3.24491	-1.96157	-0.50753
C	-1.85570	-0.13609	1.66882
C	-1.85257	-0.93541	2.83533
C	-2.64839	-0.58693	3.94071
C	-3.46449	0.55953	3.89284
C	-3.47877	1.35952	2.73619
C	-2.67524	1.01569	1.63243
C	-1.67943	1.29938	-2.22674
C	-0.63674	0.92403	-3.14969
C	-0.27651	1.81040	-4.34474
C	0.90567	2.57033	1.90378
C	2.10715	3.64086	-0.47145
C	-0.59295	4.38442	0.23212
H	2.71678	-2.25859	2.32565
H	0.74941	-2.19132	1.37596
H	4.07614	-0.29965	-1.27571
H	6.41952	-1.08317	-0.81619
H	6.89484	-2.46624	1.21813
H	5.02877	-3.04934	2.78398
H	-0.07415	-2.86094	-1.44704
H	-1.36324	-4.63291	-2.64908
H	-3.86239	-4.69970	-2.48069
H	-5.06072	-2.98703	-1.10162
H	-3.77764	-1.22900	0.10522
H	-1.22206	-1.82701	2.88269
H	-2.63283	-1.21057	4.83910
H	-4.08369	0.82768	4.75331
H	-4.11084	2.25136	2.69353
H	-2.67048	1.64517	0.73690
H	-2.04141	2.33565	-2.24229
H	-2.42977	0.55834	-1.93413
H	0.66055	1.67665	-2.30944
H	-0.52053	-0.14931	-3.35457
H	-0.33874	2.88177	-4.08582
H	-0.98781	1.62072	-5.17066
H	0.73913	1.60446	-4.72103
H	-0.01044	2.27944	2.44192
H	1.34493	3.46333	2.38191
H	1.61985	1.73350	1.96263
H	2.84887	2.83052	-0.55065
H	2.47537	4.42283	0.21567
H	1.96114	4.07472	-1.47453
H	-0.80841	4.76512	-0.77996
H	-0.11891	5.18627	0.82476
H	-1.54716	4.10484	0.70792

SHOP_2a_3b_PPh_TS

83

P	1.28851	1.18063	-0.02958
O	1.76971	-1.63951	-0.73673
C	2.81924	0.28619	0.21737
C	2.84056	-1.04643	-0.19383
C	4.05643	-1.91159	-0.03464
C	3.93304	-3.30455	-0.24884
C	5.04147	-4.15457	-0.10601
C	6.29698	-3.62845	0.24969
C	6.43435	-2.24263	0.45647
C	5.32619	-1.39203	0.31416
C	0.81018	1.75083	1.69050
C	0.82569	0.77658	2.71810
C	0.51289	1.12524	4.04282
C	0.18555	2.45593	4.36503
C	0.17219	3.43161	3.35305
C	0.48010	3.08324	2.02452
C	1.67875	2.79986	-0.86561
C	3.01113	3.20542	-1.09836
C	3.28366	4.41793	-1.75935
C	2.22908	5.23960	-2.19560
C	0.89708	4.84034	-1.97619
C	0.62331	3.62631	-1.32122
Ni	0.13726	-0.36473	-1.18633
C	1.12310	0.33472	-2.91780
C	0.29571	-0.70843	-3.36283
C	-0.95924	-0.45904	-4.18004
H	5.45484	-0.31626	0.45937
H	3.63972	0.73473	0.78290
H	2.95246	-3.69176	-0.53326
H	4.92682	-5.22959	-0.27461
H	7.16168	-4.28925	0.35973
H	7.40894	-1.82309	0.72311
H	1.10274	-0.25325	2.47876
H	0.53454	0.35866	4.82271
H	-0.04740	2.73056	5.39789
H	-0.07065	4.47044	3.59510
H	0.47638	3.85752	1.25480
H	3.83295	2.56063	-0.77693
H	4.32084	4.71750	-1.93522
H	2.44230	6.18062	-2.71024
H	0.07186	5.47006	-2.32159
H	-0.41392	3.31174	-1.16778
H	2.18281	0.15408	-2.71916
H	0.83315	1.37461	-3.09880
H	-0.45354	-1.53745	-1.86009
H	-1.37752	0.53967	-3.97187
H	-1.74383	-1.20744	-3.98708
H	-0.71186	-0.50425	-5.25832
H	0.76248	-1.69399	-3.48773
P	-1.74167	-0.62840	-0.15202
C	-2.52421	0.92439	0.51239
C	-2.73547	1.17300	1.88570
C	-3.30642	2.38878	2.30858
C	-3.67619	3.36625	1.36974
C	-3.45702	3.13346	-0.00191
C	-2.87512	1.92727	-0.42605
C	-3.16013	-1.40956	-1.10323
C	-2.91358	-2.63770	-1.76376
C	-3.94157	-3.30485	-2.44961
C	-5.23605	-2.75268	-2.49548
C	-5.49332	-1.53669	-1.84075
C	-4.46608	-0.87189	-1.14270
C	-1.66028	-1.81573	1.28398
C	-2.79525	-2.14450	2.06370
C	-2.69290	-3.09152	3.09667
C	-1.46328	-3.73115	3.34924
C	-0.33937	-3.42567	2.56216
C	-0.43227	-2.47026	1.53104
H	-2.43792	0.43151	2.62919
H	-3.45087	2.57046	3.37678
H	-4.12299	4.30725	1.70211
H	-3.73624	3.89124	-0.73972
H	-2.69329	1.75417	-1.49139
H	-1.91225	-3.07929	-1.73203
H	-3.73116	-4.25525	-2.94814
H	-6.03505	-3.26815	-3.03524
H	-6.49620	-1.10077	-1.86554
H	-4.68921	0.06660	-0.63108
H	-3.76091	-1.67627	1.85269
H	-3.57366	-3.33873	3.69631
H	-1.38805	-4.47306	4.14940
H	0.61271	-3.93278	2.74203
H	0.43225	-2.24871	0.89124

SHOP_2a_3b_TS

62

P	-1.00905	-0.44074	0.00471
O	1.83781	0.25198	-0.57298
C	0.44189	-1.36346	0.54676
C	1.68323	-0.86379	0.17694
C	2.96571	-1.53153	0.56433
C	4.14204	-1.25947	-0.17320
C	5.35741	-1.87715	0.16329
C	5.42269	-2.77117	1.24790
C	4.26124	-3.03887	1.99686
C	3.04475	-2.42351	1.66064
C	-2.07405	-1.72992	-0.82521
C	-1.44747	-2.71963	-1.62391
C	-2.21407	-3.64975	-2.34871
C	-3.61936	-3.60792	-2.29354
C	-4.25250	-2.62879	-1.50495
C	-3.48923	-1.69700	-0.77983
C	-2.02270	-0.06564	1.52874
C	-1.88032	-0.77489	2.74385
C	-2.65112	-0.43154	3.86921
C	-3.58320	0.62123	3.79672
C	-3.73375	1.33705	2.59490
C	-2.95270	1.00098	1.47313
Ni	0.19799	1.19942	-1.12609
C	0.21924	0.36030	-2.96860
C	-0.23857	1.70420	-3.16762
P	0.69463	2.77981	0.32292
C	0.96027	2.21980	2.07543
C	-0.43466	4.24288	0.55620
C	2.32796	3.58762	-0.06409
C	0.67829	2.78848	-3.72285
H	2.15480	-2.61846	2.26490
H	0.36024	-2.32144	1.06810
H	4.07694	-0.55986	-1.00877
H	6.25621	-1.66122	-0.42198
H	6.36982	-3.25044	1.51157
H	4.30535	-3.72221	2.84999
H	-0.35457	-2.76861	-1.65395
H	-1.71090	-4.41152	-2.95187
H	-4.21510	-4.33338	-2.85459
H	-5.34465	-2.59362	-1.44774
H	-3.99769	-0.95190	-0.16162
H	-1.15515	-1.58972	2.81097
H	-2.52690	-0.98864	4.80255
H	-4.18346	0.88462	4.67207
H	-4.45222	2.15994	2.53247
H	-3.05119	1.57556	0.54584
H	-0.48051	-0.47436	-3.07450
H	1.27827	0.12324	-3.11484
H	-0.77076	2.15298	-1.77239
H	1.34235	3.04702	2.69881
H	1.68589	1.39198	2.07712
H	0.01029	1.85337	2.49446
H	-0.58209	4.75146	-0.41041
H	-0.02336	4.96176	1.28529
H	-1.41337	3.88533	0.91487
H	2.25336	4.13649	-1.01660
H	3.07571	2.78707	-0.17620
H	2.64010	4.28296	0.73468
H	1.72122	2.62238	-3.40894
H	0.37309	3.79532	-3.39107
H	0.64634	2.77884	-4.82937
H	-1.28409	1.79831	-3.50302

SHOP_2a_PPh

83

P	1.36681	1.18961	-0.01894
O	1.58670	-1.70016	-0.74521
C	2.75441	0.11001	0.31182
C	2.67127	-1.21306	-0.13442
C	3.80082	-2.18270	0.07283
C	3.56985	-3.55627	-0.17439
C	4.59130	-4.50234	0.00851
C	5.86707	-4.09362	0.43841
C	6.11243	-2.72823	0.67831
C	5.09091	-1.78214	0.49606
C	0.79900	1.79635	1.65629
C	0.79918	0.86901	2.72587
C	0.40088	1.26201	4.01518
C	0.00037	2.58909	4.25773
C	-0.00387	3.51748	3.20110
C	0.38899	3.12550	1.90891
C	1.99622	2.76518	-0.78994
C	3.37128	3.08654	-0.79654
C	3.82355	4.27538	-1.39845
C	2.90861	5.15816	-2.00007
C	1.53687	4.84347	-2.00635
C	1.08457	3.65224	-1.41091
Ni	0.13856	-0.16523	-1.19093
C	1.18109	0.36199	-2.76798
C	0.24982	-0.64324	-3.35757
C	-0.70947	-0.13871	-4.45147
H	5.30607	-0.72414	0.66683
H	3.59430	0.46101	0.91696
H	2.57626	-3.85188	-0.51764
H	4.39294	-5.56053	-0.18686
H	6.66447	-4.82889	0.57991
H	7.10441	-2.39910	1.00187
H	1.13478	-0.15505	2.54478
H	0.41439	0.53273	4.83026
H	-0.29884	2.89857	5.26326
H	-0.30808	4.55265	3.38086
H	0.39195	3.86338	1.10387
H	4.08989	2.39673	-0.34731
H	4.89208	4.50914	-1.39960
H	3.26246	6.08040	-2.46918
H	0.82073	5.51951	-2.48264
H	0.01997	3.39787	-1.43831
H	2.23534	0.07690	-2.67099
H	1.03289	1.40677	-3.07096
H	-0.45663	-1.08405	-2.50433
H	-1.20282	0.79561	-4.13457
H	-1.49298	-0.87987	-4.68008
H	-0.14806	0.06862	-5.37829
H	0.77808	-1.56893	-3.64381
P	-1.76063	-0.55087	-0.11411
C	-2.62470	0.98253	0.48772
C	-2.90717	1.24783	1.84504
C	-3.51830	2.45937	2.22202
C	-3.85892	3.41657	1.25202
C	-3.56808	3.16826	-0.10356
C	-2.94567	1.96706	-0.48083
C	-3.07379	-1.37790	-1.16881
C	-2.70533	-2.57181	-1.83706
C	-3.63666	-3.26957	-2.62362
C	-4.95136	-2.78408	-2.76048
C	-5.32820	-1.60408	-2.09707
C	-4.39870	-0.90640	-1.30123
C	-1.74527	-1.72895	1.32868
C	-2.90416	-2.04353	2.07852
C	-2.83941	-2.98917	3.11574
C	-1.62406	-3.64173	3.40247
C	-0.47740	-3.35402	2.64215
C	-0.53328	-2.40089	1.60650
H	-2.63292	0.52328	2.61371
H	-3.71879	2.65308	3.27913
H	-4.33764	4.35411	1.54795
H	-3.82081	3.91158	-0.86526
H	-2.70147	1.78766	-1.53277
H	-1.68843	-2.96305	-1.72878
H	-3.33597	-4.19232	-3.12786
H	-5.67504	-3.32406	-3.37713
H	-6.34882	-1.22252	-2.19313
H	-4.70926	0.00704	-0.78902
H	-3.85872	-1.56508	1.84187
H	-3.73829	-3.22513	3.69267
H	-1.57807	-4.38090	4.20738
H	0.46309	-3.87358	2.84586
H	0.34332	-2.20050	0.97829

SHOP_2a

62

P	-0.90238	0.47619	-0.03686
O	1.91141	-0.41908	0.58355
C	0.60540	1.06726	-0.79359
C	1.82068	0.52029	-0.35799
C	3.12297	1.00314	-0.93498
C	4.31413	0.80110	-0.20002
C	5.55020	1.24134	-0.69968
C	5.62174	1.88030	-1.95178
C	4.44530	2.07213	-2.70013
C	3.20768	1.63760	-2.19717
C	-1.80927	2.00830	0.52702
C	-1.05364	3.12371	0.96081
C	-1.69450	4.28166	1.43624
C	-3.09897	4.34305	1.48979
C	-3.85935	3.23873	1.06284
C	-3.22093	2.07999	0.58605
C	-2.06180	-0.14997	-1.35992
C	-1.91725	0.23863	-2.71117
C	-2.80067	-0.24753	-3.69225
C	-3.84364	-1.12322	-3.33604
C	-3.99661	-1.51710	-1.99383
C	-3.10750	-1.03789	-1.01336
Ni	-0.09001	-0.97158	1.34194
C	-0.13027	0.29838	2.81055
C	0.30826	-0.94766	3.51008
P	0.14350	-2.84033	0.16627
C	0.45170	-2.67447	-1.65856
C	-1.14577	-4.18893	0.21826
C	1.67561	-3.74891	0.71298
C	1.74511	-0.94694	4.06363
H	2.30432	1.77074	-2.79876
H	0.58686	1.91127	-1.48916
H	4.24153	0.29307	0.76395
H	6.46045	1.08468	-0.11307
H	6.58481	2.21955	-2.34405
H	4.49320	2.55433	-3.68111
H	0.03826	3.08119	0.90869
H	-1.09479	5.13705	1.76080
H	-3.59698	5.24467	1.85720
H	-4.95209	3.27981	1.09438
H	-3.82673	1.23675	0.24439
H	-1.10128	0.90819	-2.99495
H	-2.67419	0.05768	-4.73500
H	-4.52919	-1.49983	-4.10021
H	-4.80296	-2.20019	-1.71081
H	-3.21013	-1.36216	0.02770
H	-1.12769	0.68852	3.04672
H	0.62972	1.08145	2.68773
H	0.27833	-1.87222	2.74152
H	0.77168	-3.63869	-2.08948
H	1.23831	-1.91994	-1.81224
H	-0.46443	-2.33337	-2.16422
H	-1.34171	-4.46798	1.26650
H	-0.81684	-5.08244	-0.34051
H	-2.08230	-3.81187	-0.22285
H	1.55363	-4.09651	1.75229
H	2.51167	-3.03322	0.67458
H	1.88782	-4.61546	0.06350
H	2.44768	-0.63445	3.27477
H	2.04512	-1.94518	4.42601
H	1.82215	-0.23787	4.90533
H	-0.43366	-1.29622	4.24982

SHOP_3a_4a_TS

62

Ni	0.11263	1.51795	0.12049
P	1.86680	2.49993	-0.57912
P	0.46376	-0.70476	-0.03036
O	-1.78578	1.09085	-0.06055
C	-1.23416	-1.23099	-0.24741
C	-2.15850	-0.19315	-0.23633
C	-3.62372	-0.40025	-0.44139
C	-4.43907	0.71288	-0.75471
C	-5.81779	0.55258	-0.96557
C	-6.40810	-0.72055	-0.86163
C	-5.60719	-1.83331	-0.54171
C	-4.22805	-1.67565	-0.33165
C	1.17054	-1.64149	1.41678
C	2.52615	-1.48215	1.79757
C	3.03575	-2.14101	2.93024
C	2.19641	-2.96069	3.70833
C	0.84633	-3.11666	3.34696
C	0.33651	-2.46208	2.21059
C	1.37901	-1.41029	-1.49763
C	1.01762	-0.89754	-2.76892
C	1.62876	-1.38118	-3.93734
C	2.61470	-2.38433	-3.85652
C	2.97574	-2.90405	-2.60160
C	2.36175	-2.42318	-1.42824
C	0.65510	1.88201	2.69649
C	-0.65536	1.53447	2.77754
C	-1.80797	2.49791	2.83334
C	1.70982	3.00569	-2.36424
C	2.37438	4.10574	0.21839
C	3.50068	1.59341	-0.60069
H	-3.62087	-2.54467	-0.06445
H	-1.49915	-2.26159	-0.49213
H	-3.96339	1.69272	-0.82905
H	-6.43362	1.42260	-1.21182
H	-7.48253	-0.84547	-1.02403
H	-6.05979	-2.82497	-0.44960
H	3.18726	-0.84293	1.20519
H	4.08559	-2.01040	3.20851
H	2.59177	-3.46861	4.59222
H	0.18683	-3.74770	3.94957
H	-0.71555	-2.57391	1.93388
H	0.23674	-0.13298	-2.83350

H	1.33152	-0.98114	-4.91108
H	3.09043	-2.76174	-4.76589
H	3.73061	-3.69262	-2.53094
H	2.64149	-2.84930	-0.46187
H	0.95768	2.93433	2.70462
H	1.45013	1.13214	2.72760
H	-0.26016	2.95701	-0.04127
H	-0.91539	0.46860	2.82145
H	-1.46335	3.54523	2.80354
H	-2.40189	2.35190	3.75516
H	-2.47821	2.32484	1.97288
H	1.57227	2.10331	-2.98007
H	2.60746	3.54923	-2.70725
H	0.81933	3.64325	-2.47675
H	1.52610	4.80658	0.18645
H	3.24060	4.54602	-0.30436
H	2.64146	3.92858	1.27198
H	3.81301	1.38188	0.43498
H	4.28211	2.19583	-1.09583
H	3.37977	0.64028	-1.13916

SHOP_3a

62

Ni	0.00877	-0.76377	-1.50996
P	-0.25656	-2.79911	-0.63092
P	0.80936	0.42822	0.25745
O	-1.83249	-0.17826	-0.81413
C	-0.73245	0.87873	1.03919
C	-1.88112	0.48637	0.34944
C	-3.25663	0.80104	0.85348
C	-4.34461	0.76184	-0.04960
C	-5.64648	1.05809	0.38488
C	-5.88656	1.38971	1.73135
C	-4.81291	1.41933	2.64124
C	-3.50963	1.12705	2.20721
C	1.71285	2.03000	-0.08291
C	0.94910	3.18503	-0.37789
C	1.58205	4.39713	-0.70478
C	2.98650	4.47321	-0.74738
C	3.75468	3.33081	-0.45768
C	3.12425	2.11702	-0.12831
C	1.95140	-0.34749	1.50979
C	1.83171	-0.09158	2.89458
C	2.71440	-0.69157	3.81062
C	3.73289	-1.55011	3.35533
C	3.86161	-1.81280	1.97934
C	2.97289	-1.21913	1.06326
C	1.44301	-0.40525	-2.92082
C	0.42859	0.58343	-3.01460
C	-0.62053	0.61745	-4.10670
C	-0.33971	-3.02538	1.21772
C	-1.89362	-3.52163	-1.13561
C	0.94380	-4.13157	-1.13593
H	-2.68704	1.13067	2.92743
H	-0.77980	1.51110	1.92888
H	-4.13983	0.49676	-1.08889
H	-6.47616	1.03035	-0.32768
H	-6.90090	1.61849	2.07067
H	-4.99273	1.66403	3.69226
H	-0.14266	3.12576	-0.33547
H	0.97728	5.28204	-0.92309
H	3.47862	5.41634	-1.00063
H	4.84702	3.38401	-0.48181
H	3.73545	1.24358	0.11537
H	1.03912	0.56757	3.25739
H	2.60753	-0.48805	4.87993
H	4.41882	-2.01445	4.06911
H	4.64836	-2.48235	1.61956
H	3.05925	-1.44284	-0.00494
H	1.49171	-1.21246	-3.66025
H	2.39032	-0.17448	-2.42192
H	-0.60471	-1.59442	-2.56029
H	0.61364	1.55037	-2.52911
H	-0.70854	-0.35943	-4.61231
H	-0.36012	1.37878	-4.86923
H	-1.61194	0.87843	-3.69990
H	0.63488	-2.79257	1.67219
H	-0.62793	-4.06077	1.47062
H	-1.08785	-2.32689	1.62555
H	-2.66954	-2.77150	-0.91679
H	-2.10913	-4.46068	-0.59820
H	-1.89194	-3.70695	-2.22162
H	1.00223	-4.16064	-2.23574
H	0.63235	-5.12088	-0.75867
H	1.94391	-3.89253	-0.73984

SHOP_3b_4b_TS

62

P	1.17992	-0.30738	-0.08353
O	-1.66988	-0.00691	0.02495
C	0.02452	-1.65386	-0.37001
C	-1.30809	-1.27547	-0.29164
C	-2.43935	-2.22084	-0.52848
C	-3.73575	-1.88494	-0.07276
C	-4.81685	-2.75716	-0.27672
C	-4.62565	-3.97880	-0.94809
C	-3.34239	-4.31854	-1.41674
C	-2.25993	-3.44878	-1.21062
C	2.33918	-0.86506	1.25939
C	1.97534	-1.92511	2.12073
C	2.81970	-2.30413	3.18096
C	4.03227	-1.62493	3.39669
C	4.39871	-0.56252	2.54770
C	3.55904	-0.18349	1.48665
C	2.32144	-0.20402	-1.55035
C	3.24448	-1.23869	-1.83356
C	4.05020	-1.17785	-2.98334
C	3.94750	-0.08219	-3.86198
C	3.03774	0.95365	-3.58437
C	2.22921	0.89339	-2.43440
Ni	-0.24642	1.31453	0.20084
C	0.06482	1.49468	2.89420
C	-1.26320	1.73650	3.01825
P	-1.50829	2.97381	-0.44703
C	-1.49647	3.17992	-2.29832
C	-1.14839	4.70489	0.13439
C	-3.32689	2.79059	-0.09954
C	-2.31073	0.68617	3.27171
H	-1.27437	-3.71253	-1.60301
H	0.34253	-2.67486	-0.59200
H	-3.87007	-0.93253	0.44319
H	-5.81134	-2.48383	0.08835
H	-5.46800	-4.65737	-1.10985
H	-3.18634	-5.25974	-1.95189
H	1.02893	-2.44751	1.95232
H	2.52938	-3.13042	3.83633
H	4.68784	-1.91911	4.22103
H	5.33952	-0.02928	2.71187
H	3.85203	0.64040	0.82946
H	3.33887	-2.08722	-1.15013
H	4.75964	-1.98365	-3.19264
H	4.57652	-0.03558	-4.75540
H	2.95946	1.81049	-4.25996
H	1.52281	1.69659	-2.20493
H	0.78621	2.30049	2.74181
H	0.47615	0.48893	3.02447
H	0.86404	2.28754	0.17131
H	-2.18358	3.98119	-2.62239
H	-1.79898	2.22647	-2.75968
H	-0.47415	3.41845	-2.63202
H	-1.20950	4.73979	1.23411
H	-1.85808	5.43366	-0.29300
H	-0.12148	4.97425	-0.15994
H	-3.50049	2.86432	0.98589
H	-3.62858	1.78480	-0.42914
H	-3.92486	3.55908	-0.61888
H	-1.85279	-0.30545	3.41660
H	-3.00144	0.60433	2.41300
H	-2.91561	0.92717	4.16576
H	-1.62276	2.77266	2.93598

SHOP_3b_TS$_{BHE}$

62

P	0.76438	-0.55121	0.16377
O	-1.83480	0.41613	-0.63511
C	-0.78622	-1.23590	0.73606
C	-1.92191	-0.62211	0.21321
C	-3.31292	-1.04851	0.56699
C	-4.40058	-0.23415	0.17231
C	-5.72022	-0.59581	0.48666
C	-5.98044	-1.78132	1.19813
C	-4.90712	-2.60403	1.58929
C	-3.58696	-2.24272	1.27651
C	1.77643	-0.20564	1.69681
C	1.13528	-0.10048	2.95250
C	1.87452	0.20234	4.11077
C	3.26307	0.41095	4.02988
C	3.91105	0.30929	2.78378
C	3.17462	0.00158	1.62643
C	1.78455	-1.91877	-0.60320
C	1.56462	-3.27064	-0.25238
C	2.33999	-4.29375	-0.82609
C	3.34977	-3.98168	-1.75527
C	3.57523	-2.64080	-2.11488
C	2.79426	-1.61781	-1.54578
Ni	0.01730	1.05044	-1.15974
C	-0.75124	1.79758	-2.86144
C	0.14215	0.73022	-3.24834
C	-0.37637	-0.65805	-3.59832
H	-2.76785	-2.90325	1.57242
H	-0.83620	-2.05368	1.45855
H	-4.18044	0.67808	-0.38542
H	-6.54822	0.04742	0.17408
H	-7.00824	-2.06516	1.44175
H	-5.09976	-3.53266	2.13457
H	0.05449	-0.25892	3.01321
H	3.83780	0.64556	4.93014
H	4.99202	0.46188	2.71394
H	3.69433	-0.09344	0.66876
H	0.77304	-3.52461	0.45699
H	2.15327	-5.33528	-0.54911

H	3.95068	-4.77868	-2.20181
H	4.35160	-2.39063	-2.84384
H	2.95709	-0.57852	-1.84969
H	1.36432	0.27266	5.07590
H	-0.48472	2.82967	-3.11778
H	-1.82068	1.58987	-2.75587
H	1.18669	0.76059	-2.06289
H	0.38409	-1.43406	-3.41386
H	-0.64767	-0.69931	-4.67175
H	-1.27016	-0.90390	-3.00440
H	1.00405	1.04108	-3.86209
P	0.19719	3.06427	-0.17247
C	0.63943	3.22785	1.63327
C	-1.37902	4.06613	-0.21800
C	1.41158	4.27022	-0.92745
H	0.64807	4.28508	1.95167
H	1.62838	2.78044	1.81911
H	-0.09917	2.67326	2.23362
H	-1.68865	4.21840	-1.26442
H	-1.25991	5.04767	0.27307
H	-2.17053	3.49155	0.28927
H	1.20990	4.36501	-2.00725
H	2.43307	3.87466	-0.80254
H	1.34834	5.26810	-0.45904

SHOP_3b_TS$_{BHE}$_PPh

83

P	1.49874	1.06051	0.06077
O	1.41076	-1.69483	-0.81937
C	2.70825	-0.18489	0.50520
C	2.48656	-1.44038	-0.05097
C	3.39207	-2.60581	0.18784
C	2.91585	-3.91330	-0.06788
C	3.73746	-5.03002	0.15368
C	5.05242	-4.86088	0.62544
C	5.54064	-3.56341	0.87060
C	4.71930	-2.44562	0.65347
C	0.95516	1.83508	1.66996
C	1.07119	1.09360	2.86862
C	0.65353	1.64341	4.09379
C	0.10959	2.93928	4.13804
C	-0.01692	3.68182	2.94933
C	0.40202	3.13559	1.72439
C	2.38778	2.50167	-0.73155
C	3.77130	2.70571	-0.52728
C	4.42915	3.79550	-1.12512
C	3.71397	4.69979	-1.93187
C	2.33730	4.50438	-2.14545
C	1.68111	3.40970	-1.55326
Ni	0.18641	-0.16748	-1.25553
C	-0.21997	-1.09142	-3.01083
C	0.39472	0.15854	-3.36278
C	1.86551	0.24801	-3.74512
H	5.11763	-1.44179	0.82329
H	3.52939	0.01337	1.19819
H	1.89648	-4.02545	-0.44242
H	3.35247	-6.03468	-0.04446
H	5.69399	-5.73044	0.79435
H	6.56628	-3.42223	1.22390
H	1.49830	0.08797	2.83586
H	-0.21264	3.36850	5.09096
H	-0.44200	4.68905	2.97395
H	0.30340	3.72831	0.81191
H	4.33752	2.00022	0.08576
H	5.50157	3.93640	-0.96251
H	4.22749	5.54557	-2.39729
H	1.77596	5.19741	-2.77897
H	0.61497	3.24857	-1.74328
H	0.75661	1.05830	5.01220
H	-1.28563	-1.24334	-3.20597
H	0.39904	-1.99137	-2.94364
H	0.02828	1.06622	-2.10587
H	2.28526	1.24394	-3.53196
H	1.97961	0.05806	-4.83036
H	2.45870	-0.50160	-3.19894
H	-0.24908	0.86267	-3.91535
P	-1.83711	-0.41845	-0.23645
C	-2.57504	1.18868	0.36324
C	-3.12068	1.38247	1.65129
C	-3.65392	2.63156	2.02134
C	-3.66031	3.70102	1.10933
C	-3.11189	3.52294	-0.17478
C	-2.56344	2.28137	-0.53896
C	-3.24110	-1.12090	-1.25991
C	-3.11296	-2.46151	-1.70548
C	-4.10489	-3.04903	-2.50781
C	-5.23862	-2.30635	-2.89047
C	-5.37317	-0.97551	-2.45957
C	-4.38377	-0.38588	-1.64831
C	-1.95256	-1.55065	1.24279
C	-3.19236	-1.97471	1.78158
C	-3.22935	-2.84833	2.88175
C	-2.03000	-3.31789	3.45172
C	-0.79552	-2.91448	2.91444
C	-0.75555	-2.03627	1.81470
H	-3.11985	0.56357	2.37344
H	-4.06273	2.76563	3.02676
H	-4.08158	4.66813	1.39775
H	-3.10517	4.35128	-0.88946
H	-2.11268	2.15166	-1.52815
H	-2.23556	-3.04711	-1.41422
H	-3.99123	-4.08624	-2.83581
H	-6.00907	-2.76302	-3.51780
H	-6.25278	-0.39185	-2.74656
H	-4.51021	0.64566	-1.31136
H	-4.12738	-1.63497	1.32764
H	-4.19281	-3.16934	3.28829
H	-2.06047	-4.00373	4.30316
H	0.13916	-3.29136	3.33889
H	0.20161	-1.75180	1.37218

SHOP_3b_TS$_{phosdiss}$

62

P	1.30435	-0.17188	-0.08410
O	-1.22602	-1.05622	0.87029
C	0.07532	-0.94732	-1.13790
C	-1.08480	-1.29573	-0.45698
C	-2.24785	-1.96626	-1.10960
C	-3.22377	-2.59705	-0.30252
C	-4.32463	-3.24484	-0.88539
C	-4.47480	-3.26780	-2.28404
C	-3.51487	-2.63467	-3.09640
C	-2.41171	-1.98946	-2.51592
C	2.79088	-1.27960	-0.02462
C	2.65070	-2.65777	-0.30451
C	3.75743	-3.51897	-0.19589
C	5.01097	-3.01422	0.19487
C	5.15590	-1.64246	0.47825
C	4.05308	-0.77826	0.37222
C	1.95267	1.36749	-0.88136
C	2.64855	1.31468	-2.11254
C	3.10654	2.49713	-2.71831
C	2.88174	3.74175	-2.09875
C	2.19650	3.80037	-0.87208
C	1.73190	2.61896	-0.26384
Ni	0.20330	-0.11297	1.78725
C	-0.08842	-1.14199	3.55781
C	-0.75925	0.06889	3.70974
P	-2.09014	2.80546	0.27941
C	-1.87600	2.56657	-1.57157
C	-2.56046	4.62969	0.28877
C	-3.80192	2.05174	0.46441
C	-2.25065	0.24370	3.56030
H	-1.68406	-1.48542	-3.15745
H	0.23647	-1.15579	-2.19729
H	-3.09428	-2.56705	0.78074
H	-5.06734	-3.73269	-0.24749
H	-5.33363	-3.77001	-2.73815
H	-3.62980	-2.63853	-4.18410
H	1.67339	-3.04558	-0.60608
H	3.63892	-4.58336	-0.41753
H	5.87069	-3.68466	0.27908
H	6.12807	-1.24515	0.78340
H	4.17204	0.28544	0.59593
H	2.84285	0.35075	-2.59126
H	3.64329	2.44715	-3.66981
H	3.24365	4.66016	-2.56928
H	2.02570	4.76387	-0.38371
H	1.18937	2.65970	0.68462
H	0.92497	-1.27971	3.94625
H	-0.63280	-2.04605	3.26501
H	1.34598	0.64147	2.33442
H	-2.74050	2.94941	-2.14367
H	-1.74964	1.49075	-1.77961
H	-0.96090	3.08356	-1.90577
H	-2.87315	4.92376	1.30526
H	-3.37941	4.85529	-0.41759
H	-1.67820	5.23386	0.01646
H	-4.19169	2.25220	1.47694
H	-3.72062	0.95911	0.33982
H	-4.51575	2.45028	-0.27871
H	-2.69059	-0.55933	2.95105
H	-2.49216	1.20855	3.08476
H	-2.73214	0.23874	4.55892
H	-0.22442	0.90107	4.18491

SHOP_3b

62

P	-1.04962	-0.42477	0.05244
O	1.75133	0.09297	-0.50450
C	0.31807	-1.30790	0.81346
C	1.57866	-0.88674	0.41220
C	2.84231	-1.48819	0.93894
C	4.05126	-1.30227	0.22823
C	5.25211	-1.85705	0.69910
C	5.26971	-2.60112	1.89313
C	4.07474	-2.78305	2.61453
C	2.87277	-2.23097	2.14381
C	-2.12550	-1.73008	-0.72823
C	-1.51079	-2.88101	-1.27653
C	-2.27783	-3.85246	-1.94344
C	-3.66846	-3.68616	-2.07906
C	-4.28837	-2.54340	-1.54035

C	-3.52443	-1.57191	-0.86962
C	-2.17492	0.22202	1.38993
C	-2.28180	-0.40765	2.65155
C	-3.14449	0.10761	3.63525
C	-3.91750	1.25408	3.37001
C	-3.81832	1.88952	2.11898
C	-2.94713	1.37999	1.13760
Ni	0.13808	1.00013	-1.19585
C	0.08533	-0.00018	-3.01454
C	0.81839	1.18029	-3.22723
P	0.73097	2.85083	-0.11320
C	0.84170	2.65690	1.73544
C	-0.31371	4.38437	-0.27459
C	2.43010	3.50279	-0.50646
C	2.32524	1.18972	-3.38606
H	1.95643	-2.35825	2.72618
H	0.17892	-2.16630	1.47521
H	4.02502	-0.71789	-0.69334
H	6.17672	-1.70839	0.13363
H	6.20549	-3.03088	2.26153
H	4.08080	-3.35007	3.54994
H	-0.43048	-3.01300	-1.16625
H	-1.78820	-4.73969	-2.35549
H	-4.26464	-4.44176	-2.59821
H	-5.36976	-2.40938	-1.63700
H	-4.02110	-0.69560	-0.44409
H	-1.68353	-1.29670	2.86695
H	-3.21535	-0.38719	4.60820
H	-4.58948	1.65136	4.13576
H	-4.41371	2.78280	1.90841
H	-2.85071	1.88359	0.17039
H	-0.96479	-0.07483	-3.30943
H	0.61049	-0.95166	-2.87595
H	-1.08316	1.70927	-1.57391
H	1.21556	3.57880	2.21443
H	1.52523	1.82339	1.96158
H	-0.15198	2.40967	2.14081
H	-0.37165	4.67503	-1.33600
H	0.10062	5.22239	0.31185
H	-1.33357	4.16429	0.07955
H	2.46038	3.84096	-1.55422
H	3.15358	2.68257	-0.38158
H	2.70095	4.34284	0.15660
H	2.79324	0.44227	-2.72659
H	2.76158	2.17481	-3.15290
H	2.60075	0.95232	-4.43370
H	0.28640	2.04393	-3.64737

SHOP_4a

53

Ni	-0.09853	1.69066	-0.12065
P	-0.33947	-0.53761	0.01878
O	1.77817	1.37366	-0.09505
C	1.39437	-0.98510	0.08057
C	2.24903	0.10303	-0.01480
C	3.73688	-0.00778	-0.01711
C	4.51301	1.16905	0.10471
C	5.91528	1.10170	0.11571
C	6.56708	-0.13977	0.00054
C	5.80371	-1.31574	-0.12992
C	4.40181	-1.25167	-0.13962
C	-1.10370	-1.48299	-1.38844
C	-1.35295	-0.79648	-2.60025
C	-1.84398	-1.48362	-3.72500
C	-2.09590	-2.86561	-3.65131
C	-1.84940	-3.55882	-2.45107
C	-1.35500	-2.87457	-1.32669
C	-1.13617	-1.26773	1.53290
C	-0.38315	-1.32411	2.73009
C	-0.96957	-1.78538	3.92159
C	-2.31528	-2.19736	3.93630
C	-3.07280	-2.14532	2.75184
C	-2.49025	-1.68076	1.55825
H	3.82367	-2.17141	-0.25969
H	1.73546	-2.01883	0.15721
H	3.98760	2.12219	0.18656
H	6.50118	2.02037	0.21278
H	7.65960	-0.19217	0.00732
H	6.30260	-2.28408	-0.23012
H	-1.14008	0.27615	-2.65824
H	-2.02659	-0.94110	-4.65695
H	-2.47867	-3.40096	-4.52456
H	-2.03831	-4.63450	-2.39130
H	-1.16446	-3.42263	-0.39998
H	0.66515	-1.01155	2.71519
H	-0.37316	-1.82634	4.83740
H	-2.76912	-2.56007	4.86269
H	-4.11709	-2.47118	2.75392
H	-3.08573	-1.65800	0.64139
H	0.18549	3.16134	-0.19291
P	-2.02265	2.58038	-0.12543
C	-2.32768	3.68301	1.34089
C	-3.55075	1.51074	-0.11766
C	-2.36216	3.70969	-1.56482
H	-3.33174	4.13846	1.29447
H	-1.55879	4.47033	1.35926
H	-2.23703	3.09023	2.26519
H	-3.54271	0.85340	-1.00187
H	-4.46703	2.12609	-0.12824
H	-3.54638	0.87982	0.78547
H	-2.29604	3.13748	-2.50414
H	-1.59287	4.49649	-1.58682
H	-3.36421	4.16489	-1.48578

SHOP_4b

53

Ni	0.24603	1.47457	-0.06875
P	-1.09125	-0.23909	-0.00070
O	1.72685	0.22840	-0.02401
C	0.12862	-1.55937	-0.02307
C	1.43662	-1.10013	-0.05219
C	2.61882	-2.00843	-0.08972
C	3.87662	-1.53703	0.35362
C	5.00149	-2.37703	0.33958
C	4.89287	-3.69957	-0.12842
C	3.64878	-4.17464	-0.58486
C	2.52166	-3.33794	-0.56621
C	-2.28734	-0.51561	-1.38973
C	-2.33278	0.40465	-2.46106
C	-3.18675	0.17850	-3.55642
C	-4.00299	-0.96606	-3.59010
C	-3.96678	-1.88556	-2.52391
C	-3.11575	-1.66230	-1.42846
C	-2.13270	-0.47632	1.51667
C	-1.59096	-1.14358	2.63892
C	-2.34328	-1.27229	3.82023
C	-3.64109	-0.73433	3.89477
C	-4.18487	-0.06373	2.78267
C	-3.43602	0.06793	1.60063
H	1.56593	-3.70700	-0.94759
H	-0.13026	-2.61993	-0.00033
H	3.94697	-0.50729	0.70891
H	5.96564	-1.99972	0.69306
H	5.76991	-4.35284	-0.14349
H	3.55881	-5.19674	-0.96396
H	-1.69807	1.29506	-2.42441
H	-3.21517	0.89738	-4.38019
H	-4.66674	-1.14136	-4.44136
H	-4.60253	-2.77527	-2.54562
H	-3.09918	-2.37608	-0.59998
H	-0.58169	-1.56106	2.57636
H	-1.91538	-1.79459	4.68073
H	-4.22596	-0.83635	4.81316
H	-5.19300	0.35726	2.83525
H	-3.86517	0.58989	0.74088
H	-0.90323	2.40176	-0.08814
P	1.57482	3.19541	-0.06542
C	3.02568	3.01333	-1.21175
C	2.38786	3.44251	1.59022
C	0.92396	4.88830	-0.46491
H	3.76863	3.81551	-1.06247
H	2.67119	3.03156	-2.25493
H	3.48021	2.02889	-1.02184
H	1.61767	3.66552	2.34573
H	3.12527	4.26350	1.56330
H	2.88849	2.50294	1.87224
H	0.12175	5.14071	0.24651
H	0.49112	4.87715	-1.47805
H	1.71734	5.65329	-0.41400

SHOP_5a_7a_TS

68

Ni	-0.17842	-0.38038	-1.50467
P	2.87283	-2.97591	-0.16056
C	4.25330	-2.01219	-0.99774
H	4.45904	-2.44560	-1.99149
H	5.18625	-2.01446	-0.40588
H	3.91852	-0.96997	-1.13565
C	2.95379	-2.16319	1.53340
H	2.28460	-2.69867	2.22802
H	2.59640	-1.12316	1.44545
C	3.80997	-4.56149	0.23389
H	3.18781	-5.20067	0.88341
H	4.00421	-5.11494	-0.70063
H	4.77191	-4.36448	0.74056
O	1.31218	0.82234	-1.05313
C	1.30967	1.49074	0.12342
C	2.51464	2.33021	0.38708
C	3.36634	2.67914	-0.68712
H	3.11366	2.31784	-1.68572
H	2.20933	2.50323	2.53544
C	2.83984	2.78480	1.68784
C	3.97919	3.57515	1.90440
H	4.21983	3.91412	2.91609
H	5.70241	4.54078	0.99712
C	4.81484	3.92502	0.82660
C	4.50357	3.47311	-0.46891
H	5.14888	3.73961	-1.31096
H	-0.39740	-2.22919	4.59457
H	0.22462	-0.55386	2.84619
H	0.15422	1.99665	1.91068

C	0.24162	1.39346	1.00485
C	-1.08452	-2.02421	3.76878
C	-0.73350	-1.07780	2.78933
P	-1.10335	0.38447	0.38539
C	-1.61316	-0.79459	1.71925
C	-2.31415	-2.70263	3.68907
H	0.28469	1.04103	-3.57079
C	0.04881	-0.02750	-3.53604
H	-2.58599	-3.43860	4.45065
C	-3.19394	-2.43118	2.62446
C	1.01359	-0.95134	-3.14360
H	0.88509	-2.02357	-3.31290
H	2.00791	-0.62056	-2.83768
H	-1.11220	-2.40618	-2.59158
H	-1.56135	-2.32040	-0.85978
H	-2.92374	-0.69488	-3.13544
C	-3.88892	-2.53347	-2.48979
H	-3.48497	-3.16834	-3.29842
H	-4.90212	-2.20750	-2.78606
H	-3.41776	-0.68104	-1.44505
H	-4.15104	-2.95580	2.55621
H	-3.54257	-1.27724	0.82635
C	-2.84751	-1.48530	1.64431
C	-2.57331	1.50765	0.20198
C	-3.42013	1.82559	1.28926
H	-3.27105	1.34234	2.25818
C	-4.45737	2.76219	1.12961
H	-5.10576	3.00122	1.97731
H	-5.46685	4.11841	-0.23379
C	-4.65952	3.39099	-0.11263
C	-3.82120	3.07956	-1.19919
H	-3.97608	3.56218	-2.16820
C	-2.78571	2.14226	-1.04436
H	-2.13723	1.89203	-1.88941
C	-1.54404	-1.74884	-1.81060
C	-2.96236	-1.32169	-2.22280
H	-0.86249	-0.34205	-4.05303
H	-3.98172	-3.16331	-1.58720
H	3.97814	-2.15812	1.94809

SHOP_5a

68

Ni	-0.06299	-1.07226	-1.05818
P	-0.67790	0.70942	0.23911
O	1.82654	-0.48062	-0.68120
C	0.96161	1.38070	0.55074
C	2.01914	0.65562	0.02400
C	3.44742	1.07725	0.16530
C	4.41765	0.54563	-0.71648
C	5.76397	0.93177	-0.61809
C	6.16752	1.85095	0.36760
C	5.21229	2.37871	1.25698
C	3.86537	1.99475	1.15892
C	-1.46972	0.39108	1.89745
C	-0.78139	0.67002	3.10101
C	-1.35765	0.36167	4.34689
C	-2.63147	-0.23244	4.41146
C	-3.32577	-0.51994	3.22166
C	-2.74897	-0.21495	1.97531
C	-1.65312	2.16934	-0.40102
C	-1.10414	2.87733	-1.49936
C	-1.78301	3.97063	-2.06200
C	-3.02581	4.37743	-1.54045
C	-3.57711	3.68751	-0.44701
C	-2.89766	2.59283	0.12047
C	0.13637	-0.18761	-2.93900
C	0.50285	-1.54261	-3.00686
C	-1.88465	-1.84546	-1.31263
C	-2.88979	-1.06756	-2.17230
C	-4.29436	-1.72218	-2.14959
H	3.13644	2.39537	1.86844
H	1.10554	2.35104	1.03233
H	4.09035	-0.16645	-1.47653
H	6.49965	0.51657	-1.31317
H	7.21626	2.15118	0.44561
H	5.51895	3.08640	2.03263
H	0.21479	1.11839	3.05250
H	-0.81093	0.58732	5.26718
H	-3.07871	-0.47177	5.38019
H	-4.31546	-0.98430	3.26250
H	-3.29709	-0.45167	1.05890
H	-0.13148	2.57838	-1.89845
H	-1.33948	4.50683	-2.90594
H	-3.55481	5.22838	-1.97842
H	-4.53555	4.00397	-0.02507
H	-3.33297	2.08411	0.98370
H	-0.17592	-2.28755	-3.43468
H	1.55647	-1.83063	-2.94704
H	0.90999	0.57552	-2.81629
H	-0.82546	0.16645	-3.31536
H	-2.28087	-1.98129	-0.28818
H	-1.71654	-2.84984	-1.74721
H	-2.54306	-1.02230	-3.22132
H	-2.96934	-0.02042	-1.82663
H	-4.70373	-1.74991	-1.12333
H	-4.25250	-2.76198	-2.52047
H	-5.00550	-1.16235	-2.78273
P	0.58321	-2.85390	0.18351
C	1.18126	-2.44982	1.89725
C	-0.55418	-4.29345	0.52339
C	2.06661	-3.70219	-0.55062
H	2.83862	-2.93547	-0.71576
H	1.79327	-4.14469	-1.52234
H	2.45814	-4.49249	0.11286
H	1.91701	-1.63505	1.82500
H	0.33411	-2.10232	2.50942
H	1.64663	-3.32737	2.37832
H	-0.89573	-4.73641	-0.42604
H	-1.43878	-3.94245	1.07898
H	-0.04024	-5.06786	1.11764

SHOP_5a_TS$_{BHT}$

68

Ni	0.08566	1.27138	0.02085
P	-0.93659	3.19362	0.09822
C	-2.42059	3.28470	-1.01034
C	-1.65543	3.49685	1.78411
C	-0.05360	4.78818	-0.27844
O	-1.82602	0.52044	0.24454
C	-2.02049	-0.78253	-0.03418
C	-3.44477	-1.22619	-0.13333
C	-4.45954	-0.45358	0.47821
C	-3.81701	-2.39922	-0.83358
C	-5.16313	-2.79060	-0.91035
C	-6.16334	-2.01933	-0.28850
C	-5.80496	-0.84912	0.40586
C	-0.95341	-1.65322	-0.20704
C	0.97867	-3.00594	3.62388
C	0.53137	-2.50782	2.38748
P	0.67101	-0.92826	0.02278
C	1.33082	-1.61595	1.63436
C	2.22976	-2.61664	4.13502
C	2.11142	1.74972	-2.18951
C	3.02866	-1.71842	3.40517
C	0.67522	1.62109	-2.03852
C	3.84960	3.31939	0.28117
C	2.58208	-1.21781	2.16861
C	1.72589	-1.75382	-1.27685
C	3.07099	-2.13551	-1.06454
C	3.82798	-2.70210	-2.10554
C	3.25655	-2.89324	-3.37658
C	1.91745	-2.52324	-3.59804
C	1.15715	-1.96049	-2.55805
C	1.75111	2.04017	1.06361
C	3.00868	2.04888	0.35782
H	-2.10026	3.28328	-2.06457
H	-3.01178	4.19431	-0.81099
H	-3.01949	2.38141	-0.82274
H	-0.84255	3.57610	2.52380
H	-2.27733	2.62544	2.04046
H	0.77903	4.93632	0.42629
H	0.35908	4.74467	-1.29877
H	-0.74490	5.64469	-0.20429
H	-4.16742	0.45266	1.01280
H	-3.05162	-2.99402	-1.33932
H	-5.43383	-3.69543	-1.46237
H	-7.21142	-2.32598	-0.34901
H	-6.57609	-0.24405	0.89192
H	0.34561	-3.69617	4.18891
H	-0.45081	-2.79527	2.00331
H	-1.08281	-2.72178	-0.39357
H	2.64540	0.85355	-2.53974
H	2.57583	-3.00269	5.09784
H	0.08500	2.49576	-2.34601
H	0.21302	0.67648	-2.36065
H	1.45378	3.02824	1.45097
H	1.58636	1.24637	1.81397
H	2.61733	1.89397	-1.01520
H	3.21416	4.20080	0.07864
H	4.60734	3.26078	-0.52032
H	3.60493	1.12204	0.41037
H	3.99755	-1.39889	3.79975
H	3.21044	-0.50385	1.62976
H	3.52660	-2.01539	-0.07942
H	4.86371	-3.00047	-1.91914
H	3.84701	-3.33355	-4.18478
H	1.46016	-2.67717	-4.57966
H	0.10970	-1.69598	-2.72779
H	2.47822	2.66826	-2.67767
H	4.38579	3.51165	1.23096
H	-2.26519	4.41630	1.80969

SHOP_5b_TS

68

Ni	-0.34428	-1.25547	0.26667
P	1.22954	0.37618	0.08408
O	-1.62867	0.26656	0.30623
C	0.16154	1.81728	-0.00384
C	-1.18905	1.53158	0.10583
C	-2.25721	2.57243	0.03447
C	-3.53845	2.29895	0.56839
C	-4.55540	3.26599	0.51969
C	-4.31415	4.52056	-0.07023

C	-3.04613	4.79897	-0.61452
C	-2.02716	3.83460	-0.56462
C	2.44326	0.49707	-1.33059
C	3.34070	1.58598	-1.44918
C	4.21011	1.67897	-2.54933
C	4.20531	0.67982	-3.54209
C	3.32678	-0.41187	-3.42971
C	2.45081	-0.50038	-2.33092
C	2.36093	0.65324	1.53861
C	1.88589	1.38211	2.65612
C	2.67021	1.50540	3.81618
C	3.93625	0.89326	3.88488
C	4.41496	0.15889	2.78400
C	3.63521	0.03871	1.61938
C	0.96813	-2.73896	0.37178
C	0.54223	-2.52661	1.73427
C	-1.59584	-2.05995	1.89950
C	-2.25069	-3.44024	1.84179
C	-3.66854	-3.43145	2.46663
P	-1.37626	-1.83595	-1.69704
C	-1.33174	-0.50938	-3.00945
C	-0.88492	-3.34128	-2.69552
C	-3.22431	-2.08311	-1.56495
H	-1.05383	4.05213	-1.01247
H	0.54415	2.83578	-0.10122
H	-3.71289	1.32118	1.02175
H	-5.53851	3.04102	0.94364
H	-5.10715	5.27267	-0.11055
H	-2.85322	5.76696	-1.08610
H	3.36275	2.35764	-0.67467
H	4.89392	2.52883	-2.63117
H	4.88541	0.75186	-4.39541
H	3.32466	-1.19511	-4.19349
H	1.76616	-1.34922	-2.23848
H	0.90103	1.85638	2.60311
H	2.29304	2.08160	4.66625
H	4.54491	0.98862	4.78840
H	5.39871	-0.31759	2.82895
H	4.02634	-0.51974	0.76379
H	0.17242	-3.38741	2.29754
H	1.10139	-1.81806	2.35577
H	1.95820	-2.39315	0.05495
H	0.64932	-3.66163	-0.12941
H	-2.23421	-1.27634	1.46046
H	-1.34835	-1.75843	2.93114
H	-1.63656	-4.19318	2.37402
H	-2.32010	-3.78820	0.79375
H	-4.33447	-2.73575	1.92695
H	-3.63035	-3.10860	3.52175
H	-4.12466	-4.43701	2.43411
H	-3.64090	-1.21017	-1.03834
H	-3.44468	-2.98795	-0.97531
H	-3.69761	-2.17559	-2.55821
H	-1.73842	0.41928	-2.57895
H	-0.29112	-0.31745	-3.31555
H	-1.92906	-0.79396	-3.89390
H	-1.01198	-4.24927	-2.08266
H	0.17761	-3.26743	-2.98166
H	-1.49429	-3.43900	-3.61027

SHOP_6a

49

Ni	0.05867	1.63302	-0.70328
P	0.68333	-0.24952	0.04673
O	-1.75669	1.07943	-0.50033
C	-0.91972	-0.99857	0.33249
C	-1.97848	-0.15485	0.01574
C	-3.41164	-0.52248	0.19315
C	-4.40837	0.27963	-0.41094
C	-5.76728	-0.04323	-0.27035
C	-6.15505	-1.16799	0.48077
C	-5.17141	-1.96701	1.09429
C	-3.81197	-1.64844	0.95266
C	1.66040	-0.30302	1.62194
C	1.65041	0.82882	2.46943
C	2.30807	0.79385	3.71132
C	2.98509	-0.37062	4.11844
C	3.00096	-1.50107	3.28049
C	2.34319	-1.47019	2.03794
C	1.64500	-1.31766	-1.12180
C	0.96416	-2.24152	-1.94664
C	1.67371	-3.00766	-2.88900
C	3.06616	-2.85672	-3.01957
C	3.75020	-1.93390	-2.20513
C	3.04551	-1.16575	-1.26266
C	1.67605	2.56590	-1.06380
C	0.66721	3.60522	-1.50878
C	0.66274	4.93149	-0.72341
H	-3.06030	-2.26560	1.45155
H	-1.04241	-2.00070	0.74695
H	-4.08885	1.15205	-0.98371
H	-6.52605	0.58469	-0.74628
H	-7.21389	-1.41816	0.59244
H	-5.46514	-2.83649	1.68937
H	1.12102	1.73127	2.14895
H	2.29402	1.67534	4.35833
H	3.49899	-0.39666	5.08324
H	3.52591	-2.40808	3.59319
H	2.36489	-2.35120	1.39103
H	-0.11954	-2.34990	-1.84488
H	1.13763	-3.72174	-3.52032
H	3.61635	-3.45323	-3.75243
H	4.83248	-1.81177	-2.30418
H	3.58364	-0.45235	-0.63216
H	2.28760	2.10878	-1.85563
H	2.27624	2.83144	-0.17946
H	0.70576	3.77638	-2.59901
H	-0.42432	3.18198	-1.39550
H	1.59598	5.48520	-0.92009
H	0.59927	4.74310	0.36150
H	-0.18788	5.57299	-1.00880

SHOP_6a_7b_TS

55

Ni	-0.04075	1.56446	-0.38737
P	-0.73097	-0.39895	0.01429
O	1.76399	0.91540	-0.29491
C	0.84512	-1.24136	0.16208
C	1.93692	-0.40318	-0.04292
C	3.35404	-0.86653	-0.01370
C	4.37581	0.01663	-0.43589
C	5.71990	-0.38859	-0.42823
C	6.06869	-1.68109	0.00448
C	5.06056	-2.56570	0.43271
C	3.71614	-2.16315	0.42525
C	-1.73560	-1.26985	-1.28231
C	-1.60907	-0.85020	-2.62709
C	-2.28321	-1.53357	-3.65339
C	-3.09377	-2.64311	-3.34843
C	-3.22505	-3.06774	-2.01378
C	-2.55080	-2.38643	-0.98407
C	-1.70521	-0.65558	1.57001
C	-1.07324	-1.15135	2.73260
C	-1.79553	-1.28319	3.93307
C	-3.15315	-0.91990	3.98504
C	-3.78919	-0.42080	2.83153
C	-3.07098	-0.28617	1.63158
C	-1.64594	2.53084	-0.73768
C	-0.64949	3.54783	-1.26366
C	0.99165	3.70950	1.94663
C	0.37884	2.55692	2.29064
C	-0.72674	3.84830	-2.77264
H	2.94702	-2.85724	0.77381
H	0.92572	-2.32316	0.28369
H	4.08653	1.01583	-0.76630
H	6.49737	0.30537	-0.76079
H	7.11581	-1.99676	0.01113
H	5.32362	-3.57014	0.77666
H	-0.97478	0.01079	-2.86030
H	-2.17780	-1.19905	-4.68922
H	-3.62073	-3.17303	-4.14663
H	-3.85275	-3.93003	-1.77166
H	-2.66192	-2.72164	0.05032
H	-0.01571	-1.42707	2.68758
H	-1.29631	-1.66981	4.82599
H	-3.71351	-1.02259	4.91833
H	-4.84417	-0.13476	2.86767
H	-3.57056	0.10297	0.73980
H	-2.19170	2.81192	0.17589
H	-2.31442	2.09317	-1.49518
H	0.43796	3.17060	-1.06888
H	0.92122	1.60824	2.31084
H	-0.66626	2.52761	2.61336
H	0.46647	4.67053	1.95533
H	2.04197	3.72761	1.64149
H	-1.67118	4.36831	-3.00598
H	-0.69830	2.91410	-3.35860
H	0.11020	4.48509	-3.10568
H	-0.65435	4.47417	-0.66249

SHOP_7a_7b_TS

55

Ni	0.07636	-1.08933	-1.54526
P	-0.73732	0.50844	-0.02065
O	1.81483	-0.64749	-0.86083
C	0.86021	0.91910	0.69715
C	1.95103	0.29381	0.11320
C	3.36457	0.58512	0.49255
C	4.38075	-0.33440	0.14056
C	5.71810	-0.08946	0.49133
C	6.06478	1.07926	1.19342
C	5.06244	2.00643	1.53745
C	3.72483	1.76430	1.18860
C	-1.80045	-0.17026	1.34014
C	-1.22888	-0.60711	2.55727
C	-2.03127	-1.20118	3.54949
C	-3.41214	-1.36525	3.34003
C	-3.99027	-0.93540	2.12949
C	-3.19154	-0.34763	1.13433
C	-1.54846	2.13525	-0.42013
C	-2.27544	2.88888	0.53119
C	-2.81976	4.13825	0.18400
C	-2.64512	4.65170	-1.11461
C	-1.92371	3.91012	-2.06809

C	-1.38249	2.65904	-1.72437
C	0.30260	-2.82462	-0.64224
C	-0.95999	-3.67402	-0.59386
C	-0.76531	-4.88987	0.35454
C	-1.34164	-1.41688	-2.91980
C	-0.10565	-2.01464	-3.30063
H	2.96046	2.50531	1.43679
H	0.97310	1.66111	1.49044
H	4.09672	-1.23222	-0.41129
H	6.49186	-0.81141	0.21463
H	7.10679	1.27098	1.46464
H	5.32549	2.92457	2.07051
H	-0.15515	-0.47614	2.72018
H	-1.57572	-1.53076	4.48773
H	-4.03480	-1.82478	4.11252
H	-5.06347	-1.06071	1.95954
H	-3.64996	-0.01895	0.19678
H	-2.41959	2.49654	1.54113
H	-3.37900	4.71131	0.92916
H	-3.07028	5.62285	-1.38241
H	-1.78657	4.30218	-3.07980
H	-0.82345	2.08492	-2.47017
H	0.59933	-2.44699	0.35106
H	1.15883	-3.31275	-1.13443
H	-1.81341	-3.07314	-0.23023
H	-1.22814	-4.04547	-1.59961
H	-0.54056	-4.55611	1.38187
H	0.06596	-5.53121	0.01402
H	-1.68243	-5.50356	0.38721
H	0.03415	-3.09863	-3.26429
H	0.58611	-1.48845	-3.97241
H	-1.64333	-0.44811	-3.33624
H	-2.17302	-2.02899	-2.55977

SHOP_7a_TS

55

Ni	-0.03253	-1.70230	-0.61160
P	0.47534	0.39822	0.13039
O	-1.84811	-1.18917	-0.48029
C	-1.21047	0.98286	0.30632
C	-2.17578	0.06609	-0.07758
C	-3.64038	0.35024	-0.07721
C	-4.55340	-0.71784	-0.24395
C	-5.93747	-0.48190	-0.24279
C	-6.43477	0.82387	-0.07992
C	-5.53446	1.89487	0.07744
C	-4.15056	1.66192	0.07771
C	1.38584	1.73645	-0.79021
C	1.42811	1.65225	-2.20305
C	2.04108	2.66311	-2.96404
C	2.62295	3.77249	-2.32356
C	2.58321	3.86887	-0.92027
C	1.96943	2.85943	-0.15705
C	1.24870	0.42109	1.82244
C	0.42095	0.31048	2.96448
C	0.98474	0.21777	4.24964
C	2.38187	0.23560	4.41432
C	3.21487	0.34711	3.28521
C	2.65434	0.43585	1.99871
C	1.76211	-2.38171	-1.49167
C	3.20098	-2.16387	-1.02194
C	4.14325	-1.78314	-2.18667
C	0.90145	-3.50155	-0.10122
C	-0.50540	-3.59591	-0.46252
H	-3.46435	2.50635	0.18022
H	-1.44592	1.99310	0.64544
H	-4.15051	-1.72329	-0.37696
H	-6.62986	-1.31905	-0.37099
H	-7.51291	1.00777	-0.08074
H	-5.91178	2.91494	0.19371
H	0.96221	0.79970	-2.70757
H	2.06261	2.58466	-4.05466
H	3.10143	4.55858	-2.91411
H	3.02693	4.73317	-0.41769
H	1.94274	2.94580	0.93214
H	-0.66546	0.30155	2.83557
H	0.33047	0.13535	5.12226
H	2.81884	0.16560	5.41421
H	4.30194	0.36660	3.40518
H	3.31292	0.53204	1.13061
H	1.35858	-1.46087	-1.98557
H	1.68070	-3.18537	-2.24113
H	3.22425	-1.37484	-0.25017
H	3.57709	-3.08379	-0.53385
H	3.83035	-0.83398	-2.65517
H	4.14480	-2.56376	-2.96781
H	5.18041	-1.65936	-1.83012
H	-0.77251	-4.13321	-1.38077
H	-1.28163	-3.57970	0.30853
H	1.14472	-3.18187	0.92329
H	1.59261	-4.28844	-0.42821

SHOP_7a

55

Ni	-0.06197	1.56076	-0.77964
P	-0.52595	-0.44286	0.06088
O	1.80454	1.10546	-0.40973
C	1.12070	-0.99881	0.48770
C	2.11339	-0.09084	0.14549
C	3.56691	-0.33362	0.37716
C	4.47169	0.75035	0.28919
C	5.84410	0.55656	0.51252
C	6.33833	-0.72419	0.82029
C	5.44809	-1.81203	0.89952
C	4.07531	-1.62010	0.67953
C	-1.28548	-1.64639	-1.13064
C	-1.51899	-1.25400	-2.46777
C	-2.02117	-2.17693	-3.40368
C	-2.29581	-3.49913	-3.01243
C	-2.06884	-3.89790	-1.68094
C	-1.56818	-2.97867	-0.74374
C	-1.58166	-0.61028	1.57313
C	-0.98939	-0.44667	2.84801
C	-1.77988	-0.49039	4.00956
C	-3.16957	-0.69150	3.91317
C	-3.76695	-0.84973	2.64911
C	-2.98034	-0.80889	1.48417
C	-1.93260	2.10984	-0.87108
C	-2.21773	2.91951	0.40939
C	-3.65836	3.49241	0.43683
C	0.63187	3.37296	-1.57997
C	0.50473	2.41658	-2.58445
H	3.39913	-2.47780	0.72227
H	1.31679	-1.95981	0.96614
H	4.07311	1.73603	0.04279
H	6.53000	1.40590	0.44448
H	7.40778	-0.87612	0.99141
H	5.82581	-2.81312	1.12639
H	-1.30340	-0.22435	-2.76735
H	-2.19825	-1.86138	-4.43564
H	-2.68593	-4.21654	-3.73954
H	-2.28180	-4.92531	-1.37256
H	-1.39978	-3.29618	0.28911
H	0.09135	-0.29247	2.92018
H	-1.30962	-0.36880	4.98934
H	-3.78302	-0.72588	4.81761
H	-4.84595	-1.00849	2.56831
H	-3.45196	-0.94551	0.50758
H	-2.62841	1.25289	-0.95267
H	-2.06772	2.73720	-1.77490
H	-2.07037	2.28395	1.30286
H	-1.49962	3.75775	0.50274
H	-4.40283	2.67834	0.39255
H	-3.83420	4.15923	-0.42588
H	-3.83919	4.07130	1.35999
H	-0.35178	2.41906	-3.26571
H	1.35944	1.79861	-2.87465
H	1.58506	3.51319	-1.06364
H	-0.12779	4.14730	-1.43680

SHOP_7b_TS

55

Ni	-0.10938	1.46647	-0.70122
P	0.95381	-0.26449	0.04834
O	-1.73228	0.41747	-0.45271
C	-0.40278	-1.39457	0.34168
C	-1.63918	-0.83772	0.04690
C	-2.93322	-1.55600	0.22585
C	-4.09588	-1.06202	-0.41067
C	-5.32536	-1.72466	-0.26860
C	-5.41734	-2.88758	0.51787
C	-4.26839	-3.38172	1.16432
C	-3.03738	-2.72303	1.02068
C	1.92033	-0.10403	1.62553
C	1.69779	1.02079	2.45299
C	2.33974	1.12843	3.69952
C	3.21333	0.11446	4.13237
C	3.44106	-1.00915	3.31580
C	2.79980	-1.12020	2.06951
C	2.14119	-1.08055	-1.12012
C	1.65669	-2.04624	-2.03262
C	2.51668	-2.61623	-2.98796
C	3.86775	-2.22743	-3.04589
C	4.35734	-1.26424	-2.14387
C	3.50071	-0.69073	-1.18759
C	-1.50098	3.02694	-1.24555
C	-1.97358	3.52600	0.12444
C	-3.43614	4.03130	0.07494
C	0.50345	3.32936	-1.56610
C	1.52585	2.45982	-1.01465
H	-2.15787	-3.10438	1.54601
H	-0.26576	-2.40413	0.73263
H	-4.00937	-0.15566	-1.01255
H	-6.21423	-1.33247	-0.77128
H	-6.37573	-3.40208	0.63144
H	-4.33370	-4.27844	1.78724
H	1.01240	1.80526	2.11746
H	2.15842	2.00339	4.32998
H	3.71436	0.19845	5.10063
H	4.11815	-1.80074	3.64912

H	2.98478	-1.99562	1.44120
H	0.60530	-2.34461	-1.98527
H	2.13054	-3.36440	-3.68591
H	4.53564	-2.67224	-3.78865
H	5.40689	-0.95913	-2.18335
H	3.89276	0.05124	-0.48636
H	-2.06130	2.14322	-1.59694
H	-1.60977	3.81383	-2.00826
H	-1.90017	2.71446	0.87022
H	-1.31711	4.34801	0.47378
H	-4.11939	3.21697	-0.21996
H	-3.54938	4.85385	-0.65403
H	-3.75768	4.40445	1.06304
H	2.17378	1.91329	-1.71186
H	2.02819	2.76744	-0.08801
H	0.38284	4.31110	-1.09278
H	0.43229	3.36935	-2.65922

SHOP_7b

55

Ni	-0.30091	1.58824	-0.65873
P	1.00955	-0.22914	0.04022
O	-1.75592	0.38213	-0.40758
C	-0.31379	-1.41882	0.25481
C	-1.57335	-0.90241	0.01158
C	-2.83379	-1.68519	0.16253
C	-4.03383	-1.18108	-0.39182
C	-5.23326	-1.90132	-0.27397
C	-5.25701	-3.13309	0.40489
C	-4.07010	-3.63885	0.96890
C	-2.86922	-2.92281	0.85001
C	1.92547	-0.13544	1.65549
C	1.46825	0.80547	2.61016
C	2.06781	0.88548	3.87891
C	3.13674	0.03196	4.20870
C	3.59908	-0.90562	3.26683
C	2.99831	-0.99176	1.99787
C	2.23662	-0.95921	-1.13960
C	1.84041	-1.98602	-2.02849
C	2.73237	-2.46895	-3.00271
C	4.02846	-1.93166	-3.10642
C	4.43007	-0.90382	-2.23247
C	3.54105	-0.41647	-1.25846
C	-1.68597	2.90749	-1.10419
C	-2.41654	3.32418	0.17586
C	-3.59757	4.28894	-0.11118
C	1.09182	3.06711	-0.46818
C	1.09006	2.55003	-1.77683
H	-1.96057	-3.31782	1.31160
H	-0.14155	-2.44296	0.59029
H	-3.99891	-0.22109	-0.90931
H	-6.15180	-1.49960	-0.71130
H	-6.19188	-3.69264	0.49963
H	-4.08244	-4.59006	1.50861
H	0.63331	1.46720	2.35775
H	1.70250	1.61509	4.60696
H	3.60635	0.09665	5.19400
H	4.42645	-1.57459	3.52025
H	3.36355	-1.72557	1.27490
H	0.83061	-2.39875	-1.95011
H	2.41354	-3.26633	-3.67984
H	4.72091	-2.30927	-3.86362
H	5.43566	-0.48056	-2.30845
H	3.86789	0.37761	-0.58029
H	-2.33428	2.33090	-1.78820
H	-1.25184	3.77811	-1.63230
H	-2.79632	2.42277	0.68761
H	-1.71596	3.82285	0.87568
H	-4.33894	3.81191	-0.77585
H	-3.24571	5.21231	-0.60504
H	-4.11114	4.57543	0.82403
H	0.57556	3.07442	-2.58775
H	1.83444	1.81238	-2.09495
H	1.84735	2.75581	0.26070
H	0.58037	4.00640	-0.23624

Anilinotropone catalyst (II)

Anilinotropone_1a_1b_TS

67

C	2.35933	-0.80682	1.41242
C	2.75073	-2.28585	1.31611
C	3.35303	-2.81383	2.64414
O	0.80036	-1.97552	-1.22235
P	3.01133	0.86052	-0.76107
C	4.67887	0.02790	-0.87117
C	3.44029	2.42401	0.16413
C	2.80050	1.47515	-2.51074
H	1.54853	-0.62601	2.14766
H	3.22862	-0.18700	1.70880
H	1.86941	-2.89007	1.04102
H	3.48189	-2.43244	0.49984
H	2.62990	-2.71761	3.47323
H	4.26112	-2.24922	2.92327
H	3.62866	-3.87959	2.55510
H	5.43971	0.71390	-1.28212
H	4.59184	-0.85702	-1.52141
H	4.99765	-0.30599	0.12882
H	2.57412	3.10394	0.13397
H	4.32100	2.92848	-0.27113
H	3.64640	2.17981	1.21874
H	1.90420	2.11104	-2.57419
H	2.66344	0.60977	-3.17865
H	3.68289	2.05418	-2.83519
Ni	1.34912	-0.26718	-0.15729
N	-0.62368	-0.10855	-0.10544
C	-1.34970	-1.06530	-0.75730
C	-0.49666	-2.11677	-1.38357
C	-1.29614	0.95636	0.59551
C	-2.77143	-1.02289	-0.81918
C	-0.95982	-3.23568	-2.12751
C	-1.66990	0.78014	1.96406
C	-2.30476	1.84584	2.63480
C	-2.57370	3.06192	1.98952
C	-2.19769	3.22664	0.64819
C	-1.56096	2.19328	-0.06949
C	-1.41150	-0.53148	2.71263
C	-1.18391	2.41509	-1.53713
C	-0.65377	-0.29950	4.04454
C	-2.72783	-1.31088	2.97368
C	-2.43479	2.43525	-2.45468
C	-0.35715	3.71102	-1.73151
C	-2.25126	-3.64556	-2.48201
C	-3.69683	-1.87739	-1.43440
C	-3.48774	-3.05058	-2.18063
H	-2.59660	1.71720	3.68200
H	-3.07216	3.87375	2.52705
H	-2.40837	4.17535	0.14422
H	-0.77250	-1.15888	2.06594
H	-0.38620	-1.26666	4.50571
H	-1.27416	0.25521	4.77086
H	0.27204	0.27796	3.88273
H	-2.51463	-2.26728	3.48377
H	-3.25443	-1.53471	2.03145
H	-3.40893	-0.72508	3.61710
H	-0.55329	1.56052	-1.84351
H	-2.13795	2.55906	-3.51161
H	-3.10260	3.27370	-2.18657
H	-3.00854	1.49828	-2.36677
H	-0.01331	3.79707	-2.77809
H	0.52523	3.72478	-1.06850
H	-0.95717	4.61071	-1.50784
H	-0.13387	-3.86655	-2.47314
H	-2.29787	-4.56513	-3.07757
H	-4.38201	-3.55241	-2.56473
H	-4.74497	-1.57875	-1.31050
H	-3.21268	-0.16778	-0.29524

Anilinotropone_1a_2a_TS_PPh

88

Ni	-0.21899	-0.45683	1.19814
C	-1.16194	-1.63122	2.40315
C	0.19068	-1.63261	3.01555
C	0.91382	-2.98815	3.12685
N	-1.72676	0.02078	0.14494
C	-1.91297	1.35437	-0.11303
C	-1.03628	2.26187	0.66888
C	-2.74904	-0.93161	-0.23681
C	-2.88215	1.78252	-1.07376
C	-1.05069	3.68519	0.61712
C	-2.51390	-1.84784	-1.30465
C	-3.52586	-2.76777	-1.65065
C	-4.74953	-2.79729	-0.96807
C	-4.96895	-1.90269	0.08825
C	-3.99113	-0.96390	0.47991
C	-1.21555	-1.82407	-2.11167
C	-4.30946	-0.02719	1.65294
C	-0.63325	-3.23803	-2.34511
C	-1.41601	-1.09288	-3.46587
C	-5.39609	1.01656	1.27849
C	-4.76261	-0.80597	2.91658
O	-0.20409	1.68327	1.50992
C	-1.77176	4.58351	-0.17848
C	-3.22137	3.05718	-1.54083
C	-2.73952	4.32484	-1.16218
H	-1.50842	-2.55295	1.91510
H	-1.95290	-1.08262	2.92677
H	0.92114	-0.96066	2.33727
H	0.23206	-1.06332	3.96076
H	0.46026	-3.58224	3.93808
H	0.81125	-3.56272	2.19125
H	1.98732	-2.86571	3.34647
H	-3.35230	-3.46598	-2.47461

H	-5.52520	-3.51331	-1.25497
H	-5.92122	-1.93239	0.62689
H	-0.47772	-1.25638	-1.51475
H	0.35591	-3.16640	-2.82785
H	-1.28201	-3.84527	-3.00130
H	-0.51023	-3.77823	-1.39146
H	-0.46097	-1.02913	-4.01725
H	-1.80328	-0.07019	-3.31815
H	-2.14014	-1.63853	-4.09757
H	-3.38530	0.52109	1.90631
H	-5.58113	1.69632	2.12908
H	-6.34880	0.51479	1.02987
H	-5.08981	1.62560	0.41389
H	-4.86235	-0.11280	3.77044
H	-4.04456	-1.59596	3.19147
H	-5.74580	-1.28469	2.76209
H	-0.35049	4.12419	1.33534
H	-1.54250	5.64157	-0.00196
H	-3.17111	5.19007	-1.67571
H	-3.98864	3.06079	-2.32533
H	-3.43263	0.96141	-1.54495
P	1.85948	-0.03992	0.03408
C	2.69699	-1.36045	-0.98513
C	2.52228	-2.71003	-0.59827
C	3.15754	-3.74801	-1.30172
C	3.96183	-3.45314	-2.41835
C	4.12906	-2.11621	-2.82360
C	3.50608	-1.07534	-2.11027
C	1.96587	1.44139	-1.09106
C	0.98503	1.58435	-2.10073
C	1.01573	2.68186	-2.97776
C	2.02116	3.65780	-2.85280
C	2.99559	3.52952	-1.84688
C	2.97040	2.42866	-0.97088
C	3.16799	0.34063	1.31300
C	4.45946	-0.23476	1.30082
C	5.38313	0.06743	2.31960
C	5.03192	0.95158	3.35508
C	3.74959	1.53300	3.37098
C	2.81713	1.22844	2.36367
H	1.87297	-2.94427	0.25080
H	3.01406	-4.78549	-0.98686
H	4.44851	-4.26021	-2.97284
H	4.74726	-1.88035	-3.69455
H	3.64564	-0.03981	-2.42985
H	0.18934	0.84196	-2.19464
H	0.24489	2.78029	-3.74655
H	2.03980	4.51656	-3.52950
H	3.77753	4.28686	-1.73994
H	3.72831	2.34036	-0.18933
H	4.74500	-0.92093	0.49995
H	6.37765	-0.38772	2.29945
H	5.75165	1.18579	4.14458
H	3.47011	2.22337	4.17220
H	1.81720	1.67624	2.37491

Anilinotropone_1a_2a_TS

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Ni	-1.12665	-0.36173	-0.96529
C	-0.37063	-1.80309	-2.01413
C	-1.74519	-1.73301	-2.56483
C	-2.64359	-2.97054	-2.38176
N	0.45154	0.12603	-0.04405
C	0.70832	1.46039	0.12405
C	-0.17840	2.35627	-0.65813
C	1.42953	-0.85193	0.38336
C	1.74416	1.90044	1.00853
C	-0.10305	3.77974	-0.69438
C	1.19720	-1.63123	1.55356
C	2.15826	-2.58918	1.93894
C	3.33236	-2.78059	1.19790
C	3.55174	-2.01252	0.04539
C	2.62022	-1.04588	-0.38895
C	-0.05358	-1.44052	2.41171
C	2.92424	-0.24722	-1.66293
C	-0.86129	-2.75526	2.54067
C	0.29461	-0.86347	3.80781
C	4.06689	0.77985	-1.43810
C	3.28556	-1.16646	-2.85933
O	-1.09552	1.76616	-1.39678
C	0.70330	4.69081	0.00103
C	2.16306	3.18346	1.37458
C	1.71576	4.44804	0.94218
H	-0.10690	-2.66950	-1.39176
H	0.44765	-1.44885	-2.65128
H	-2.34942	-0.85023	-1.99303
H	-1.77350	-1.34137	-3.59716
H	-2.29521	-3.78396	-3.04014
H	-2.59856	-3.32999	-1.34028
H	-3.69704	-2.75614	-2.63078
H	1.98542	-3.18677	2.83973
H	4.07095	-3.52267	1.51469
H	4.46641	-2.16652	-0.53535
H	-0.68839	-0.70777	1.88392
H	-1.77571	-2.59182	3.13922
H	-0.27382	-3.54451	3.04220
H	-1.15783	-3.12936	1.54586
H	-0.62435	-0.69193	4.39725
H	0.83132	0.09587	3.71848
H	0.93552	-1.55947	4.37802
H	2.01096	0.31270	-1.93125
H	4.23796	1.36732	-2.35755
H	5.00991	0.26317	-1.18281
H	3.82490	1.48073	-0.62380
H	3.37453	-0.56617	-3.78183
H	2.52160	-1.94453	-3.02301
H	4.25352	-1.67389	-2.70010
H	-0.82220	4.20580	-1.40230
H	0.51000	5.74579	-0.22968
H	2.21343	5.32164	1.37521
H	2.97095	3.19984	2.11688
H	2.28021	1.08410	1.50381
P	-3.01356	0.28301	0.33084
C	-2.70141	1.52846	1.68832
C	-4.14422	-0.92004	1.21840
C	-4.25503	1.22019	-0.70373
H	-3.64903	1.85600	2.15062
H	-2.18546	2.40417	1.26448
H	-2.05392	1.08865	2.46369
H	-4.51653	-1.66919	0.50045
H	-5.00572	-0.40553	1.67958
H	-3.57809	-1.44900	2.00185
H	-4.71100	0.53960	-1.44270
H	-3.70867	2.00712	-1.24641
H	-5.05400	1.66837	-0.08757

Anilinotropone_1a_5a_TS

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C	2.14159	-0.28933	-2.95607
H	0.45125	1.00614	-3.13549
H	0.09376	-0.81048	-3.33140
C	0.82335	-0.02119	-3.13865
H	2.53827	-1.30719	-3.01962
H	2.86787	0.51837	-2.84497
C	0.32758	-2.85917	-1.36925
H	0.54203	-2.22923	0.70525
H	2.07488	-2.64931	-0.11738
C	1.09829	-2.14754	-0.24810
C	0.02087	-4.33682	-1.01792
H	0.90839	-2.82955	-2.31095
H	-0.62441	-2.33601	-1.56209
H	-0.60886	-4.39716	-0.11338
H	0.95244	-4.89835	-0.82219
H	-0.51499	-4.84288	-1.84140
C	3.37966	0.61123	1.95873
C	4.36430	-1.73475	0.60787
C	4.57398	0.85676	-0.64168
P	3.35068	-0.20373	0.28140
H	2.90429	1.60037	1.87088
H	2.79979	0.00568	2.67342
H	4.41181	0.72931	2.33333
H	4.52058	-2.28947	-0.33136
H	3.83832	-2.39370	1.31656
H	5.34506	-1.46032	1.03211
H	4.07643	1.80570	-0.89271
H	4.87709	0.35292	-1.57354
H	5.47189	1.05308	-0.03082
Ni	1.29922	-0.20949	-0.50364
C	0.44659	2.46291	-0.30717
O	1.50808	1.73661	-0.65575
C	-0.72690	1.67978	0.12079
C	0.55865	3.86877	-0.39746
N	-0.54311	0.33218	0.02328
C	-1.93591	2.25714	0.63592
C	-0.35926	4.88811	-0.08518
H	1.53451	4.18773	-0.77846
C	-1.61339	-0.55512	0.41583
C	-2.32818	3.58801	0.77569
H	-2.67188	1.51946	0.97100
C	-1.64966	4.78430	0.44329
H	0.00201	5.90639	-0.27282
C	-2.65767	-0.88193	-0.50487
C	-1.60249	-1.11944	1.72903
H	-3.32793	3.72321	1.20668
H	-2.18830	5.71931	0.62761
C	-3.66685	-1.77582	-0.08796
C	-2.74090	-0.26423	-1.90683
C	-2.63450	-2.00996	2.09194
C	-0.53305	-0.73077	2.75568
C	-3.66100	-2.34028	1.19532
H	-4.47319	-2.02963	-0.78292
C	-2.93765	-1.32594	-3.01913
C	-3.87746	0.79065	-1.99636
H	-1.78310	0.25081	-2.09457
H	-2.63595	-2.44724	3.09463
C	-1.05363	0.37179	3.71800
C	-0.00821	-1.93733	3.57082
H	0.31613	-0.31028	2.18511
H	-4.45391	-3.03114	1.49639
H	-2.89970	-0.84336	-4.01165
H	-3.91884	-1.82529	-2.93205
H	-2.15894	-2.10514	-2.98278
H	-3.90006	1.24289	-3.00387
H	-3.73822	1.59961	-1.26210
H	-4.86029	0.32069	-1.81138
H	-0.26185	0.66544	4.43040
H	-1.91751	0.00200	4.29932
H	-1.37036	1.27254	3.16738

H	0.83670	-1.62255	4.20928
H	0.33932	-2.74979	2.91083
H	-0.78458	-2.34922	4.24002

Anilinotropone_1a_PPh

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Ni	0.05046	-0.08119	0.09940
C	0.10808	-2.00883	-0.17530
C	-0.00040	-2.75698	1.16462
C	0.14444	-4.29040	1.00259
N	1.96299	0.22232	0.03976
C	2.33745	1.53293	0.15201
C	1.20253	2.43007	0.43318
C	2.98231	-0.77475	-0.19778
C	3.69037	1.96401	-0.01103
C	1.23479	3.82430	0.65207
C	3.63126	-1.40283	0.90853
C	4.61871	-2.37475	0.64062
C	4.95907	-2.72891	-0.67348
C	4.30306	-2.11488	-1.74957
C	3.30987	-1.13549	-1.53818
C	3.30009	-1.03189	2.35913
C	2.62236	-0.48493	-2.74236
C	3.23426	-2.26444	3.29499
C	4.31184	-0.00233	2.93345
C	3.61617	0.37088	-3.57051
C	1.92377	-1.53358	-3.64505
O	0.02155	1.81953	0.48980
C	2.30833	4.72985	0.62450
C	4.25665	3.23934	0.07336
C	3.66297	4.48668	0.36222
H	1.08506	-2.21371	-0.64886
H	-0.68688	-2.33659	-0.87203
H	0.77775	-2.39215	1.85976
H	-0.96753	-2.53451	1.65647
H	-0.63929	-4.68774	0.33319
H	1.12432	-4.54287	0.56019
H	0.06260	-4.81072	1.97454
H	5.12666	-2.86408	1.47646
H	5.72872	-3.48436	-0.85694
H	4.56450	-2.39865	-2.77381
H	2.30184	-0.55601	2.35045
H	2.83296	-1.96649	4.27940
H	4.23564	-2.69790	3.46749
H	2.58745	-3.05628	2.88334
H	4.03735	0.26476	3.96955
H	4.33696	0.92279	2.33608
H	5.33054	-0.43068	2.94856
H	1.83863	0.18710	-2.34891
H	3.08988	0.87623	-4.39976
H	4.41142	-0.25916	-4.00808
H	4.09596	1.14338	-2.94683
H	1.39510	-1.03041	-4.47427
H	1.18817	-2.12238	-3.07290
H	2.65264	-2.23490	-4.08949
H	0.24381	4.23793	0.86489
H	2.03917	5.77254	0.83019
H	4.33301	5.35233	0.38166
H	5.33770	3.26797	-0.10988
H	4.39327	1.15829	-0.24419
P	-2.14364	-0.00392	0.01352
C	-2.68748	1.41742	-1.06490
C	-3.88496	2.13140	-0.84064
C	-4.25905	3.17904	-1.70131
C	-3.44421	3.52219	-2.79559
C	-2.24779	2.81822	-3.02365
C	-1.86814	1.77547	-2.16002
C	-3.13971	-1.41991	-0.67680
C	-3.53065	-1.43181	-2.03616
C	-4.20359	-2.54181	-2.57823
C	-4.49646	-3.65612	-1.77259
C	-4.11268	-3.65542	-0.41920
C	-3.43788	-2.54876	0.12503
C	-2.96681	0.33405	1.65096
C	-4.32616	0.03174	1.90768
C	-4.89713	0.32768	3.15895
C	-4.12096	0.92971	4.16596
C	-2.77083	1.23661	3.91741
C	-2.19382	0.93983	2.66989
H	-4.51908	1.88385	0.01391
H	-5.18492	3.72975	-1.51255
H	-3.73558	4.33909	-3.46167
H	-1.60264	3.08795	-3.86442
H	-0.92216	1.24787	-2.31418
H	-3.31562	-0.57039	-2.67295
H	-4.50033	-2.53113	-3.63069
H	-5.01992	-4.51813	-2.19496
H	-4.33660	-4.51683	0.21610
H	-3.14909	-2.56336	1.17868
H	-4.93696	-0.44446	1.13662
H	-5.94731	0.08543	3.34528
H	-4.56569	1.15612	5.13901
H	-2.16213	1.70547	4.69553
H	-1.14899	1.18931	2.46844

Anilinotropone_1a

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Ni	1.33636	0.14017	0.00354
C	1.49165	-1.79283	0.20512
C	1.93657	-2.50113	-1.09051
C	1.92998	-4.04436	-0.96154
N	-0.59257	0.25944	-0.01422
C	-1.08943	1.52384	-0.15722
C	-0.03428	2.53389	-0.36149
C	-1.51121	-0.83232	0.21124
C	-2.48717	1.81440	-0.08031
C	-0.19772	3.91503	-0.60005
C	-2.05108	-1.54744	-0.89914
C	-2.94618	-2.60730	-0.64038
C	-3.29352	-2.96633	0.67079
C	-2.73358	-2.27199	1.75284
C	-1.83699	-1.20191	1.54923
C	-1.68956	-1.18196	-2.34313
C	-1.23746	-0.47187	2.75459
C	-1.40473	-2.42800	-3.21764
C	-2.79116	-0.31376	-3.00965
C	-2.31965	0.29755	3.55512
C	-0.45664	-1.43968	3.67975
O	1.20660	2.05070	-0.31418
C	-1.36019	4.70237	-0.66746
C	-3.17636	3.02130	-0.22341
C	-2.69671	4.32109	-0.49682
P	3.48217	0.41452	0.12624
C	4.24253	0.90389	-1.50091
C	4.64421	-0.89986	0.74514
C	3.91956	1.85318	1.21942
H	0.48205	-2.13835	0.49380
H	2.17851	-2.04762	1.03852
H	1.27293	-2.20551	-1.92472
H	2.95282	-2.17193	-1.38975
H	2.60563	-4.37400	-0.15149
H	0.91659	-4.40913	-0.71804
H	2.25488	-4.53360	-1.89789
H	-3.37510	-3.16234	-1.47965
H	-3.99103	-3.79030	0.84777
H	-2.99573	-2.56329	2.77492
H	-0.76461	-0.57749	-2.29926
H	-1.00691	-2.11608	-4.19919
H	-2.32331	-3.01174	-3.40613
H	-0.66895	-3.09684	-2.74159
H	-2.49574	-0.04578	-4.03973
H	-2.96601	0.61928	-2.45022
H	-3.74494	-0.86969	-3.06070
H	-0.51272	0.26462	2.36360
H	-1.85570	0.85753	4.38647
H	-3.06340	-0.39618	3.98742
H	-2.85565	1.01667	2.91354
H	0.01789	-0.87784	4.50389
H	0.33240	-1.96913	3.12033
H	-1.12407	-2.19626	4.12959
H	0.75586	4.43277	-0.74767
H	-1.18719	5.76534	-0.87306
H	-3.45014	5.11115	-0.57930
H	-4.26426	2.93884	-0.11095
H	-3.11489	0.94100	0.12242
H	5.31143	1.15629	-1.39196
H	3.69155	1.77690	-1.88413
H	4.13180	0.07781	-2.22135
H	4.37324	-1.17226	1.77764
H	5.68311	-0.52982	0.72969
H	4.57226	-1.80138	0.11764
H	3.67335	1.60485	2.26451
H	3.30190	2.70860	0.90842
H	4.99141	2.10566	1.14540

Anilinotropone_1b_2b_TS

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Ni	-1.25400	-0.17214	-0.93829
C	-1.19709	-0.53010	-2.89648
C	-1.31598	-1.87755	-2.33053
C	-0.18988	-2.89656	-2.57942
N	0.49401	0.18196	0.05528
C	0.68093	1.50104	0.30608
C	-0.30762	2.36564	-0.36608
C	1.48572	-0.79039	0.42089
C	1.72256	1.98256	1.17338
C	-0.34119	3.77823	-0.38697
C	1.24061	-1.68272	1.50930
C	2.19186	-2.68140	1.80059
C	3.36825	-2.81074	1.04712
C	3.60413	-1.92866	-0.01781
C	2.68658	-0.91152	-0.35408
C	-0.00614	-1.53218	2.38339
C	3.01314	0.02792	-1.52290
C	-0.72676	-2.87880	2.63124
C	0.33459	-0.83743	3.72848
C	4.21261	0.95458	-1.18887
C	3.30178	-0.74025	-2.83835
O	-1.26385	1.73203	-1.05650
C	0.45427	4.72434	0.28714
C	2.07591	3.27559	1.54847

C	1.52778	4.52336	1.15962
H	-0.22844	-0.21632	-3.30510
H	-2.06778	-0.06401	-3.37041
H	-1.30916	-1.78649	-1.07824
H	-2.31817	-2.31812	-2.46797
H	-0.19135	-3.20271	-3.63900
H	0.79194	-2.45976	-2.34088
H	-0.31679	-3.79877	-1.95809
H	2.01148	-3.36230	2.63822
H	4.09727	-3.58906	1.29057
H	4.52333	-2.02778	-0.60427
H	-0.70209	-0.87674	1.82787
H	-1.65960	-2.71341	3.20015
H	-0.10486	-3.57661	3.21958
H	-0.98279	-3.37295	1.67830
H	-0.57816	-0.69643	4.33573
H	0.79239	0.15164	3.56002
H	1.04482	-1.44661	4.31629
H	2.12847	0.66417	-1.69801
H	4.40016	1.65523	-2.02184
H	5.13124	0.36169	-1.02859
H	4.02194	1.54723	-0.28015
H	3.47508	-0.02642	-3.66304
H	2.45959	-1.39272	-3.12160
H	4.20322	-1.37203	-2.74869
H	-1.13233	4.17236	-1.03303
H	0.18301	5.76958	0.09517
H	1.99687	5.41666	1.58425
H	2.91305	3.33391	2.25534
H	2.32055	1.18236	1.62360
P	-3.27371	-0.15402	0.16319
C	-3.41034	0.94116	1.67312
C	-4.24353	-1.65549	0.72676
C	-4.52678	0.66998	-0.95378
H	-4.45825	1.06411	1.99888
H	-2.98736	1.92936	1.43061
H	-2.82233	0.50864	2.49873
H	-4.35735	-2.35590	-0.11782
H	-5.24584	-1.38450	1.10279
H	-3.68509	-2.17025	1.52574
H	-4.71553	0.02365	-1.82744
H	-4.09065	1.61589	-1.31222
H	-5.48295	0.86991	-0.43830

Anilinotropone_1b

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Ni	1.36060	0.48827	-0.37566
C	3.18415	1.18305	-0.66240
C	3.64981	1.90938	0.61104
C	4.99138	2.65866	0.41128
N	-0.56393	0.27125	-0.02425
C	-1.28097	1.43326	-0.03071
C	-0.44229	2.60512	-0.33374
C	-1.25284	-0.96485	0.25055
C	-2.68356	1.48411	0.23851
C	-0.84332	3.95374	-0.44022
C	-1.88791	-1.67358	-0.81286
C	-2.53525	-2.89202	-0.51526
C	-2.56581	-3.40098	0.79183
C	-1.94122	-2.69113	1.82923
C	-1.27694	-1.47056	1.58518
C	-1.89297	-1.14247	-2.25095
C	-0.62946	-0.69869	2.74000
C	-1.28496	-2.15794	-3.25119
C	-3.32051	-0.73867	-2.70437
C	-1.69474	0.06339	3.57343
C	0.22332	-1.60047	3.66562
O	0.84299	2.32346	-0.52843
C	-2.10963	4.54325	-0.28574
C	-3.56604	2.56743	0.26311
C	-3.33419	3.94054	0.02821
H	2.97606	1.90071	-1.47860
H	3.97138	0.48674	-1.01353
H	2.87185	2.62970	0.91901
H	3.76227	1.19013	1.44708
H	5.79866	1.96041	0.12268
H	4.89995	3.41423	-0.38889
H	5.30481	3.17651	1.33582
H	-3.02867	-3.44647	-1.32003
H	-3.07946	-4.34351	1.00264
H	-1.97528	-3.08914	2.84789
H	-1.26011	-0.23785	-2.27019
H	-1.25320	-1.72075	-4.26453
H	-1.88407	-3.08448	-3.30391
H	-0.25523	-2.43508	-2.96719
H	-3.29200	-0.31037	-3.72187
H	-3.75674	0.01469	-2.02866
H	-3.99290	-1.61536	-2.72310
H	0.04562	0.05081	2.28755
H	-1.20843	0.65081	4.37236
H	-2.39982	-0.64335	4.04752
H	-2.27502	0.75660	2.94312
H	0.72930	-0.98392	4.42878
H	0.99827	-2.14583	3.09934
H	-0.39480	-2.34474	4.19802
H	-0.01160	4.62281	-0.68284
H	-2.13353	5.62983	-0.42975
H	-4.20425	4.60088	0.10315
H	-4.60315	2.30356	0.50389
H	-3.13509	0.51194	0.46071
P	2.27222	-1.46018	-0.44996
C	1.30913	-3.02197	-0.11667
C	3.72063	-1.75229	0.69076
C	2.98239	-1.87615	-2.12514
H	1.96727	-3.89778	-0.25177
H	0.45002	-3.10161	-0.79879
H	0.91587	-3.01543	0.91064
H	4.48587	-0.97447	0.55388
H	4.16668	-2.74273	0.49696
H	3.36648	-1.71514	1.73365
H	3.69151	-1.09802	-2.44394
H	2.16135	-1.91706	-2.85898
H	3.49457	-2.85336	-2.10004

Anilinotropone_2a_2b_TS

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Ni	-1.25961	-0.36263	-1.08309
C	-0.27184	-0.76946	-2.71236
C	-1.16732	-1.93507	-2.58474
C	-0.50852	-3.31411	-2.38738
N	0.43251	0.18072	0.02690
C	0.53653	1.50819	0.24745
C	-0.43289	2.32950	-0.53278
C	1.44223	-0.73999	0.45967
C	1.48935	2.05104	1.17603
C	-0.51336	3.74538	-0.54462
C	1.15492	-1.65995	1.51884
C	2.12816	-2.60861	1.88926
C	3.37360	-2.66599	1.24559
C	3.65146	-1.76446	0.20926
C	2.71324	-0.79624	-0.20733
C	-0.16892	-1.57813	2.27954
C	3.10061	0.14945	-1.35264
C	-0.71907	-2.95937	2.70383
C	-0.04249	-0.64339	3.51275
C	4.20217	1.15440	-0.92113
C	3.57493	-0.62046	-2.61359
O	-1.27782	1.66876	-1.30946
C	0.18944	4.72872	0.17378
C	1.76647	3.36174	1.56330
C	1.20256	4.58169	1.12722
H	0.79743	-0.93449	-2.54917
H	-0.51311	0.01035	-3.44449
H	-1.83948	-1.80491	-1.55125
H	-1.97411	-1.95541	-3.33690
H	-0.04092	-3.64111	-3.33163
H	0.27369	-3.26002	-1.61345
H	-1.24276	-4.08004	-2.08455
H	1.91130	-3.30857	2.70115
H	4.11989	-3.40555	1.54984
H	4.62265	-1.81048	-0.29384
H	-0.89721	-1.12339	1.57961
H	-1.72715	-2.84861	3.14275
H	-0.08633	-3.43813	3.47196
H	-0.78855	-3.64499	1.84215
H	-1.00630	-0.56912	4.05009
H	0.26728	0.37246	3.21559
H	0.70969	-1.03660	4.22021
H	2.20319	0.73003	-1.62910
H	4.44116	1.84084	-1.75283
H	5.12885	0.62122	-0.64195
H	3.87922	1.76037	-0.06039
H	3.72823	0.08213	-3.45156
H	2.84198	-1.38110	-2.93057
H	4.53430	-1.13648	-2.43190
H	-1.26710	4.10854	-1.25145
H	-0.10996	5.75993	-0.05068
H	1.60238	5.49679	1.57577
H	2.55027	3.45423	2.32581
H	2.09294	1.28446	1.67535
P	-3.11798	-0.12224	0.14058
C	-3.07123	1.02244	1.61186
C	-4.09148	-1.56609	0.81633
C	-4.38861	0.72063	-0.93130
H	-4.08623	1.20762	2.00449
H	-2.62011	1.97805	1.30197
H	-2.44667	0.58788	2.40771
H	-4.31412	-2.27002	-0.00268
H	-5.03964	-1.23680	1.27497
H	-3.48959	-2.09663	1.57179
H	-4.68063	0.04705	-1.75366
H	-3.91264	1.61319	-1.36597
H	-5.28771	1.00839	-0.35899

Anilinotropone_2a_3a_TS

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Ni	-1.24526	-0.34102	-1.08480
C	-0.10516	-1.17588	-2.53280
C	-1.37287	-1.79124	-2.65377
C	-1.64523	-3.20086	-2.15442
N	0.36970	0.12450	-0.02022

C	0.60464	1.43998	0.24736
C	-0.18666	2.38876	-0.58855
C	1.32984	-0.87297	0.38952
C	1.53470	1.83137	1.26244
C	-0.08422	3.81176	-0.54552
C	1.00362	-1.82243	1.40580
C	1.95032	-2.80625	1.75883
C	3.20273	-2.87129	1.13288
C	3.51450	-1.94708	0.12632
C	2.60455	-0.94435	-0.27020
C	-0.32568	-1.75466	2.15762
C	3.02451	0.01725	-1.39099
C	-0.98809	-3.14104	2.33739
C	-0.15183	-1.05133	3.52970
C	4.15493	0.97603	-0.92978
C	3.47922	-0.73330	-2.67086
O	-1.01698	1.85744	-1.45470
C	0.65434	4.67801	0.27092
C	1.92902	3.08959	1.73071
C	1.55149	4.37867	1.30813
H	0.70188	-1.70884	-2.02254
H	0.19034	-0.37532	-3.21781
H	-2.48852	-0.74323	-1.77744
H	-1.99432	-1.48106	-3.50599
H	-1.44775	-3.92837	-2.96577
H	-0.99355	-3.45299	-1.30278
H	-2.69305	-3.33300	-1.83832
H	1.70428	-3.52613	2.54512
H	3.92805	-3.63632	1.42449
H	4.48847	-2.00342	-0.36976
H	-1.00029	-1.14121	1.53227
H	-1.98388	-3.03212	2.80388
H	-0.39397	-3.80046	2.99420
H	-1.11469	-3.64993	1.36694
H	-1.12037	-0.97334	4.05711
H	0.26243	-0.03607	3.40949
H	0.53889	-1.62435	4.17416
H	2.14545	0.62889	-1.65652
H	4.40364	1.68783	-1.73673
H	5.07056	0.40900	-0.68213
H	3.85567	1.55562	-0.04283
H	3.68138	-0.00824	-3.47881
H	2.71244	-1.44033	-3.02711
H	4.40944	-1.30233	-2.49537
H	-0.71124	4.28313	-1.31031
H	0.50458	5.74488	0.06337
H	2.00962	5.22430	1.83108
H	2.64741	3.05836	2.55968
H	2.00286	0.98498	1.77712
P	-2.94724	0.29260	0.18745
C	-2.62170	1.35460	1.68591
C	-4.11099	-0.99385	0.87661
C	-4.11419	1.36997	-0.77991
H	-3.57346	1.64613	2.16260
H	-2.07906	2.26081	1.37625
H	-2.00087	0.81128	2.41389
H	-4.48295	-1.61780	0.04786
H	-4.96767	-0.52489	1.39093
H	-3.57594	-1.64616	1.58504
H	-4.59967	0.76701	-1.56456
H	-3.51640	2.15619	-1.26595
H	-4.88675	1.81920	-0.13302

Anilinotropone_2a_PPh

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Ni	-0.14672	-0.44454	1.19511
C	-1.20093	-1.17106	2.64153
C	0.17125	-1.53220	3.06485
C	0.50857	-3.03078	3.16447
N	-1.67761	0.02761	0.12299
C	-1.88550	1.35205	-0.14338
C	-1.06031	2.29197	0.66768
C	-2.67591	-0.95039	-0.25052
C	-2.83299	1.74900	-1.13854
C	-1.11637	3.71511	0.59147
C	-2.40023	-1.91201	-1.26933
C	-3.38409	-2.86912	-1.59388
C	-4.62224	-2.89545	-0.93785
C	-4.88473	-1.95478	0.06745
C	-3.93810	-0.97532	0.43435
C	-1.08574	-1.90220	-2.04910
C	-4.31501	0.01062	1.54946
C	-0.45671	-3.30939	-2.17462
C	-1.27499	-1.26812	-3.45299
C	-5.44735	0.97417	1.10354
C	-4.74161	-0.71583	2.85250
O	-0.25033	1.75552	1.55123
C	-1.83543	4.58525	-0.23617
C	-3.19747	3.00853	-1.62769
C	-2.76440	4.29248	-1.24742
H	-1.86051	-1.97983	2.30151
H	-1.70775	-0.35905	3.17523
H	0.95869	-1.09511	2.25073
H	0.51337	-0.96504	3.94840
H	0.02336	-3.46194	4.05649
H	0.13577	-3.57136	2.27874
H	1.59502	-3.20256	3.25078
H	-3.17536	-3.60059	-2.38020
H	-5.37517	-3.64229	-1.20602
H	-5.84876	-1.97855	0.58517
H	-0.37914	-1.27501	-1.47548
H	0.54253	-3.23897	-2.63709
H	-1.07112	-3.97781	-2.80399
H	-0.34290	-3.78037	-1.18407
H	-0.30798	-1.20409	-3.98290
H	-1.70274	-0.25293	-3.38473
H	-1.96177	-1.88044	-4.06504
H	-3.42441	0.61931	1.78043
H	-5.67089	1.69755	1.90763
H	-6.37363	0.41350	0.88306
H	-5.16274	1.54063	0.20332
H	-4.90984	0.02144	3.65743
H	-3.97419	-1.42986	3.19224
H	-5.68414	-1.27397	2.71115
H	-0.45620	4.18357	1.32902
H	-1.64162	5.65084	-0.06165
H	-3.20363	5.14098	-1.78201
H	-3.93985	2.98169	-2.43550
H	-3.34223	0.90681	-1.61984
P	1.82199	-0.01785	0.04811
C	2.65168	-1.39248	-0.90380
C	2.62222	-2.69604	-0.35291
C	3.25069	-3.76746	-1.00929
C	3.89985	-3.55669	-2.24081
C	3.92065	-2.26920	-2.80606
C	3.30657	-1.19113	-2.14045
C	1.92765	1.41273	-1.14064
C	0.91280	1.56138	-2.11479
C	0.95932	2.61901	-3.03955
C	2.01495	3.54758	-2.99819
C	3.02455	3.41277	-2.02844
C	2.98367	2.35228	-1.10499
C	3.13200	0.41714	1.30709
C	4.44370	-0.10915	1.27256
C	5.37643	0.24052	2.26753
C	5.01279	1.12326	3.29997
C	3.71068	1.65743	3.33560
C	2.76960	1.30696	2.35113
H	2.09438	-2.87054	0.58944
H	3.22262	-4.76733	-0.56719
H	4.38051	-4.39176	-2.75773
H	4.41922	-2.09897	-3.76455
H	3.33616	-0.19284	-2.58313
H	0.07797	0.85854	-2.14134
H	0.16077	2.72430	-3.77840
H	2.04568	4.37564	-3.71170
H	3.84552	4.13421	-1.98613
H	3.77053	2.26088	-0.35302
H	4.73770	-0.79464	0.47401
H	6.38685	-0.17698	2.23185
H	5.73913	1.39335	4.07179
H	3.42237	2.34740	4.13393
H	1.75540	1.72107	2.37523

Anilinotropone_2a

67

Ni	-1.20251	-0.38946	-0.95001
C	-0.27794	-1.21803	-2.43958
C	-1.68826	-1.56832	-2.70639
C	-2.07371	-3.05826	-2.66755
N	0.39264	0.11824	-0.00412
C	0.66126	1.44267	0.17976
C	-0.17630	2.37330	-0.63403
C	1.34878	-0.88404	0.41052
C	1.67143	1.85518	1.10640
C	-0.04724	3.79563	-0.64695
C	1.06729	-1.72875	1.52616
C	2.00000	-2.72227	1.88821
C	3.19511	-2.89436	1.17651
C	3.46769	-2.06114	0.08269
C	2.57060	-1.05057	-0.32365
C	-0.19750	-1.55181	2.36694
C	2.95586	-0.17454	-1.52313
C	-0.96234	-2.88284	2.56182
C	0.12506	-0.89463	3.73447
C	4.15127	0.75717	-1.18601
C	3.29533	-1.01593	-2.78156
O	-1.07783	1.83253	-1.41837
C	0.76684	4.67771	0.07548
C	2.12280	3.12138	1.49356
C	1.73760	4.40110	1.05029
H	0.39098	-2.01939	-2.10154
H	0.19385	-0.45627	-3.07040
H	-2.40231	-1.05885	-1.84223
H	-2.10222	-1.04769	-3.58783
H	-1.68679	-3.56514	-3.56775
H	-1.63596	-3.54760	-1.78245
H	-3.16749	-3.20147	-2.63753
H	1.78827	-3.36510	2.74830
H	3.90927	-3.66799	1.47308
H	4.40138	-2.19404	-0.47279
H	-0.85423	-0.86757	1.80120
H	-1.89204	-2.71334	3.13479
H	-0.36335	-3.62088	3.12384
H	-1.22847	-3.32893	1.58842
H	-0.79979	-0.73538	4.31866
H	0.62270	0.08036	3.59933
H	0.79573	-1.53795	4.33183

H	2.08923	0.46224	-1.76882
H	4.38334	1.40716	-2.04820
H	5.05457	0.16496	-0.95272
H	3.92730	1.40183	-0.32160
H	3.47478	-0.34874	-3.64316
H	2.47751	-1.70635	-3.04359
H	4.21034	-1.61577	-2.63052
H	-0.72647	4.25142	-1.37576
H	0.61741	5.73862	-0.16097
H	2.25013	5.25646	1.50203
H	2.90225	3.10581	2.26585
H	2.16142	1.02060	1.61971
P	-2.95343	0.28028	0.33007
C	-2.64622	1.50351	1.70419
C	-4.08588	-0.94367	1.17646
C	-4.16540	1.22643	-0.72384
H	-3.59900	1.82956	2.15609
H	-2.11914	2.38031	1.29804
H	-2.01235	1.04942	2.48201
H	-4.44941	-1.67548	0.43643
H	-4.95114	-0.43845	1.63956
H	-3.52760	-1.49109	1.95245
H	-4.62049	0.54941	-1.46620
H	-3.59827	2.00306	-1.25987
H	-4.96483	1.68547	-0.11711

Anilinotropone_2b_3b_TS

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Ni	-1.33050	-0.24036	-1.00579
C	-0.58437	-0.45160	-2.89477
C	-1.08387	-1.74230	-2.56044
C	-0.14444	-2.94393	-2.43406
N	0.47958	0.18500	0.05031
C	0.60814	1.50253	0.31213
C	-0.41953	2.34396	-0.34924
C	1.48260	-0.76118	0.44059
C	1.63166	2.02104	1.18187
C	-0.50398	3.75504	-0.33396
C	1.20630	-1.68459	1.49875
C	2.16452	-2.66611	1.81965
C	3.38222	-2.75215	1.12734
C	3.64868	-1.84520	0.09209
C	2.72367	-0.84462	-0.27405
C	-0.09276	-1.57645	2.29793
C	3.08438	0.10539	-1.42341
C	-0.66802	-2.94866	2.71852
C	0.08931	-0.66058	3.53810
C	4.27347	1.03077	-1.05243
C	3.40749	-0.66176	-2.73214
O	-1.34753	1.69797	-1.05631
C	0.27079	4.72424	0.33094
C	1.94837	3.32225	1.56311
C	1.36183	4.55480	1.18744
H	0.49445	-0.27291	-2.91179
H	-1.19891	0.25338	-3.46250
H	-1.46476	-1.72857	-1.04935
H	-2.08512	-1.99195	-2.93987
H	0.10572	-3.31829	-3.44288
H	0.79103	-2.66529	-1.92430
H	-0.60588	-3.77176	-1.87035
H	1.95604	-3.37160	2.62898
H	4.11631	-3.51814	1.39353
H	4.59806	-1.91129	-0.44925
H	-0.82607	-1.09200	1.62499
H	-1.66139	-2.81809	3.18487
H	-0.02782	-3.45515	3.46278
H	-0.77729	-3.62026	1.84971
H	-0.86310	-0.55482	4.08997
H	0.43119	0.34605	3.24505
H	0.83747	-1.08889	4.22921
H	2.20693	0.74650	-1.61807
H	4.48491	1.73374	-1.87769
H	5.18820	0.43960	-0.86628
H	4.05466	1.62069	-0.14827
H	3.58602	0.04975	-3.55781
H	2.58145	-1.33108	-3.02528
H	4.31596	-1.27970	-2.62044
H	-1.32385	4.12960	-0.95590
H	-0.03993	5.76052	0.15016
H	1.80802	5.45983	1.61196
H	2.78946	3.40008	2.26370
H	2.26308	1.24097	1.62181
P	-3.24099	-0.22049	0.08202
C	-3.33349	0.81641	1.62939
C	-4.10520	-1.78556	0.61277
C	-4.55068	0.59937	-0.96431
H	-4.37191	0.91459	1.99137
H	-2.92937	1.81578	1.40315
H	-2.71383	0.36416	2.41960
H	-4.22403	-2.44760	-0.26071
H	-5.09915	-1.57696	1.04454
H	-3.48802	-2.30943	1.36040
H	-4.73418	-0.00911	-1.86479
H	-4.16733	1.58210	-1.28073
H	-5.49763	0.72759	-0.41031

Anilinotropone_2b

67

Ni	-1.32734	-0.26239	-1.08782
C	-0.48500	-0.49921	-2.85318
C	-0.97034	-1.84593	-2.53238
C	0.06137	-2.98192	-2.39741
N	0.46753	0.18859	0.05420
C	0.55356	1.50806	0.31162
C	-0.47314	2.32845	-0.38221
C	1.48645	-0.73023	0.45895
C	1.54108	2.05225	1.20784
C	-0.58873	3.73772	-0.36200
C	1.20452	-1.68253	1.49134
C	2.17678	-2.64690	1.82108
C	3.41566	-2.68936	1.16277
C	3.68784	-1.75617	0.15257
C	2.74966	-0.77114	-0.22181
C	-0.11907	-1.61819	2.25389
C	3.11931	0.20404	-1.34760
C	-0.64773	-3.00439	2.68826
C	-0.00989	-0.67339	3.48125
C	4.28078	1.14592	-0.93409
C	3.49078	-0.53643	-2.65927
O	-1.36689	1.67260	-1.12315
C	0.13701	4.72267	0.33454
C	1.81531	3.35839	1.60456
C	1.20605	4.57726	1.22238
H	0.59409	-0.31588	-2.83972
H	-1.05131	0.12089	-3.55753
H	-1.47284	-1.83148	-1.37433
H	-1.85808	-2.14659	-3.11348
H	0.44659	-3.24930	-3.39596
H	0.90863	-2.66804	-1.76765
H	-0.38380	-3.88556	-1.94777
H	1.96362	-3.37363	2.61008
H	4.16082	-3.44240	1.43493
H	4.65304	-1.79075	-0.36320
H	-0.85428	-1.17648	1.55228
H	-1.66272	-2.90715	3.11415
H	-0.01459	-3.46137	3.46942
H	-0.69428	-3.70254	1.83494
H	-0.97837	-0.60520	4.01098
H	0.29019	0.34398	3.17995
H	0.74162	-1.05434	4.19611
H	2.23455	0.83073	-1.55553
H	4.50218	1.86193	-1.74548
H	5.20019	0.56810	-0.73013
H	4.02789	1.72196	-0.02996
H	3.66573	0.19106	-3.47162
H	2.69064	-1.22510	-2.97812
H	4.41423	-1.12981	-2.53684
H	-1.39454	4.09711	-1.01069
H	-0.19639	5.75121	0.15003
H	1.61497	5.49101	1.66538
H	2.63634	3.45260	2.32661
H	2.18036	1.28556	1.66032
P	-3.22838	-0.26505	0.07841
C	-3.31788	0.76919	1.62964
C	-4.10399	-1.82488	0.61667
C	-4.53783	0.55655	-0.96611
H	-4.35501	0.85017	1.99899
H	-2.93242	1.77688	1.40704
H	-2.68588	0.32364	2.41424
H	-4.24444	-2.48360	-0.25644
H	-5.08972	-1.60663	1.06293
H	-3.48355	-2.35906	1.35449
H	-4.73876	-0.06629	-1.85312
H	-4.13861	1.52474	-1.30682
H	-5.47792	0.71227	-0.40771

Anilinotropone_3a_4a_TS

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Ni	-0.96202	-1.41453	-0.06576
C	-1.56835	-1.86827	2.01597
C	-0.44534	-2.64062	1.76971
C	-0.48274	-4.11596	1.45036
N	0.45466	0.00475	0.08653
C	1.71134	-0.45522	-0.19537
C	1.72019	-1.80857	-0.78466
C	0.27381	1.42411	0.30110
C	2.88135	0.33481	0.04317
C	2.85682	-2.55083	-1.20327
C	0.18497	2.28711	-0.84210
C	-0.01532	3.66759	-0.63298
C	-0.12856	4.20548	0.65779
C	-0.02765	3.35689	1.76778
C	0.18307	1.96890	1.61606
C	0.32158	1.76008	-2.27696
C	0.36815	1.10699	2.86710
C	-0.72554	2.36841	-3.24516
C	1.74320	2.01896	-2.84810
C	1.71982	1.40881	3.56842
C	-0.79860	1.27621	3.87240
O	0.52903	-2.35638	-0.97077

C	4.22580	-2.26396	-1.11959
C	4.23825	0.03938	-0.12072
C	4.86681	-1.11682	-0.62564
H	-2.56276	-2.32595	1.99479
H	-1.49962	-0.89123	2.49614
H	-1.86362	-2.51059	-0.43129
H	0.54442	-2.22359	1.99814
H	-0.07594	-4.70852	2.29295
H	-1.51537	-4.45599	1.26119
H	0.12114	-4.34311	0.55606
H	-0.08234	4.33332	-1.49842
H	-0.28597	5.27914	0.79574
H	-0.09696	3.77836	2.77553
H	0.16242	0.66657	-2.23930
H	-0.67030	1.85975	-4.22373
H	-0.53592	3.44136	-3.42573
H	-1.75475	2.27032	-2.86193
H	1.82407	1.60585	-3.86927
H	2.52287	1.55268	-2.22664
H	1.94563	3.10425	-2.89997
H	0.39564	0.05553	2.53374
H	1.84648	0.75869	4.45217
H	1.76046	2.45925	3.90804
H	2.57064	1.23400	2.88993
H	-0.70118	0.55306	4.70090
H	-1.77808	1.12105	3.38840
H	-0.80294	2.28871	4.31368
H	2.58050	-3.50814	-1.65734
H	4.88606	-3.05179	-1.50197
H	5.96119	-1.11029	-0.64982
H	4.91712	0.84149	0.19501
H	2.67123	1.32980	0.44889
P	-2.81234	-0.52032	-0.78500
C	-3.20756	1.25484	-0.36480
C	-4.37535	-1.33881	-0.17667
C	-3.09587	-0.59079	-2.62727
H	-4.16231	1.56398	-0.82527
H	-2.39840	1.91893	-0.70132
H	-3.28561	1.34946	0.73042
H	-4.37542	-2.39887	-0.47619
H	-5.26787	-0.83978	-0.59137
H	-4.41381	-1.28806	0.92331
H	-3.03697	-1.64444	-2.94482
H	-2.30245	-0.03294	-3.14723
H	-4.08022	-0.17533	-2.90617

Anilinotropone_3a

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Ni	1.19170	-0.28311	1.17905
C	0.60269	-2.03866	1.97299
C	0.07794	-0.97188	2.75187
C	0.58119	-0.60588	4.13317
N	-0.35432	0.10737	-0.04298
C	-0.40059	1.39224	-0.49438
C	0.51424	2.30623	0.22903
C	-1.42369	-0.80744	-0.35832
C	-1.25260	1.78118	-1.57752
C	0.62447	3.71075	0.04487
C	-1.19045	-1.91619	-1.22935
C	-2.23997	-2.82294	-1.48504
C	-3.50405	-2.65657	-0.90407
C	-3.72725	-1.57266	-0.04463
C	-2.71272	-0.63788	0.25191
C	0.15014	-2.10060	-1.94101
C	-3.04975	0.51223	1.21161
C	0.65045	-3.56473	-1.91383
C	0.07352	-1.57987	-3.40112
C	-4.03433	1.52605	0.56891
C	-3.64411	0.00128	2.55141
O	1.26872	1.74746	1.16178
C	0.02348	4.57252	-0.88438
C	-1.45022	3.01936	-2.19481
C	-0.89458	4.28258	-1.90445
H	1.43435	-2.63903	2.35970
H	-0.02286	-2.53021	1.21915
H	2.34069	-0.45705	2.06285
H	-0.94197	-0.64014	2.52986
H	-0.09118	-1.01625	4.91333
H	1.59363	-1.00653	4.31163
H	0.62021	0.48782	4.27386
H	-2.06521	-3.66815	-2.15736
H	-4.30809	-3.36671	-1.11751
H	-4.71265	-1.44803	0.41445
H	0.88250	-1.48265	-1.39053
H	1.65602	-3.63348	-2.36639
H	-0.00923	-4.23575	-2.49149
H	0.70804	-3.94877	-0.88153
H	1.04919	-1.69057	-3.90895
H	-0.21544	-0.51597	-3.43255
H	-0.67505	-2.15230	-3.97774
H	-2.11275	1.04861	1.44173
H	-4.22843	2.36128	1.26469
H	-5.00036	1.04009	0.34189
H	-3.63021	1.94583	-0.36524
H	-3.75782	0.84228	3.25756
H	-3.00208	-0.76190	3.02142
H	-4.64287	-0.44568	2.40275
H	1.30745	4.16893	0.76805
H	0.32138	5.62433	-0.79553
H	-1.22023	5.11855	-2.53165
H	-2.15228	2.99888	-3.03771
H	-1.82937	0.95291	-2.00349
P	3.05299	-0.26257	-0.15765
C	3.97670	-1.84745	-0.49622
C	4.37543	0.77753	0.63937
C	2.98231	0.52179	-1.85392
H	4.92632	-1.66172	-1.02743
H	3.34907	-2.52278	-1.09927
H	4.19123	-2.34392	0.46420
H	3.92368	1.74204	0.91832
H	5.23390	0.93931	-0.03445
H	4.71959	0.28137	1.56104
H	2.57756	1.54275	-1.76006
H	2.31468	-0.05301	-2.51405
H	3.98707	0.57413	-2.30827

Anilinotropone_3b_4b_TS

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Ni	1.26886	-0.06690	0.42421
C	1.00868	0.07396	2.81993
C	2.36434	-0.07007	2.84777
C	3.07257	-1.36741	3.15024
N	-0.61093	0.13272	0.01058
C	-1.00402	1.41502	-0.23136
C	0.08061	2.39697	-0.03661
C	-1.53456	-0.96286	-0.19015
C	-2.32717	1.73990	-0.68039
C	-0.00396	3.80212	-0.14696
C	-1.50347	-1.67433	-1.42670
C	-2.39041	-2.75482	-1.61046
C	-3.29516	-3.13431	-0.60840
C	-3.31855	-2.42731	0.60164
C	-2.45141	-1.33862	0.83623
C	-0.54944	-1.28344	-2.55730
C	-2.53143	-0.60230	2.17644
C	0.33588	-2.47583	-2.99560
C	-1.31387	-0.68708	-3.76769
C	-3.86798	0.17037	2.33165
C	-2.33320	-1.56940	3.37194
O	1.26637	1.87056	0.28292
C	-1.09059	4.63248	-0.47981
C	-2.92313	2.97302	-0.93820
C	-2.39669	4.28365	-0.83683
H	0.34883	-0.77637	3.01028
H	0.54581	1.06079	2.75629
H	1.26022	-1.53314	0.41504
H	2.99051	0.82551	2.74846
H	3.50552	-1.34701	4.16947
H	2.37948	-2.22247	3.09151
H	3.91075	-1.56015	2.45700
H	-2.37439	-3.30356	-2.55758
H	-3.97754	-3.97382	-0.77022
H	-4.02579	-2.72181	1.38343
H	0.12001	-0.50103	-2.15771
H	1.05787	-2.15639	-3.76927
H	-0.26752	-3.29500	-3.42573
H	0.89605	-2.88071	-2.13552
H	-0.60488	-0.36395	-4.55103
H	-1.91468	0.18715	-3.46594
H	-1.99636	-1.43256	-4.21420
H	-1.71251	0.13607	2.19591
H	-3.88633	0.71584	3.29194
H	-4.72801	-0.52301	2.31822
H	-4.00425	0.90305	1.51949
H	-2.27184	-1.00356	4.31824
H	-1.41098	-2.16404	3.25943
H	-3.17738	-2.27640	3.45900
H	0.94693	4.29962	0.07032
H	-0.86833	5.70634	-0.46825
H	-3.08186	5.10392	-1.07388
H	-3.96792	2.91410	-1.26744
H	-2.96903	0.86688	-0.83836
P	3.22297	-0.23975	-0.51485
C	3.15258	0.39629	-2.26502
C	4.06245	-1.88479	-0.73406
C	4.58675	0.82350	0.18522
H	4.15212	0.41217	-2.73467
H	2.73795	1.41636	-2.24080
H	2.47921	-0.24007	-2.86057
H	4.26227	-2.33276	0.25216
H	5.01059	-1.78272	-1.28909
H	3.38601	-2.55801	-1.28384
H	4.89329	0.43743	1.17038
H	4.19116	1.84331	0.31506
H	5.46489	0.84776	-0.48332

Anilinotropone_3b_TS$_{BHE}$

67

Ni	1.31880	-0.97964	0.25323
N	-0.43821	-0.09168	0.07602
C	-1.43542	-0.91696	-0.35562
C	-0.93625	-2.19572	-0.89837
C	-0.73178	1.28362	0.41255

C	-2.81788	-0.55895	-0.24661
C	-1.70288	-3.20660	-1.53454
C	-0.83898	1.68092	1.77915
C	-1.04669	3.04269	2.08235
C	-1.17255	4.00354	1.07048
C	-1.10304	3.60197	-0.27115
C	-0.88658	2.25464	-0.63176
C	-0.78766	0.66549	2.92182
C	-0.86867	1.88536	-2.12180
C	0.32939	0.99457	3.94266
C	-2.16162	0.54812	3.63316
C	-2.30347	1.86282	-2.71764
C	0.00895	2.84088	-2.97127
O	0.37321	-2.38077	-0.80219
C	-3.08729	-3.32725	-1.72416
C	-3.97172	-1.23294	-0.65431
C	-4.11980	-2.46439	-1.32732
C	2.61518	-2.34774	0.90281
C	1.77786	-2.03741	2.04137
C	0.61974	-2.93599	2.44756
H	-1.12539	3.34954	3.13020
H	-1.33581	5.05515	1.32337
H	-1.22190	4.35093	-1.05979
H	-0.55861	-0.31479	2.47234
H	0.39879	0.20019	4.70702
H	0.12940	1.94604	4.46702
H	1.30891	1.08298	3.44198
H	-2.12056	-0.22179	4.42430
H	-2.95567	0.26688	2.92132
H	-2.44844	1.50503	4.10461
H	-0.45036	0.86599	-2.20580
H	-2.27046	1.56126	-3.77971
H	-2.75901	2.86801	-2.66097
H	-2.95501	1.15607	-2.18185
H	0.07529	2.46783	-4.00856
H	1.03140	2.93358	-2.57180
H	-0.42834	3.85373	-3.01703
H	-1.07903	-4.01896	-1.92171
H	-3.40199	-4.23643	-2.25071
H	-5.14302	-2.77522	-1.56135
H	-4.90876	-0.71501	-0.41439
H	-2.98927	0.40025	0.25376
H	3.66879	-2.05257	0.93110
H	2.38819	-3.23144	0.29623
H	1.50823	-0.46910	1.64704
H	0.98420	-3.74118	3.11666
H	0.15605	-3.40463	1.56656
H	-0.16064	-2.38429	2.99772
H	2.29544	-1.58310	2.90108
P	2.81716	0.20792	-0.95965
C	2.92235	2.03264	-0.57084
C	2.66784	0.19447	-2.82524
C	4.62867	-0.23880	-0.80816
H	3.57591	2.57352	-1.27774
H	3.32377	2.14472	0.45033
H	1.91376	2.47288	-0.58133
H	2.78350	-0.84501	-3.17407
H	3.43181	0.82968	-3.30748
H	1.66642	0.54122	-3.12179
H	4.78337	-1.27606	-1.14779
H	4.94449	-0.16672	0.24599
H	5.25622	0.43598	-1.41564

Anilinotropone_3b

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Ni	1.24426	-0.14659	0.86264
C	0.83301	-0.13078	2.87644
C	2.23201	-0.20590	2.69830
C	3.02902	-1.44895	3.04543
N	-0.53679	0.11035	-0.00919
C	-0.79395	1.39006	-0.38109
C	0.26408	2.34074	0.02099
C	-1.54196	-0.91498	-0.17162
C	-1.98470	1.75357	-1.09962
C	0.28818	3.73655	-0.19908
C	-1.46575	-1.81897	-1.27176
C	-2.45087	-2.81887	-1.40526
C	-3.49592	-2.93918	-0.47864
C	-3.55680	-2.05440	0.60688
C	-2.59496	-1.03794	0.78758
C	-0.35691	-1.70711	-2.31755
C	-2.71819	-0.11162	2.00193
C	0.34994	-3.06170	-2.56625
C	-0.88861	-1.11392	-3.64891
C	-3.94273	0.83405	1.88353
C	-2.79066	-0.91155	3.32793
O	1.29494	1.80632	0.68100
C	-0.62270	4.58196	-0.85987
C	-2.42216	2.98479	-1.58158
C	-1.83132	4.26797	-1.48809
H	0.27212	-1.01626	3.19122
H	0.34695	0.83405	3.04622
H	1.20805	-1.59884	0.87680
H	2.79589	0.73716	2.70389
H	3.40834	-1.38615	4.08480
H	2.40549	-2.35518	2.96675
H	3.90760	-1.58460	2.39053
H	-2.40095	-3.50989	-2.25263
H	-4.25520	-3.71716	-0.59992
H	-4.36897	-2.15281	1.33409
H	0.38893	-1.00629	-1.90463
H	1.20434	-2.92920	-3.25478
H	-0.33087	-3.79746	-3.02928
H	0.72113	-3.49214	-1.62075
H	-0.07004	-1.00943	-4.38422
H	-1.33885	-0.11968	-3.49120
H	-1.65889	-1.77188	-4.08986
H	-1.80940	0.51229	2.03641
H	-3.99228	1.50760	2.75751
H	-4.88370	0.25592	1.84532
H	-3.88382	1.45565	0.97534
H	-2.75786	-0.22347	4.19095
H	-1.94988	-1.61928	3.41489
H	-3.72833	-1.49100	3.39868
H	1.17511	4.21327	0.23103
H	-0.33395	5.63981	-0.87950
H	-2.38105	5.09432	-1.94980
H	-3.37832	2.94971	-2.11839
H	-2.64637	0.90661	-1.30920
P	2.99921	-0.27196	-0.55029
C	2.82219	0.49902	-2.24263
C	3.80658	-1.90220	-0.95043
C	4.42977	0.72208	0.11272
H	3.79843	0.56557	-2.75354
H	2.40254	1.51093	-2.12708
H	2.13132	-0.09384	-2.86203
H	4.06792	-2.41379	-0.01019
H	4.71723	-1.77299	-1.56047
H	3.09027	-2.53692	-1.49597
H	4.79507	0.26954	1.04800
H	4.06398	1.73676	0.33538
H	5.25908	0.77366	-0.61372

Anilinotropone_4a

58

Ni	0.58095	-1.78399	-0.08233
N	-0.47910	-0.17362	0.01904
C	-1.82642	-0.38805	0.04815
C	-2.16092	-1.82535	-0.00049
C	0.04225	1.16906	0.04226
C	-2.77624	0.67411	0.11158
C	-3.44374	-2.41052	0.00996
C	0.41353	1.75749	1.28859
C	0.97408	3.05235	1.27938
C	1.16671	3.75482	0.07937
C	0.78969	3.16746	-1.13775
C	0.21884	1.87772	-1.18323
C	0.19015	1.02467	2.61570
C	-0.20130	1.27930	-2.52998
C	1.43762	1.04946	3.53214
C	-1.03894	1.59699	3.37195
C	-1.29701	2.13436	-3.21736
C	1.00848	1.08416	-3.47855
O	-1.10813	-2.64030	-0.06349
C	-4.71605	-1.81580	0.06432
C	-4.17344	0.64077	0.14480
C	-5.05865	-0.45850	0.12440
H	1.24164	-3.11097	-0.14172
H	1.26086	3.51872	2.22700
H	1.60198	4.75829	0.09412
H	0.93169	3.72212	-2.07104
H	-0.02441	-0.03114	2.36988
H	1.25619	0.43760	4.43293
H	1.67883	2.07307	3.86955
H	2.32640	0.64523	3.01743
H	-1.21554	1.03049	4.30340
H	-1.95091	1.53596	2.75610
H	-0.87508	2.65643	3.64037
H	-0.62605	0.28063	-2.32982
H	-1.62562	1.65202	-4.15461
H	-0.92073	3.14216	-3.46896
H	-2.17778	2.25157	-2.56475
H	0.67897	0.63561	-4.43219
H	1.75907	0.41142	-3.02899
H	1.50139	2.04574	-3.70793
H	-3.40803	-3.50375	-0.03367
H	-5.55553	-2.52081	0.05766
H	-6.12721	-0.22211	0.15895
H	-4.65222	1.62630	0.19465
H	-2.33131	1.67454	0.13808
P	2.67007	-1.39760	-0.12572
C	3.57519	-2.12007	1.33211
C	3.37069	0.33163	-0.18059
C	3.54907	-2.18668	-1.56528
H	4.66385	-1.96579	1.23882
H	3.35411	-3.19661	1.39289
H	3.21774	-1.64134	2.25785
H	3.03357	0.84382	-1.09491
H	4.47397	0.29700	-0.16545
H	3.00835	0.91679	0.67828
H	3.14928	-1.77755	-2.50706
H	3.35685	-3.27033	-1.55249
H	4.63524	-1.99795	-1.51778

Anilinotropone_4b

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Ni	1.43373	-0.09686	-0.01004
N	-0.43175	0.17267	-0.00698
C	-0.82884	1.47675	-0.00947
C	0.31802	2.40984	-0.01048
C	-1.39671	-0.90195	0.00505
C	-2.20353	1.85749	-0.00949
C	0.27382	3.81809	-0.01371
C	-1.84973	-1.45048	-1.22829
C	-2.74173	-2.54258	-1.18904
C	-3.18411	-3.07767	0.03012
C	-2.73044	-2.52402	1.23677
C	-1.83769	-1.43189	1.25102
C	-1.35653	-0.91611	-2.57530
C	-1.33264	-0.87703	2.58546
C	-0.41507	-1.94086	-3.25989
C	-2.52215	-0.51733	-3.51361
C	-2.49005	-0.44984	3.52137
C	-0.39709	-1.89666	3.28556
O	1.51524	1.81804	-0.00684
C	-0.82454	4.69663	-0.01774
C	-2.79137	3.12463	-0.01357
C	-2.19428	4.40458	-0.01786
H	1.35701	-1.56937	-0.02438
H	-3.09136	-2.98083	-2.12916
H	-3.87592	-3.92510	0.03984
H	-3.07151	-2.94789	2.18661
H	-0.76003	-0.00933	-2.37371
H	-0.02176	-1.53106	-4.20752
H	-0.95012	-2.88002	-3.48853
H	0.43739	-2.18109	-2.60214
H	-2.12766	-0.07484	-4.44534
H	-3.18346	0.22378	-3.03386
H	-3.13685	-1.39181	-3.79297
H	-0.72876	0.02007	2.36383
H	-2.08720	0.00676	4.44268
H	-3.11089	-1.31348	3.82001
H	-3.14702	0.28795	3.03070
H	0.00260	-1.47238	4.22412
H	0.45134	-2.15619	2.62999
H	-0.93832	-2.82726	3.53381
H	1.26958	4.27337	-0.01292
H	-0.56308	5.76134	-0.02068
H	-2.87877	5.25922	-0.02112
H	-3.88802	3.11957	-0.01366
H	-2.90143	1.01339	-0.00679
P	3.52723	-0.50056	-0.00110
C	4.62082	0.99630	0.13903
C	4.18588	-1.35517	-1.51629
C	4.14093	-1.59320	1.37273
H	5.68949	0.72216	0.12209
H	4.38410	1.52340	1.07615
H	4.39385	1.67975	-0.69333
H	3.66334	-2.31641	-1.64050
H	5.27249	-1.53116	-1.43863
H	3.97873	-0.73167	-2.40063
H	3.63358	-2.56840	1.30854
H	3.88528	-1.13400	2.34105
H	5.23323	-1.73820	1.31342

Anilinotropone_5a_7a_TS

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C	1.68784	-1.67663	-2.64704
H	0.37894	-0.26598	-3.65910
H	-0.38510	-1.91747	-3.30837
C	0.44613	-1.22843	-3.14152
H	1.85619	-2.73266	-2.41770
H	2.58289	-1.06435	-2.78308
C	-0.73882	-3.51119	-1.30758
H	-0.64961	-2.15887	0.38863
H	0.95323	-2.83532	-0.09294
C	-0.01833	-2.45150	-0.46826
C	-1.07062	-4.77801	-0.47905
H	-0.12702	-3.81428	-2.17882
H	-1.68269	-3.09774	-1.71251
H	-1.71698	-4.52679	0.37986
H	-0.14899	-5.24154	-0.08411
H	-1.59540	-5.53167	-1.09324
C	3.62207	0.94517	1.42738
C	4.37440	-1.79892	1.70339
C	4.64018	-0.48096	-0.82246
P	3.37489	-0.69651	0.54595
H	3.22749	1.75921	0.79752
H	3.06107	0.94645	2.37713
H	4.68809	1.14104	1.64205
H	4.47687	-2.80359	1.25928
H	3.83869	-1.90547	2.66196
H	5.38203	-1.39051	1.90047
H	4.25739	0.26514	-1.53781
H	4.77295	-1.43712	-1.35669
H	5.61982	-0.14897	-0.43480
Ni	0.59572	-0.74278	-1.19439
C	0.92942	2.03533	-1.05976
O	1.43929	0.96579	-1.66109
C	-0.19765	1.75247	-0.14909
C	1.50077	3.29461	-1.35346
N	-0.51905	0.42688	-0.09339
C	-0.91083	2.74479	0.59447
C	1.18979	4.57914	-0.87592
H	2.31644	3.22503	-2.08063
C	-1.67379	0.01392	0.67093
C	-0.73746	4.12850	0.67238
H	-1.72624	2.34392	1.20450
C	0.19627	4.97036	0.02985
H	1.81422	5.38493	-1.27945
C	-2.95202	-0.01712	0.03693
C	-1.52401	-0.38783	2.03086
H	-1.44140	4.63696	1.34236
H	0.12999	6.03843	0.26046
C	-4.06857	-0.42403	0.79657
C	-3.14086	0.39719	-1.42606
C	-2.67320	-0.78827	2.74561
C	-0.16007	-0.37685	2.72741
C	-3.93822	-0.80209	2.14137
H	-5.05633	-0.44317	0.32570
C	-3.87838	-0.68889	-2.24805
C	-3.88431	1.75487	-1.53812
H	-2.13497	0.51999	-1.86510
H	-2.57174	-1.09411	3.79145
C	-0.06010	0.78560	3.75090
C	0.15705	-1.72794	3.41551
H	0.60350	-0.21477	1.94529
H	-4.81775	-1.11160	2.71338
H	-3.91563	-0.39931	-3.31300
H	-4.91891	-0.82407	-1.90318
H	-3.36561	-1.66230	-2.17086
H	-3.97719	2.05612	-2.59658
H	-3.34658	2.55289	-0.99998
H	-4.90195	1.67997	-1.11398
H	0.93849	0.79924	4.22365
H	-0.81275	0.66710	4.55115
H	-0.22441	1.76294	3.26765
H	1.18004	-1.71017	3.83183
H	0.09066	-2.56370	2.69996
H	-0.53639	-1.93250	4.25053

Anilinotropone_5a_7a_TS_PPh

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C	0.37328	-0.82365	-3.12040
C	-0.99457	-0.55585	-3.33568
C	-1.58511	-3.21519	-1.65161
C	-0.71531	-2.22335	-0.87622
C	-1.56078	-4.62784	-1.01482
Ni	-0.59445	-0.33809	-1.37464
C	-0.98243	2.39186	-0.84530
O	-0.26736	1.58819	-1.62646
C	-1.93970	1.70244	0.04198
C	-0.77055	3.78478	-0.96041
N	-1.91251	0.34453	-0.09395
C	-2.83626	2.36333	0.94163
C	-1.35580	4.86394	-0.27730
C	-2.93283	-0.45242	0.55007
C	-3.00472	3.71845	1.23356
C	-2.35038	4.85437	0.70818
C	-4.17891	-0.65167	-0.12233
C	-2.68802	-1.05372	1.82021
C	-5.16834	-1.43003	0.51337
C	-4.47639	-0.02465	-1.48975
C	-3.71211	-1.82620	2.40983
C	-1.36477	-0.85412	2.56592
C	-4.94560	-2.01124	1.77044
C	-5.05138	-1.04871	-2.49973
C	-5.43841	1.18710	-1.36049
C	-1.51066	0.18964	3.70595
C	-0.79252	-2.17699	3.13190
H	-1.31160	0.43947	-3.66378
H	-1.71778	-1.35966	-3.49449
H	0.74288	-1.85378	-3.11019
H	1.12514	-0.05094	-3.30073
H	-1.05447	-2.16487	0.17314
H	0.34745	-2.53673	-0.89488
H	-1.24560	-3.29905	-2.70212
H	-2.63097	-2.85595	-1.67780
H	-1.94129	-4.59612	0.02084
H	-0.53197	-5.02861	-0.98457
H	-2.18742	-5.33493	-1.58738
H	-0.01839	4.03408	-1.71564
H	-3.48952	1.68278	1.49669
H	-0.97881	5.85166	-0.56751
H	-3.76899	3.92803	1.99188
H	-2.66179	5.82530	1.10654
H	-6.12887	-1.58439	0.01261
H	-3.51758	0.34101	-1.89753
H	-3.53668	-2.28846	3.38568
H	-0.63661	-0.46131	1.83246
H	-5.72774	-2.61002	2.24611
H	-5.15812	-0.57916	-3.49343
H	-6.05042	-1.40681	-2.19408
H	-4.39219	-1.92674	-2.60155
H	-5.60969	1.64758	-2.34973
H	-5.02802	1.95872	-0.68919
H	-6.41677	0.86670	-0.95868

H	-0.53927	0.35057	4.20589
H	-2.23233	-0.16521	4.46376
H	-1.86696	1.16084	3.32403
H	0.21654	-2.00512	3.54417
H	-0.71439	-2.94914	2.34916
H	-1.42152	-2.57579	3.94758
P	2.21397	-0.11075	-0.02331
C	2.63239	1.13299	1.31135
C	3.96286	1.47475	1.65493
C	4.22015	2.43012	2.65243
C	3.15238	3.06368	3.31809
C	1.82758	2.73967	2.97972
C	1.56965	1.78090	1.98093
C	2.97525	-1.67721	0.63916
C	3.12494	-2.78156	-0.23971
C	3.59171	-4.01982	0.23256
C	3.90146	-4.18689	1.59556
C	3.74462	-3.10499	2.47947
C	3.28671	-1.86057	2.00738
C	3.43771	0.41222	-1.33669
C	4.72891	-0.13989	-1.50440
C	5.58660	0.34405	-2.51029
C	5.17021	1.38823	-3.35546
C	3.88715	1.94404	-3.19570
C	3.02222	1.45747	-2.19967
H	4.79677	1.00021	1.13098
H	5.25306	2.68590	2.90586
H	3.35478	3.81104	4.09043
H	0.99306	3.23603	3.48227
H	0.53766	1.54402	1.71016
H	2.88488	-2.66735	-1.30118
H	3.70891	-4.85530	-0.46361
H	4.25969	-5.15208	1.96378
H	3.98299	-3.22470	3.54033
H	3.17794	-1.02641	2.70481
H	5.06566	-0.95177	-0.85483
H	6.58185	-0.09449	-2.62909
H	5.83880	1.76303	-4.13558
H	3.55353	2.75152	-3.85402
H	2.01425	1.87212	-2.09056

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C	1.93915	-0.93167	-2.78982
H	0.39964	0.53842	-3.22673
H	-0.20594	-1.20857	-3.13420
C	0.60401	-0.50047	-2.95136
H	2.19505	-1.99456	-2.85562
H	2.76260	-0.23434	-2.97461
C	-0.30637	-3.09579	-1.35044
H	0.48815	-2.28403	0.51090
H	1.73206	-2.89098	-0.63923
C	0.77002	-2.34978	-0.55666
C	-0.55738	-4.51317	-0.77548
H	-0.00526	-3.19548	-2.41094
H	-1.25641	-2.53276	-1.33295
H	-0.90940	-4.45413	0.26930
H	0.36802	-5.11695	-0.78950
H	-1.32376	-5.05032	-1.36234
C	3.15619	0.78216	1.74062
C	3.63602	-2.02263	1.26001
C	4.54669	-0.03956	-0.62667
P	3.04023	-0.48763	0.37582
H	2.90315	1.77186	1.33008
H	2.43683	0.54459	2.54040
H	4.17299	0.81379	2.16916
H	3.80706	-2.82958	0.52922
H	2.86768	-2.36446	1.97231
H	4.57526	-1.82908	1.80559
H	4.34258	0.91001	-1.14590
H	4.73199	-0.81959	-1.38269
H	5.44199	0.06876	0.00960
Ni	1.14712	-0.45169	-0.96759
C	0.82963	2.34251	-0.56435
O	1.62996	1.46846	-1.17179
C	-0.34987	1.76074	0.10848
C	1.18731	3.70889	-0.63918
N	-0.41827	0.40822	0.00979
C	-1.34644	2.53206	0.80088
C	0.57022	4.85701	-0.10986
H	2.10244	3.86868	-1.21898
C	-1.59064	-0.28814	0.47957
C	-1.44834	3.90160	1.03644
H	-2.15587	1.92665	1.22151
C	-0.60208	4.96579	0.64370
H	1.08915	5.79836	-0.32743
C	-2.74180	-0.38217	-0.36602
C	-1.58791	-0.90915	1.76541
H	-2.32842	4.19734	1.62105
H	-0.90163	5.97088	0.95707
C	-3.86571	-1.09410	0.10234
C	-2.80153	0.28358	-1.74618
C	-2.73777	-1.61279	2.18255
C	-0.39407	-0.77331	2.71468
C	-3.87181	-1.70698	1.36356
H	-4.75196	-1.16804	-0.53542
C	-3.24855	-0.69811	-2.85907
C	-3.73424	1.52488	-1.73846
H	-1.78149	0.62407	-1.99239
H	-2.74643	-2.08751	3.16817
C	-0.63911	0.33991	3.76963
C	-0.02992	-2.10100	3.42290
H	0.46805	-0.46693	2.09466
H	-4.75509	-2.25367	1.70625
H	-3.19203	-0.20218	-3.84406
H	-4.29232	-1.02890	-2.71383
H	-2.60998	-1.59632	-2.88850
H	-3.73202	2.01021	-2.73061
H	-3.40996	2.26868	-0.99307
H	-4.77376	1.23199	-1.50432
H	0.23954	0.44751	4.43125
H	-1.51133	0.08819	4.39928
H	-0.83110	1.31427	3.29149
H	0.90440	-1.98051	3.99995
H	0.11075	-2.92035	2.69763
H	-0.81400	-2.41071	4.13613

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Ni	0.51142	1.75719	-0.59556
N	-0.20014	0.14020	-0.06673
C	-1.55548	0.14366	0.11785
C	-2.15391	1.46731	-0.15503
C	0.58312	-1.05577	0.13583
C	-2.26944	-1.01966	0.52541
C	-3.51428	1.82528	-0.06283
C	2.37896	1.43152	-0.74966
C	2.30610	2.88989	-1.08549
C	3.00314	3.86476	-0.11682
C	0.77060	-1.96441	-0.94596
C	1.55497	-3.11606	-0.72345
C	2.14260	-3.36680	0.52516
C	1.96079	-2.45469	1.57568
C	1.18824	-1.28692	1.40565
C	0.15201	-1.72086	-2.32609
C	1.00446	-0.31154	2.57225
C	1.23262	-1.64720	-3.43454
C	-0.91174	-2.79419	-2.67456
C	0.02347	-0.87678	3.63324
C	2.35145	0.07440	3.23220
O	-1.28032	2.40454	-0.52744
C	-4.63654	1.05745	0.29278
C	-3.63541	-1.20564	0.75786
C	-4.70780	-0.29344	0.65902
H	2.63164	0.73510	-1.56121
H	2.86172	1.16532	0.20214
H	2.56539	3.09869	-2.13860
H	1.16471	3.23717	-1.09098
H	4.09705	3.75502	-0.20653
H	2.71998	3.64542	0.92601
H	2.74146	4.91449	-0.33073
H	1.70657	-3.82590	-1.54253
H	2.74426	-4.26741	0.67802
H	2.42803	-2.65037	2.54546
H	-0.35287	-0.73929	-2.29424
H	0.76548	-1.41310	-4.40731
H	1.77075	-2.60554	-3.54133
H	1.97666	-0.86369	-3.21233
H	-1.37783	-2.56932	-3.64999
H	-1.70884	-2.82932	-1.91372
H	-0.45574	-3.79838	-2.73972
H	0.56132	0.61174	2.15653
H	-0.13318	-0.14250	4.44320
H	0.42493	-1.80260	4.08344
H	-0.95768	-1.10962	3.18749
H	2.18882	0.85137	3.99951
H	3.06338	0.46833	2.48706
H	2.82585	-0.78988	3.73000
H	-3.69250	2.87506	-0.31688
H	-5.58937	1.59927	0.27907
H	-5.70194	-0.68610	0.89604
H	-3.91104	-2.22143	1.06530
H	-1.64094	-1.90329	0.67804

Anilinotropone_6a_7b_TS

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Ni	0.76589	-1.55730	-0.08534
N	-0.23031	0.01272	-0.02309
C	-1.57277	-0.14460	-0.24352
C	-1.93868	-1.54561	-0.52923
C	0.33117	1.32766	0.18574
C	-2.48401	0.95328	-0.19546
C	-3.22484	-2.05405	-0.81302
C	2.56333	-0.93700	0.04388
C	2.88289	-2.23650	-0.66210
C	3.47568	-2.11210	-2.07825
C	0.45685	1.84352	1.50752
C	1.00891	3.13066	1.67781
C	1.42999	3.89307	0.57881
C	1.31432	3.36679	-0.71649
C	0.77209	2.08393	-0.94154
C	0.00963	1.04537	2.73462
C	0.65406	1.54619	-2.37124

C	1.18327	0.81341	3.71976
C	-1.18370	1.72301	3.45649
C	-0.52317	2.21340	-3.13171
C	1.96914	1.71044	-3.17294
O	-0.91423	-2.39733	-0.51512
C	-4.47046	-1.40510	-0.87043
C	-3.86895	0.98830	-0.37649
C	-4.77670	-0.05222	-0.67501
C	0.98341	-3.92600	1.55761
C	0.65238	-2.76347	2.17421
H	2.91320	-0.83721	1.08289
H	2.74426	-0.01862	-0.53436
H	3.48299	-2.91656	-0.03002
H	1.89576	-2.84426	-0.77558
H	4.48916	-1.67923	-2.02815
H	2.85250	-1.45174	-2.70408
H	3.54406	-3.09303	-2.57855
H	1.10672	3.54055	2.68815
H	1.85027	4.89147	0.73070
H	1.65124	3.96199	-1.57061
H	-0.32748	0.05730	2.37692
H	0.85773	0.17620	4.56088
H	1.54837	1.76638	4.14209
H	2.03245	0.32110	3.21591
H	-1.51421	1.10782	4.31206
H	-2.04088	1.85216	2.77493
H	-0.90074	2.71831	3.84358
H	0.43979	0.46436	-2.29600
H	-0.61607	1.78725	-4.14637
H	-0.35594	3.30123	-3.23047
H	-1.47964	2.05934	-2.60602
H	1.87603	1.21788	-4.15674
H	2.82443	1.26134	-2.64044
H	2.20490	2.77355	-3.35707
H	-3.21824	-3.13088	-1.01037
H	-5.31972	-2.05814	-1.10354
H	-5.82964	0.23298	-0.76730
H	-4.31678	1.98362	-0.26907
H	-2.01645	1.91800	0.02726
H	2.00808	-4.31096	1.56599
H	0.23720	-4.51617	1.01969
H	1.38063	-2.18921	2.75418
H	-0.38588	-2.42709	2.22734

Anilinotropone_7a_7b_TS

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Ni	0.88505	-1.63423	0.46650
C	2.08796	-1.50846	-1.06861
C	3.57000	-1.17515	-0.94963
C	4.27850	-1.25980	-2.32846
C	2.28913	-1.65368	1.86158
C	2.00459	-2.97365	1.39631
H	1.54699	-0.76507	-1.67398
H	1.91319	-2.52997	-1.45863
H	3.69760	-0.15800	-0.53621
H	4.07864	-1.87202	-0.25940
H	3.83323	-0.55671	-3.05309
H	4.19784	-2.27628	-2.75169
H	5.35037	-1.01419	-2.22995
H	2.70710	-3.49989	0.74135
H	1.32036	-3.62939	1.94837
H	1.81704	-1.28824	2.78338
H	3.22145	-1.14550	1.60545
C	0.02956	1.19725	2.72724
C	0.00571	1.38246	-2.45974
C	1.16685	1.38756	3.75969
C	-1.32871	1.64732	3.33075
C	-1.22003	2.04454	-3.14488
C	1.23820	1.48318	-3.39506
O	-0.78099	-2.66450	0.05288
C	-4.37608	-2.06953	-0.60216
C	-4.03246	0.41152	-0.39550
C	-4.81944	-0.74051	-0.59974
N	-0.32272	-0.11325	0.12587
C	-1.62743	-0.44782	-0.09109
C	-1.85385	-1.91518	-0.14946
C	0.08373	1.27248	0.14347
C	-2.65611	0.53733	-0.18608
C	-3.08159	-2.57308	-0.39733
C	0.30909	1.91153	1.40221
C	0.74664	3.25143	1.41310
C	0.96094	3.95931	0.22135
C	0.72499	3.32829	-1.00712
C	0.27956	1.99055	-1.07800
H	0.91780	3.74988	2.37173
H	1.30410	4.99742	0.25083
H	0.88440	3.88514	-1.93574
H	-0.04846	0.11846	2.50230
H	0.98486	0.75593	4.64706
H	1.22835	2.43320	4.10962
H	2.14624	1.11548	3.33242
H	-1.53791	1.09442	4.26380
H	-2.16005	1.46345	2.63005
H	-1.31214	2.72640	3.56792
H	-0.22828	0.31201	-2.31907
H	-1.41617	1.56700	-4.12110
H	-1.03649	3.11930	-3.32242
H	-2.12820	1.94823	-2.52895
H	1.04573	0.94426	-4.33930
H	2.13885	1.05315	-2.92677
H	1.46199	2.53400	-3.65014
H	-2.96850	-3.66191	-0.41837
H	-5.14566	-2.83041	-0.77694
H	-5.88896	-0.57688	-0.76681
H	-4.58003	1.36166	-0.40814
H	-2.29826	1.56483	-0.06078

Anilinotropone_7a_TS

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N	0.42650	0.08511	-0.02944
C	1.77408	-0.10544	0.01372
C	2.52116	1.14003	-0.23688
C	-0.46904	-1.01932	0.20088
C	2.37278	-1.37517	0.28108
C	3.91816	1.31828	-0.28000
C	-0.98283	-1.24035	1.51614
C	-1.88154	-2.30895	1.71438
C	-2.27675	-3.13604	0.65091
C	-1.77604	-2.90037	-0.63731
C	-0.86938	-1.84779	-0.89082
C	-0.53829	-0.37270	2.69932
C	-0.31986	-1.64668	-2.30836
C	-1.70787	0.03507	3.62759
C	0.57191	-1.07763	3.52530
C	0.61365	-2.81503	-2.72309
C	-1.44751	-1.46669	-3.35609
O	1.75831	2.21776	-0.44172
C	4.96053	0.39132	-0.10360
C	3.71730	-1.74908	0.34800
C	4.88882	-0.97912	0.17538
H	-2.27722	-2.49817	2.71653
H	-2.97345	-3.96073	0.82705
H	-2.08827	-3.54727	-1.46332
H	-0.10589	0.55238	2.27414
H	-1.34838	0.74322	4.39449
H	-2.13314	-0.83508	4.15811
H	-2.52243	0.52179	3.06545
H	0.91180	-0.42369	4.34792
H	1.44556	-1.32312	2.90006
H	0.18996	-2.01554	3.96785
H	0.28178	-0.72020	-2.30186
H	1.03451	-2.63074	-3.72718
H	0.05877	-3.76998	-2.75587
H	1.45157	-2.92844	-2.01610
H	-1.01237	-1.26070	-4.34971
H	-2.11264	-0.62733	-3.09187
H	-2.06664	-2.37705	-3.44397
H	4.20586	2.35370	-0.48841
H	5.96971	0.80910	-0.19698
H	5.83990	-1.51210	0.27498
H	3.88414	-2.80998	0.57075
H	1.65369	-2.18142	0.45967
Ni	-0.09662	1.94792	-0.39629
C	-0.40008	3.86522	-0.45319
C	-1.62747	3.33933	0.10322
C	-2.18587	1.67277	-0.84438
C	-3.37593	1.23164	0.01631
C	-4.37997	0.36311	-0.77458
H	0.38848	4.24503	0.20466
H	-1.66295	3.15808	1.18625
H	-2.58137	3.74291	-0.25811
H	-1.62209	0.77969	-1.17939
H	-2.50121	2.21179	-1.75250
H	-3.00514	0.65893	0.88464
H	-3.90505	2.11803	0.41736
H	-4.76571	0.90604	-1.65596
H	-3.90677	-0.56942	-1.12477
H	-5.24202	0.08784	-0.14240
H	-0.42931	4.32451	-1.44926

Anilinotropone_7a

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Ni	0.18302	1.93396	-0.14432
N	-0.31260	0.06616	0.00631
C	-1.66456	-0.16442	-0.01064
C	-2.45197	1.04869	-0.29612
C	0.58178	-1.04811	0.22937
C	-2.22610	-1.44751	0.25840
C	-3.85334	1.15141	-0.45379
C	2.10287	1.69207	0.06248
C	2.78351	1.37138	-1.27502
C	4.30682	1.13359	-1.11739
C	0.22370	3.83408	0.59116
C	0.46368	3.85029	-0.79151
C	0.98638	-1.86856	-0.86884
C	1.85346	-2.95121	-0.60741
C	2.31750	-3.22147	0.68802
C	1.92499	-2.39870	1.75345
C	1.05886	-1.30354	1.55083
C	0.48631	-1.63221	-2.30096
C	0.62366	-0.44363	2.74291
C	1.61624	-1.72910	-3.35782
C	-0.64684	-2.62385	-2.68401

C	-0.47144	-1.15651	3.58143
C	1.80999	-0.03522	3.65016
O	-1.73072	2.15397	-0.42782
C	-4.86128	0.18396	-0.33431
C	-3.55785	-1.87854	0.26803
C	-4.74700	-1.17453	-0.00484
H	2.22243	0.85754	0.77699
H	2.53984	2.60562	0.51074
H	2.32504	0.46997	-1.71787
H	2.62044	2.19227	-1.99971
H	-0.78743	3.98712	0.97925
H	-0.35794	4.01698	-1.49438
H	1.47452	3.98758	-1.18544
H	4.50093	0.29028	-0.43214
H	4.80481	2.02850	-0.70339
H	4.77806	0.90070	-2.08926
H	2.17104	-3.59200	-1.43504
H	2.98669	-4.06840	0.86540
H	2.29539	-2.60925	2.76095
H	0.07111	-0.60837	-2.33870
H	1.22950	-1.42429	-4.34582
H	1.99019	-2.76370	-3.45615
H	2.47221	-1.08150	-3.10903
H	-1.00285	-2.41712	-3.70882
H	-1.50767	-2.54677	-2.00212
H	-0.27464	-3.66389	-2.65460
H	0.18306	0.48303	2.33093
H	-0.80229	-0.50760	4.41174
H	-0.08131	-2.09513	4.01511
H	-1.35339	-1.40311	2.96771
H	1.46510	0.67265	4.42397
H	2.61062	0.45218	3.06939
H	2.24619	-0.90602	4.17073
H	1.03947	3.95305	1.31017
H	-4.17162	2.16883	-0.70303
H	-5.87878	0.54987	-0.51382
H	-5.67749	-1.74845	0.05056
H	-3.68889	-2.93697	0.52326
H	-1.48918	-2.21944	0.50010

Anilinotropone_7b_TS$_{nonagostic}$

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C	1.14381	-2.29180	-0.02367
C	2.57883	-2.25971	-0.03618
C	3.66851	-0.45134	-0.01462
C	5.02107	-1.17943	0.01890
C	6.18754	-0.16485	-0.00540
H	0.61863	-2.56806	0.89818
H	3.10047	-2.58438	0.86991
H	3.08501	-2.55271	-0.96192
H	3.56427	0.18857	0.87841
H	3.58462	0.15710	-0.93155
H	5.10608	-1.80361	0.92853
H	5.12229	-1.86442	-0.84400
H	6.15775	0.45289	-0.91955
H	6.14031	0.51659	0.86151
H	7.15977	-0.68726	0.02279
H	0.60123	-2.54435	-0.94217
N	-0.27938	0.16407	-0.00046
C	-0.48635	1.51536	0.00393
C	0.77658	2.27073	-0.00110
C	-1.41649	-0.72869	0.00290
C	-1.79161	2.09307	0.01305
C	0.94547	3.67105	0.00063
C	-1.96741	-1.16800	-1.23627
C	-3.07889	-2.03656	-1.20511
C	-3.62991	-2.47110	0.00959
C	-3.06424	-2.04581	1.22082
C	-1.95248	-1.17737	1.24518
C	-1.39490	-0.70908	-2.58124
C	-1.36415	-0.72825	2.58657
C	-1.06312	-1.90143	-3.51368
C	-2.35008	0.28219	-3.29759
C	-2.31241	0.25534	3.32240
C	-1.01826	-1.92755	3.50476
O	1.86403	1.50280	-0.00805
C	-0.01084	4.70127	0.00793
C	-2.18562	3.43377	0.01831
C	-1.40899	4.61351	0.01594
H	-3.51865	-2.37469	-2.14844
H	-4.49500	-3.14055	0.01226
H	-3.49269	-2.39108	2.16677
H	-0.44959	-0.17710	-2.37004
H	-0.57822	-1.53742	-4.43640
H	-1.97336	-2.45274	-3.80963
H	-0.37945	-2.61669	-3.02546
H	-1.89950	0.63418	-4.24245
H	-2.55955	1.16324	-2.66902
H	-3.31214	-0.20492	-3.53908
H	-0.42251	-0.19273	2.36821
H	-1.85098	0.60084	4.26441
H	-3.27056	-0.23548	3.57178
H	-2.53120	1.14081	2.70324
H	-0.52351	-1.57012	4.42483
H	-0.33830	-2.63633	3.00215
H	-1.92339	-2.48407	3.80660
H	1.99804	3.97158	-0.00467
H	0.40430	5.71594	0.00744
H	-1.96143	5.55870	0.02105
H	-3.27131	3.58866	0.02532
H	-2.60771	1.36354	0.01670
Ni	1.52869	-0.39917	-0.00980

Anilinotropone_7b_TS

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N	0.24021	0.15859	0.02009
C	0.19590	1.52167	0.10694
C	-1.18203	2.04382	0.03821
C	1.50904	-0.53158	0.05114
C	1.37164	2.31621	0.26069
C	-1.59172	3.39316	0.08389
C	1.99276	-1.04476	1.28949
C	3.22699	-1.72748	1.29671
C	3.96594	-1.90866	0.11771
C	3.46887	-1.41315	-1.09653
C	2.23962	-0.72203	-1.15844
C	1.21401	-0.85895	2.59479
C	1.73014	-0.20168	-2.50740
C	0.96422	-2.20504	3.31888
C	1.92310	0.14678	3.53927
C	2.62350	0.94418	-3.05099
C	1.61339	-1.33500	-3.55859
O	-2.11814	1.10396	-0.07943
C	-0.83638	4.57133	0.21527
C	1.52045	3.70161	0.36545
C	0.54984	4.72720	0.34387
H	3.61440	-2.12162	2.24140
H	4.92271	-2.43818	0.14454
H	4.04288	-1.56530	-2.01616
H	0.22789	-0.43795	2.32825
H	0.33304	-2.04573	4.21080
H	1.90876	-2.66800	3.65596
H	0.45132	-2.92242	2.65633
H	1.32666	0.29962	4.45610
H	2.05863	1.12601	3.05066
H	2.91870	-0.22817	3.83787
H	0.71682	0.20611	-2.34314
H	2.21279	1.33471	-3.99881
H	3.64973	0.58486	-3.24700
H	2.68368	1.77928	-2.33400
H	1.18240	-0.94158	-4.49597
H	0.96632	-2.15354	-3.19990
H	2.60138	-1.76641	-3.79822
H	-2.67733	3.50840	0.00297
H	-1.42373	5.49702	0.22133
H	0.92329	5.75185	0.43981
H	2.55689	4.04078	0.48182
H	2.30086	1.73899	0.30597
Ni	-1.42393	-0.70846	-0.10740
C	-0.85243	-2.51728	-0.47037
C	-2.20755	-2.43252	-0.99396
C	-3.39474	-1.39031	0.27000
C	-4.57601	-0.99763	-0.61808
C	-5.82928	-0.63716	0.21182
H	0.00052	-2.44618	-1.15408
H	-2.33578	-2.03745	-2.01197
H	-2.90284	-3.25861	-0.80587
H	-3.14849	-0.56187	0.96950
H	-3.58597	-2.28036	0.88884
H	-4.28150	-0.12974	-1.23422
H	-4.82308	-1.82343	-1.31341
H	-6.15286	-1.48736	0.83857
H	-5.62441	0.21813	0.87861
H	-6.67141	-0.36136	-0.44641
H	-0.67422	-3.17180	0.39321

Anilinotropone_7b

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Ni	-1.53888	-0.65195	-0.57794
N	0.20614	0.15835	-0.06083
C	0.15899	1.50473	0.12416
C	-1.18375	2.06068	-0.12624
C	1.43755	-0.56237	0.14264
C	1.29540	2.27323	0.52936
C	-1.59108	3.40555	-0.04114
C	-3.39986	-1.08928	-0.97523
C	-4.24767	-0.95203	0.29532
C	-5.76101	-1.14656	0.01691
C	-1.14984	-2.59851	-0.19409
C	-0.86972	-2.29024	-1.53794
C	1.69784	-1.15422	1.41772
C	2.89419	-1.88163	1.58842
C	3.81229	-2.03185	0.53840
C	3.53941	-1.45781	-0.71143
C	2.35710	-0.72144	-0.93948
C	0.73006	-0.97883	2.59463
C	2.10834	-0.09212	-2.31618
C	0.50052	-2.28901	3.38756
C	1.20798	0.14336	3.55594
C	2.98935	1.16868	-2.53165

C	2.33735	-1.09126	-3.47881
O	-2.10772	1.16029	-0.47548
C	-0.86258	4.56177	0.29557
C	1.43328	3.64304	0.75556
C	0.48376	4.68511	0.65252
H	-3.50306	-2.09592	-1.42361
H	-3.65588	-0.31894	-1.72645
H	-3.92641	-1.69411	1.05324
H	-4.08654	0.04714	0.73806
H	-0.33786	-2.64091	0.53874
H	0.15873	-2.08290	-1.84795
H	-1.56457	-2.55197	-2.34142
H	-5.96208	-2.14806	-0.40368
H	-6.12406	-0.39685	-0.70781
H	-6.35256	-1.04048	0.94395
H	3.10915	-2.33693	2.55943
H	4.73520	-2.59811	0.69308
H	4.25617	-1.58280	-1.52844
H	-0.24241	-0.66651	2.17067
H	-0.29117	-2.13728	4.14163
H	1.41111	-2.60630	3.92588
H	0.19153	-3.11770	2.72822
H	0.48116	0.28040	4.37605
H	1.31668	1.10628	3.03097
H	2.18443	-0.11778	4.00229
H	1.05027	0.22612	-2.34663
H	2.77225	1.62357	-3.51421
H	4.06125	0.90168	-2.50726
H	2.80604	1.92876	-1.75523
H	2.03805	-0.62991	-4.43590
H	1.75277	-2.01725	-3.34630
H	3.40101	-1.37504	-3.56636
H	-2.07340	-3.11198	0.08860
H	-2.64956	3.54183	-0.28415
H	-1.44072	5.49275	0.27566
H	0.84329	5.69372	0.88014
H	2.43896	3.95610	1.06089
H	2.20225	1.67945	0.68472

Salicylaldiminato catalyst (III)

Salicylaldiminato_1a_1b_TS

89

C	-0.94152	-1.04613	2.39427
C	0.46097	-1.58955	2.68703
C	0.42296	-2.75138	3.71387
Ni	-0.92719	0.18192	0.88271
O	0.74734	-0.07774	-0.12614
C	-1.52482	-0.81769	-1.85818
N	-2.03813	-0.35244	-0.71923
C	2.29903	-0.61890	-1.86557
C	0.94946	-0.52834	-1.35687
C	-0.14193	-0.93139	-2.22159
C	0.15047	-1.44734	-3.52154
C	1.45727	-1.55299	-3.98146
C	2.52572	-1.12825	-3.14810
C	-4.15919	0.92148	-0.90482
C	-3.48584	-0.30576	-0.62175
C	-4.21416	-1.46809	-0.23313
C	-5.61611	-1.36678	-0.10441
C	-6.28887	-0.16318	-0.35578
C	-5.56006	0.96755	-0.75801
C	-3.53004	-2.81789	0.00544
C	-3.95348	-3.47153	1.34444
C	-3.79163	-3.79113	-1.17538
C	-3.38731	2.14053	-1.41684
C	-3.96716	3.48698	-0.92450
C	-3.30495	2.13683	-2.96803
C	4.03235	-2.52365	-0.42766
C	4.26783	-1.10680	-0.34524
C	3.44049	-0.15710	-1.01079
C	3.70485	1.23642	-0.87573
C	2.90901	2.23379	-1.53747
C	3.18441	3.58311	-1.39519
C	4.27815	4.02208	-0.58322
C	5.07404	3.09591	0.06589
C	4.82167	1.68631	-0.05629
C	5.63429	0.73437	0.59006
C	5.38922	-0.64663	0.46499
C	6.21887	-1.61830	1.12273
C	5.96248	-2.97206	1.00622
C	4.85266	-3.42703	0.22592
H	-1.59679	-1.80139	1.91511
H	-1.43974	-0.70860	3.32420
H	0.93443	-1.93261	1.75240
H	1.11149	-0.78397	3.07260
H	-0.18678	-3.59257	3.33893
H	-0.01188	-2.42332	4.67555
H	1.44081	-3.13082	3.91170
H	-2.23708	-1.14885	-2.63487
H	-0.68581	-1.75512	-4.15987
H	1.66628	-1.94744	-4.97882
H	3.55524	-1.19246	-3.51454
H	-6.18914	-2.25066	0.19202
H	-7.37605	-0.10743	-0.24981
H	-6.09216	1.89896	-0.97068
H	-2.44152	-2.63733	0.05116
H	-3.79270	-2.78569	2.19302
H	-5.01977	-3.75866	1.33715
H	-4.87089	-4.00581	-1.27217
H	-3.26350	-4.74743	-1.01357
H	-3.44649	-3.36371	-2.13198
H	-2.35304	2.05092	-1.03177
H	-4.95041	3.69883	-1.38009
H	-3.29472	4.31571	-1.20809
H	-4.09370	3.50008	0.17172
H	-4.31630	2.19902	-3.40774
H	-2.82662	1.21782	-3.34449
H	-2.71712	3.00054	-3.32678
H	3.18315	-2.87713	-1.01722
H	2.07563	1.90531	-2.16279
H	2.56715	4.32360	-1.91223
H	4.48385	5.09185	-0.48498
H	5.91763	3.42073	0.68377
H	6.47767	1.07557	1.20093
H	7.06193	-1.26002	1.72251
H	6.60234	-3.70040	1.51240
H	4.65204	-4.49955	0.15035
H	-3.36477	-4.38842	1.52307
P	-1.15209	1.75595	2.26426
C	0.01593	1.86732	3.71434
C	-2.80111	2.02990	3.09584
C	-0.83310	3.39497	1.43117
H	-0.17927	2.77479	4.31171
H	1.04968	1.89358	3.33495
H	-0.09648	0.98117	4.35828
H	-3.57938	2.12840	2.32246
H	-2.79199	2.93168	3.73297
H	-3.04581	1.15208	3.71565
H	-1.58063	3.56767	0.64230
H	0.16666	3.36840	0.96909
H	-0.87961	4.22075	2.16262

Salicylaldiminato_1a_2a_TS

89

C	1.91110	0.97001	-2.28102
C	0.84849	0.38993	-3.13806
P	0.47118	-2.65275	-0.96116
C	0.32342	-3.34043	0.76890
C	1.30560	-4.08513	-1.83906
C	-1.27729	-2.86398	-1.57610
C	-0.33737	1.29963	-3.50521
H	2.95917	0.75270	-2.52280
H	1.74079	1.99087	-1.91428
H	0.34831	-0.53823	-2.55371
H	-0.13265	-4.34596	0.76351
H	-0.29994	-2.65987	1.36976
H	1.31985	-3.39782	1.23697
H	1.35633	-3.86698	-2.91895
H	0.75284	-5.02951	-1.68979
H	2.33563	-4.20848	-1.46802
H	-1.29946	-2.73401	-2.67176
H	-1.89536	-2.07584	-1.11960
H	-1.68627	-3.85821	-1.32651
H	-0.75946	1.76576	-2.60092
H	-1.14464	0.73467	-4.00000
H	-0.00126	2.09482	-4.19198
H	1.25521	-0.15584	-4.00861
Ni	1.14157	-0.35227	-1.07956
O	-0.73499	-0.03494	-0.15738
C	1.63338	0.20684	1.63775
N	2.17418	0.06479	0.42427
C	-2.19344	0.41354	1.69303
C	-0.87460	0.19024	1.13680
C	0.25797	0.20800	2.05207
C	0.02308	0.35873	3.45465
C	-1.25898	0.51235	3.96926
C	-2.36036	0.54712	3.07631
C	3.96167	1.80320	0.40780
C	3.58683	0.42820	0.31742
C	4.56665	-0.58888	0.14049
C	5.92239	-0.20932	0.05899
C	6.30908	1.13566	0.14603
C	5.33352	2.12594	0.31813
C	4.19088	-2.07090	0.11314
C	4.92983	-2.85208	-0.99832
C	4.43332	-2.72433	1.49987
C	2.94902	2.93843	0.61084
C	3.14732	4.09292	-0.40486
C	3.00949	3.49555	2.05860
C	-4.07699	-1.84762	1.48745
C	-4.28455	-0.64391	0.72649
C	-3.38266	0.45933	0.78197
C	-3.63095	1.61859	-0.00907
C	-2.76556	2.76529	0.02404
C	-3.02780	3.88538	-0.74622
C	-4.17687	3.93168	-1.59791

C	-5.04087	2.85358	-1.65419
C	-4.80445	1.67267	-0.87018
C	-5.68772	0.57600	-0.90899
C	-5.46066	-0.57706	-0.13363
C	-6.36326	-1.69490	-0.17030
C	-6.12808	-2.82861	0.58568
C	-4.96779	-2.90503	1.41964
H	2.35224	0.40954	2.44657
H	0.88738	0.36128	4.12915
H	-1.41968	0.62205	5.04437
H	-3.37203	0.68685	3.47117
H	6.68772	-0.98063	-0.06466
H	7.36617	1.40959	0.08375
H	5.63971	3.17401	0.38706
H	3.10836	-2.11846	-0.10582
H	4.74992	-2.39936	-1.98791
H	4.57982	-3.89926	-1.02719
H	6.02017	-2.88093	-0.82709
H	5.50402	-2.68553	1.76893
H	4.12209	-3.78452	1.49021
H	3.86725	-2.20395	2.29099
H	1.93807	2.52593	0.45126
H	4.09754	4.62810	-0.23244
H	2.33044	4.82868	-0.30296
H	3.15229	3.72208	-1.44315
H	4.00859	3.91429	2.27445
H	2.80393	2.71069	2.80504
H	2.26408	4.29886	2.19293
H	-3.19372	-1.91249	2.12714
H	-1.89059	2.73781	0.67748
H	-2.35567	4.74724	-0.70264
H	-4.36954	4.82528	-2.19838
H	-5.92647	2.88144	-2.29738
H	-6.57231	0.62276	-1.55399
H	-7.24534	-1.62789	-0.81551
H	-6.82412	-3.67139	0.54796
H	-4.78711	-3.80917	2.00821
C	3.99408	1.28183	0.84976
C	-5.67555	2.99902	1.48362
H	-4.22124	3.39799	3.06792
H	-6.64182	0.23734	-1.36995
H	-6.95341	2.34413	-0.12588
C	-4.79891	-3.31184	-2.21686
H	-3.12450	-4.57128	-1.59039
H	-6.36110	-1.87726	-2.61177
C	5.73549	-0.94187	0.69214
C	3.82292	-2.61090	0.56192
C	5.39351	1.45036	0.89418
C	3.05970	2.47802	1.05123
H	-6.23071	3.92467	1.65970
H	-5.12631	-4.00807	-2.99400
C	6.26161	0.35143	0.80997
H	6.41676	-1.79649	0.64411
C	4.51576	-3.44521	-0.54527
C	3.97864	-3.33165	1.92894
H	2.74636	-2.56731	0.32283
H	5.80921	2.45518	1.00738
C	3.57940	3.78107	0.40127
C	2.78081	2.70509	2.56214
H	2.09821	2.21575	0.56836
H	7.34428	0.50275	0.84679
H	5.58711	-3.59973	-0.32725
H	4.04598	-4.44200	-0.61482
H	4.43752	-2.95771	-1.53075
H	5.04339	-3.39747	2.21494
H	3.44768	-2.79867	2.73517
H	3.57460	-4.35775	1.87115
H	3.82675	3.62934	-0.66317
H	2.80892	4.56935	0.46924
H	4.48074	4.16458	0.91138
H	3.71670	2.94288	3.09860
H	2.07918	3.54679	2.70254
H	2.33767	1.80951	3.02840

Salicylaldiminato_1a_5a_TS

95

C	-0.01126	-1.47816	-2.54728
H	0.23932	-2.66601	-0.78669
H	1.72578	-2.56104	-1.90110
C	0.69428	-2.26542	-1.69631
H	0.41605	-1.12308	-3.49015
H	-1.06210	-1.25113	-2.36018
C	3.26177	-0.32564	-2.63313
H	2.97479	1.53099	-1.52276
H	1.95503	1.34380	-2.97680
C	2.36941	0.80790	-2.10365
C	4.48522	0.22216	-3.41026
H	2.68005	-0.98285	-3.30689
H	3.62373	-0.95597	-1.80454
H	5.12248	0.83575	-2.74994
H	4.16378	0.85588	-4.25690
H	5.10443	-0.59848	-3.81593
C	-0.90354	3.06817	-0.28378
C	0.26206	3.21039	-2.90941
C	-1.99246	1.48018	-2.42508
P	-0.35928	1.95705	-1.67436
H	-1.42257	2.45200	0.46481
H	-0.02493	3.54014	0.18497
H	-1.58748	3.85305	-0.65002
H	0.44515	2.73120	-3.88446
H	1.20723	3.65378	-2.55813
H	-0.48680	4.00985	-3.03971
H	-2.48990	0.78248	-1.73531
H	-1.82601	0.97567	-3.39046
H	-2.63317	2.36452	-2.58380
Ni	0.89076	0.29369	-0.89363
C	-0.96298	-0.66883	1.24759
O	-0.78843	-0.09881	0.05672
C	-2.29821	-0.96188	1.70414
C	0.14372	-0.98978	2.11362
C	-2.48974	-1.56258	2.95628
C	-3.48018	-0.62428	0.84483
C	1.51081	-0.69036	1.78773
C	-0.10791	-1.58716	3.38392
C	-1.40166	-1.88180	3.80447
H	-3.51212	-1.78478	3.27825
C	-4.19808	0.58625	1.06794
C	-3.90510	-1.52593	-0.17288
N	2.02729	-0.22276	0.65257
H	2.22256	-0.87535	2.60735
H	0.74704	-1.81792	4.02952
H	-1.58044	-2.34882	4.77578
C	-3.81470	1.52927	2.08474
C	-5.36326	0.89915	0.24914
C	-3.22652	-2.76793	-0.42455
C	-5.06923	-1.20379	-0.98834
C	3.47584	-0.03736	0.70158
C	-4.52994	2.69751	2.28672
H	-2.94455	1.30087	2.70530
C	-5.76503	-0.00064	-0.75738
C	-6.07746	2.12231	0.49238
C	-3.65789	-3.63305	-1.41514
H	-2.35832	-3.02031	0.18881
C	-5.48436	-2.12922	-2.00639
C	4.34283	-1.16818	0.63777

Salicylaldiminato_1a

89

O	-0.69094	0.10894	0.05102
C	1.56534	1.29974	1.44766
N	2.07374	0.53880	0.47519
C	-2.24083	1.19385	1.53090
C	-0.89820	0.92467	1.08417
C	0.19596	1.55351	1.77742
C	-0.07064	2.43642	2.86647
C	-1.37260	2.70252	3.27522
C	-2.44972	2.07316	2.60187
C	4.30183	1.39494	-0.23111
C	3.53455	0.45695	0.51383
C	4.15036	-0.54323	1.31715
C	5.56104	-0.57456	1.36611
C	6.33545	0.34664	0.64562
C	5.70805	1.32012	-0.14578
C	3.32307	-1.53147	2.14959
C	3.93776	-2.95099	2.20112
C	3.11091	-1.00729	3.59688
C	3.62933	2.47727	-1.08248
C	4.29054	2.64453	-2.47137
C	3.59519	3.83535	-0.33159
C	-3.12827	-1.51795	2.24113
C	-3.82957	-0.75771	1.24201
C	-3.41627	0.55007	0.85734
C	-4.14581	1.26397	-0.13676
C	-3.76146	2.58064	-0.57123
C	-4.48537	3.25576	-1.53882
C	-5.64288	2.65910	-2.13253
C	-6.04571	1.39332	-1.74783
C	-5.31971	0.65505	-0.75114
C	-5.71649	-0.63742	-0.35628
C	-5.00304	-1.35911	0.62102
C	-5.40820	-2.67641	1.02824
C	-4.70279	-3.37335	1.99233
C	-3.54976	-2.78577	2.60349
H	2.29549	1.79729	2.10373
H	0.77678	2.90326	3.38098
H	-1.56875	3.38107	4.10865
H	-3.47770	2.27059	2.92177
H	6.05875	-1.33156	1.97817
H	7.42720	0.30494	0.69991
H	6.31816	2.03244	-0.70848
H	2.32923	-1.61097	1.66917
H	4.15644	-3.33838	1.19250
H	3.23255	-3.64466	2.69105
H	4.87472	-2.96939	2.78574
H	4.08211	-0.87903	4.10737
H	2.50687	-1.72524	4.17933
H	2.58933	-0.03659	3.60890
H	2.58409	2.15630	-1.24871
H	5.31638	3.04650	-2.39326
H	3.70508	3.35289	-3.08322
H	4.33822	1.68251	-3.00820
H	4.61998	4.19165	-0.12341
H	3.06359	3.75075	0.63109
H	3.08135	4.59991	-0.94069
H	-2.24909	-1.07265	2.71281
H	-2.87793	3.03979	-0.12130
H	-4.17330	4.25504	-1.85512
H	-6.20509	3.20963	-2.89200

H	-6.92911	0.92865	-2.19772
H	-6.60176	-1.09016	-0.81675
H	-6.29328	-3.11664	0.55760
H	-5.02301	-4.37460	2.29381
H	-3.00024	-3.34631	3.36491
Ni	0.97492	-0.35176	-0.83706
P	-0.43583	-1.32081	-2.22654
C	-1.44387	-2.62137	-1.36758
C	-1.71371	-0.14277	-2.87783
C	0.08194	-2.19278	-3.78979
C	2.46828	-0.94128	-1.95951
C	2.95093	-2.36963	-1.64718
C	4.15381	-2.79995	-2.52179
H	3.28803	-0.22538	-1.77481
H	2.20171	-0.85210	-3.03131
H	3.24106	-2.43368	-0.58281
H	2.12797	-3.10092	-1.77772
H	5.00889	-2.11931	-2.36518
H	3.89190	-2.76918	-3.59516
H	4.48600	-3.82640	-2.28146
H	0.82098	-2.97889	-3.57086
H	0.53422	-1.47456	-4.49177
H	-0.80150	-2.65040	-4.26625
H	-0.79290	-3.46434	-1.08455
H	-1.86242	-2.17227	-0.45524
H	-2.25985	-2.98972	-2.01248
H	-1.22201	0.62023	-3.50291
H	-2.19137	0.35318	-2.02119
H	-2.47344	-0.67226	-3.47737

Salicylaldiminato_1b_2b_TS

89

C	-0.64571	0.97421	-2.39940
C	-1.74740	0.16089	-2.91932
P	-0.10555	-2.54451	-1.19059
C	0.29468	-3.45074	0.39521
C	1.58977	-2.46287	-1.96568
C	-0.88193	-3.92410	-2.19721
C	-3.09591	0.83327	-3.23422
H	0.36741	0.83750	-2.78893
H	-0.86504	1.98640	-2.03667
H	-2.06911	-0.66842	-2.03827
H	0.87454	-4.37174	0.20796
H	-0.63809	-3.70830	0.92369
H	0.88322	-2.77749	1.03865
H	1.49847	-2.15372	-3.02061
H	2.11536	-3.43260	-1.91744
H	2.17007	-1.69645	-1.42885
H	-1.05794	-3.57142	-3.22761
H	-1.85503	-4.20019	-1.75873
H	-0.23616	-4.81906	-2.23390
H	-3.43985	1.44498	-2.38612
H	-3.87927	0.08676	-3.44647
H	-2.98829	1.48373	-4.11852
H	-1.43349	-0.53300	-3.71754
Ni	-0.90952	-0.36010	-0.93236
O	0.73509	0.07729	-0.07340
C	-1.59696	0.43194	1.79942
N	-2.10664	0.10381	0.62085
C	2.22283	0.71676	1.66749
C	0.88508	0.43950	1.20820
C	-0.20264	0.55035	2.15246
C	0.08519	0.88449	3.50785
C	1.38678	1.11453	3.94723
C	2.44740	1.03230	3.01627
C	-4.36072	-0.90404	0.35350
C	-3.54004	0.25773	0.46344
C	-4.10630	1.56862	0.38890
C	-5.49850	1.67978	0.18080
C	-6.31327	0.54693	0.05070
C	-5.74313	-0.73288	0.14220
C	-3.27020	2.84671	0.55068
C	-3.54357	3.89514	-0.55740
C	-3.50211	3.49060	1.94460
C	-3.76267	-2.29805	0.54834
C	-4.43642	-3.38383	-0.32033
C	-3.79827	-2.70354	2.04730
C	2.72803	2.81577	-0.33510
C	3.59486	1.67394	-0.23747
C	3.37738	0.63616	0.71466
C	4.28122	-0.46498	0.78553
C	4.10353	-1.54998	1.71417
C	4.99842	-2.60485	1.76852
C	6.13103	-2.64597	0.89498
C	6.33468	-1.63131	-0.02207
C	5.42778	-0.52006	-0.11421
C	5.62231	0.51113	-1.05285
C	4.73661	1.60339	-1.13905
C	4.94023	2.65993	-2.09151
C	4.07490	3.73646	-2.15742
C	2.95852	3.81418	-1.26559
H	-2.30240	0.68485	2.60892
H	-0.75303	0.96480	4.20940
H	1.58732	1.36864	4.99068
H	3.47465	1.22352	3.34208
H	-5.95000	2.67477	0.12143
H	-7.38919	0.65907	-0.11106
H	-6.38650	-1.61304	0.05850
H	-2.20475	2.56636	0.48010
H	-3.37471	3.47769	-1.56364
H	-2.86935	4.75994	-0.42880
H	-4.57959	4.27443	-0.51536
H	-4.55688	3.79779	2.06006
H	-2.86751	4.38603	2.06661
H	-3.26635	2.78778	2.76067
H	-2.69998	-2.22899	0.24439
H	-5.48039	-3.57080	-0.01226
H	-3.89436	-4.34056	-0.21688
H	-4.44030	-3.10109	-1.38698
H	-4.84027	-2.76852	2.40843
H	-3.26540	-1.96828	2.67298
H	-3.32156	-3.68962	2.19414
H	1.87526	2.88270	0.34422
H	3.24127	-1.52611	2.38474
H	4.84116	-3.41708	2.48401
H	6.83066	-3.48445	0.95491
H	7.19532	-1.65568	-0.69850
H	6.48433	0.46557	-1.72778
H	5.80182	2.59448	-2.76387
H	4.24184	4.53511	-2.88575
H	2.28493	4.67413	-1.32134

Salicylaldiminato_1b

89

O	0.77055	-0.09590	0.11714
C	-1.43387	-1.82457	0.83884
N	-1.93968	-0.71582	0.28953
C	2.35579	-1.64453	1.01226
C	0.99825	-1.25344	0.72879
C	-0.06825	-2.13915	1.10956
C	0.23045	-3.37732	1.75318
C	1.54383	-3.74067	2.02746
C	2.59715	-2.86745	1.65113
C	-3.95187	-1.20167	-1.08070
C	-3.39229	-0.77480	0.15598
C	-4.20946	-0.46316	1.27824
C	-5.60830	-0.59379	1.13641
C	-6.17962	-1.01770	-0.07273
C	-5.35537	-1.31630	-1.16945
C	-3.60659	-0.00911	2.61330
C	-4.32082	1.23376	3.20090
C	-3.60860	-1.16133	3.65307
C	-3.05713	-1.56607	-2.26979
C	-3.61690	-1.07191	-3.62456
C	-2.79541	-3.09532	-2.32168
C	3.09338	0.73094	2.58930
C	3.83972	0.37012	1.41505
C	3.50115	-0.76107	0.61918
C	4.27437	-1.07888	-0.53534
C	3.95922	-2.19215	-1.39043
C	4.72899	-2.48318	-2.50338
C	5.86622	-1.68014	-2.83399
C	6.19959	-0.59377	-2.04615
C	5.42340	-0.25287	-0.88583
C	5.74779	0.85861	-0.08417
C	4.98594	1.19293	1.05269
C	5.31855	2.32475	1.87323
C	4.56976	2.63867	2.99262
C	3.44465	1.83092	3.35250
H	-2.15787	-2.60564	1.11964
H	-0.59854	-4.03878	2.02942
H	1.76929	-4.68645	2.52578
H	3.63351	-3.14869	1.86276
H	-6.25723	-0.36257	1.98653
H	-7.26520	-1.11940	-0.15984
H	-5.80870	-1.65003	-2.10727
H	-2.55518	0.27081	2.41884
H	-4.35661	2.06414	2.47507
H	-3.78267	1.58681	4.09765
H	-5.35739	1.00518	3.50533
H	-4.63754	-1.51750	3.83907
H	-3.18498	-0.81566	4.61228
H	-3.01056	-2.01988	3.30559
H	-2.08336	-1.06578	-2.10532
H	-4.54141	-1.60520	-3.90836
H	-2.87597	-1.24996	-4.42293
H	-3.84135	0.00876	-3.60151
H	-3.74348	-3.64946	-2.44230
H	-2.30649	-3.45088	-1.39961
H	-2.13828	-3.34334	-3.17363
H	2.23389	0.11816	2.87077
H	3.08918	-2.80679	-1.14809
H	4.46654	-3.33229	-3.14085
H	6.46538	-1.92729	-3.71493
H	7.06344	0.03136	-2.29462
H	6.61325	1.47620	-0.34915
H	6.18293	2.93483	1.59149
H	4.83417	3.50275	3.60875
H	2.86011	2.08778	4.24057
Ni	-0.85648	0.80778	-0.33001
P	-2.26647	2.37737	-0.86284
C	-2.10751	3.15520	-2.55461
C	-4.12545	2.17463	-0.86776
C	-2.15041	3.83947	0.29524
C	0.46347	2.17616	-0.94498
C	1.11548	1.69828	-2.25052
C	2.30702	2.59559	-2.67119
H	1.16520	2.10979	-0.09634

H	0.13936	3.23059	-1.04246
H	1.47059	0.66339	-2.11266
H	0.37408	1.67630	-3.07463
H	3.08025	2.60413	-1.88406
H	1.98300	3.63963	-2.83969
H	2.77313	2.22849	-3.60305
H	-1.11234	4.19288	0.37488
H	-2.48509	3.51783	1.29508
H	-2.79647	4.66370	-0.05279
H	-1.08117	3.49259	-2.75157
H	-2.38192	2.40674	-3.31596
H	-2.79586	4.01368	-2.63500
H	-4.49239	1.88189	0.12559
H	-4.42920	1.39364	-1.58045
H	-4.58627	3.13472	-1.15891

Salicylaldiminato_3b_TS$_{BHE}$

89

C	-0.24335	-1.11884	-2.54789
C	0.59342	-2.20957	-2.09441
Ni	0.91148	-0.35871	-1.10035
C	-0.96902	-0.40169	1.21574
O	-0.78055	-0.05901	-0.05016
C	-2.31296	-0.42954	1.74898
C	0.12080	-0.74675	2.10491
C	-2.52811	-0.80617	3.08022
C	-3.47120	-0.08069	0.86325
C	1.50249	-0.66776	1.72084
C	-0.15695	-1.11297	3.45580
C	-1.45856	-1.15221	3.94450
C	-3.76653	1.28265	0.57502
C	-4.29268	-1.11477	0.32677
N	2.02284	-0.41753	0.52434
C	-2.97877	2.36259	1.10267
C	-4.90826	1.61612	-0.26589
C	-4.03199	-2.50888	0.56963
C	-5.43725	-0.77062	-0.50888
C	3.46765	-0.19864	0.48816
C	-3.28603	3.68194	0.81650
C	-5.71298	0.58259	-0.78392
C	-5.19317	2.99798	-0.53930
C	-4.84596	-3.49528	0.03990
C	-6.25926	-1.82547	-1.03499
C	4.33605	-1.22124	0.01128
C	3.99433	1.04844	0.95027
C	-4.40472	4.00596	-0.01537
C	-5.97576	-3.15237	-0.76845
C	5.71892	-0.95223	-0.06335
C	3.83655	-2.62450	-0.33811
C	5.38704	1.26107	0.85815
C	3.11831	2.12994	1.59791
C	6.24598	0.28091	0.34236
C	4.26069	-3.06326	-1.76050
C	4.31118	-3.65719	0.71942
C	3.47893	3.56570	1.14125
C	3.20025	2.05585	3.14818
C	0.07659	-3.24933	-1.10870
H	1.85321	-1.33465	-1.74764
H	-0.08426	-0.72515	-3.55692
H	-1.25564	-1.01013	-2.14673
H	-3.55588	-0.82704	3.45704
H	2.21975	-0.81444	2.54411
H	0.68498	-1.36402	4.11149
H	-1.65892	-1.43625	4.98018
H	-2.12716	2.12024	1.74256
H	-3.17078	-2.77824	1.18559
H	-2.67455	4.48768	1.23281
H	-6.57407	0.83705	-1.41204
H	-6.05466	3.23536	-1.17198
H	-4.62561	-4.54826	0.23730
H	-7.11855	-1.55275	-1.65633
H	-4.63433	5.05376	-0.22902
H	-6.60981	-3.94478	-1.17609
H	6.39349	-1.73252	-0.42864
H	2.73530	-2.60158	-0.30305
H	5.80511	2.21041	1.20444
H	2.07143	1.93400	1.30450
H	7.32117	0.47026	0.27689
H	5.35768	-3.15851	-1.84433
H	3.82164	-4.04634	-2.00585
H	3.92641	-2.33221	-2.51629
H	5.41326	-3.72703	0.73988
H	3.97164	-3.37651	1.73072
H	3.90978	-4.65906	0.48481
H	3.48308	3.66111	0.04351
H	2.74443	4.28338	1.54672
H	4.47236	3.87335	1.51220
H	4.23645	2.23290	3.48713
H	2.55128	2.82370	3.60480
H	2.88489	1.07167	3.53008
H	-0.67595	-2.81527	-0.43324
H	0.88548	-3.67687	-0.49252
H	-0.39753	-4.08709	-1.65739
H	1.26025	-2.64106	-2.85959
P	1.18073	1.67486	-2.10770
C	0.32815	1.94079	-3.75206
C	2.90016	2.25653	-2.56161
C	0.49178	3.14175	-1.17904
H	0.47654	2.97357	-4.11209
H	-0.75115	1.74970	-3.63741
H	0.72981	1.24101	-4.50347
H	3.55920	2.20005	-1.68117
H	2.89744	3.28735	-2.95777
H	3.30700	1.57627	-3.32862
H	1.02162	3.25859	-0.22138
H	-0.56898	2.94195	-0.95699
H	0.58086	4.07692	-1.75950

Salicylaldiminato_2a_3b_TS

89

C	1.46777	1.28779	-2.09908
C	0.85495	0.47116	-3.07569
P	0.47933	-2.56812	-0.81865
C	0.36759	-3.11613	0.95817
C	1.30669	-4.03803	-1.61455
C	-1.26490	-2.76193	-1.41844
C	-0.62450	0.55472	-3.40330
H	2.54008	1.49702	-2.15316
H	0.85560	1.98168	-1.51565
H	1.12186	-1.22689	-2.49498
H	-0.07682	-4.12436	1.02366
H	-0.25421	-2.40205	1.51874
H	1.37212	-3.13084	1.40968
H	1.30989	-3.89890	-2.70782
H	0.77163	-4.97139	-1.36908
H	2.35111	-4.12103	-1.27619
H	-1.27305	-2.72291	-2.51983
H	-1.85180	-1.91583	-1.03173
H	-1.70311	-3.71693	-1.08297
H	-1.21945	0.73664	-2.49566
H	-0.98914	-0.36968	-3.88092
H	-0.79798	1.38691	-4.11270
H	1.49721	0.11379	-3.89313
Ni	1.18908	-0.52050	-1.20154
O	-0.70539	0.05854	-0.18542
C	1.65539	0.29672	1.61759
N	2.19318	0.06069	0.42535
C	-2.17503	0.49521	1.66361
C	-0.85147	0.28334	1.10678
C	0.27608	0.32792	2.02633
C	0.04296	0.53412	3.42053
C	-1.23922	0.69617	3.93341
C	-2.34098	0.67927	3.04134
C	3.98304	1.79897	0.36557
C	3.59843	0.42207	0.28425
C	4.57729	-0.59067	0.05952
C	5.92554	-0.21017	-0.09115
C	6.31579	1.13530	-0.02275
C	5.34896	2.12140	0.20598
C	4.20026	-2.07150	0.06732
C	4.96763	-2.89927	-0.98835
C	4.38948	-2.67616	1.48446
C	2.99586	2.94560	0.63083
C	3.11910	4.08715	-0.41175
C	3.17572	3.52111	2.06162
C	-4.03342	-1.79353	1.57152
C	-4.25946	-0.62710	0.75916
C	-3.36975	0.48800	0.75910
C	-3.63819	1.60825	-0.08049
C	-2.78744	2.76618	-0.10365
C	-3.06877	3.84762	-0.92054
C	-4.22328	3.84193	-1.76595
C	-5.07392	2.75186	-1.76910
C	-4.81777	1.60994	-0.93510
C	-5.68843	0.50264	-0.91825
C	-5.44261	-0.61186	-0.09386
C	-6.33334	-1.73966	-0.07282
C	-6.08074	-2.83552	0.73176
C	-4.91348	-2.86204	1.55902
H	2.36563	0.55719	2.42114
H	0.90957	0.57068	4.09146
H	-1.39912	0.85085	5.00304
H	-3.35403	0.82173	3.43207
H	6.68479	-0.97966	-0.25456
H	7.36758	1.41104	-0.14078
H	5.65702	3.16969	0.26485
H	3.12441	-2.11783	-0.18609
H	4.83334	-2.47671	-1.99831
H	4.60233	-3.94179	-0.99679
H	6.04966	-2.94224	-0.77349
H	5.45070	-2.63168	1.78775
H	4.07347	-3.73510	1.50309
H	3.80049	-2.12369	2.23614
H	1.97148	2.54356	0.55770
H	4.09512	4.59832	-0.34123
H	2.33528	4.84440	-0.23474
H	3.00672	3.70955	-1.44108
H	4.18691	3.94764	2.18631
H	3.04184	2.74417	2.83260
H	2.43962	4.32223	2.24964
H	-3.14511	-1.82021	2.20696
H	-1.90756	2.77812	0.54341
H	-2.40648	4.71808	-0.92107
H	-4.43050	4.70545	-2.40438
H	-5.96372	2.74024	-2.40694
H	-6.57823	0.51060	-1.55769
H	-7.22119	-1.71085	-0.71296
H	-6.76857	-3.68583	0.73839
H	-4.71950	-3.73604	2.18763

Salicylaldiminato_2a

89

C	1.46944	1.24920	-2.08141
C	0.77658	0.42784	-3.09630
P	0.55578	-2.60212	-0.87070
C	0.46056	-3.24211	0.87660
C	1.40457	-4.02130	-1.74490
C	-1.19503	-2.83520	-1.45751
C	-0.64391	0.85760	-3.50371
H	2.53514	1.46479	-2.22471
H	0.89146	2.05724	-1.61600
H	0.61580	-0.70177	-2.64790
H	0.02414	-4.25547	0.90456
H	-0.16255	-2.55667	1.47164
H	1.46749	-3.26785	1.32337
H	1.42438	-3.81639	-2.82817
H	0.87401	-4.97325	-1.56871
H	2.44479	-4.11776	-1.39672
H	-1.22521	-2.75686	-2.55739
H	-1.80585	-2.02394	-1.03323
H	-1.59958	-3.81646	-1.15661
H	-1.26463	1.00819	-2.60684
H	-1.13109	0.10094	-4.14202
H	-0.59780	1.80454	-4.06750
H	1.41913	0.17507	-3.95776
Ni	1.19794	-0.42995	-1.13135
O	-0.75143	0.02401	-0.19921
C	1.64701	0.25928	1.59783
N	2.20674	0.05507	0.40521
C	-2.19146	0.44012	1.67246
C	-0.87406	0.23571	1.09564
C	0.26755	0.26936	2.00481
C	0.04294	0.44555	3.40687
C	-1.23354	0.59328	3.93519
C	-2.34515	0.59415	3.05403
C	3.96751	1.82270	0.37857
C	3.61018	0.44052	0.28542
C	4.60791	-0.55689	0.08423
C	5.95405	-0.15422	-0.02473
C	6.32041	1.19705	0.05840
C	5.33183	2.16798	0.25868
C	4.25891	-2.04480	0.06536
C	5.01754	-2.82451	-1.03315
C	4.49836	-2.68184	1.46022
C	2.95078	2.94861	0.61472
C	3.08080	4.08804	-0.42896
C	3.07960	3.53045	2.04828
C	-4.02956	-1.86189	1.52638
C	-4.27194	-0.67502	0.74928
C	-3.39361	0.44835	0.77717
C	-3.67852	1.59025	-0.02676
C	-2.83852	2.75621	-0.02124
C	-3.13484	3.85838	-0.80459
C	-4.29453	3.86635	-1.64295
C	-5.13478	2.76860	-1.67322
C	-4.86281	1.60517	-0.87470
C	-5.72161	0.48862	-0.88671
C	-5.45970	-0.64712	-0.09696
C	-6.33817	-1.78462	-0.10509
C	-6.06970	-2.90084	0.66567
C	-4.89825	-2.93895	1.48657
H	2.35386	0.50682	2.40657
H	0.91471	0.46998	4.07161
H	-1.38269	0.72330	5.00967
H	-3.35445	0.72569	3.45810
H	6.72964	-0.91176	-0.16705
H	7.37089	1.48947	-0.02676
H	5.62118	3.22098	0.32769
H	3.17920	-2.10918	-0.16313
H	4.83743	-2.38255	-2.02765
H	4.68450	-3.87751	-1.05527
H	6.10682	-2.83635	-0.85403
H	5.56578	-2.62296	1.73829
H	4.20478	-3.74726	1.45823
H	3.91732	-2.16253	2.24118
H	1.93801	2.52401	0.51462
H	4.04175	4.62252	-0.32959
H	2.27395	4.82738	-0.28205
H	3.01147	3.70171	-1.45886
H	4.07903	3.97510	2.20147
H	2.93605	2.75311	2.81707
H	2.32441	4.31888	2.21259
H	-3.13793	-1.89716	2.15672
H	-1.95477	2.75699	0.62077
H	-2.48078	4.73481	-0.78337
H	-4.51391	4.74618	-2.25453
H	-6.02808	2.76702	-2.30630
H	-6.61456	0.50592	-1.52158
H	-7.22936	-1.74669	-0.74011
H	-6.74812	-3.75858	0.65015
H	-4.69177	-3.82898	2.08811

Salicylaldiminato_2b_3b_TS

89

C	-0.94002	1.40044	-2.08631
C	-1.63967	0.46251	-2.90168
P	-0.03700	-2.40366	-1.25422
C	0.33632	-3.34040	0.31552
C	1.65763	-2.29457	-2.01734
C	-0.83918	-3.72524	-2.30135
C	-3.10940	0.68409	-3.27591
H	0.12958	1.57593	-2.22846
H	-1.49674	2.19159	-1.57449
H	-1.92350	-0.75161	-2.04237
H	0.91099	-4.26072	0.11108
H	-0.60331	-3.60250	0.82833
H	0.92408	-2.68501	0.97710
H	1.56927	-1.96759	-3.06650
H	2.18680	-3.26276	-1.98048
H	2.22618	-1.53367	-1.46101
H	-0.99520	-3.33698	-3.32152
H	-1.82208	-3.98834	-1.87866
H	-0.21335	-4.63273	-2.35587
H	-3.68791	1.05428	-2.41513
H	-3.58851	-0.24251	-3.63360
H	-3.16868	1.43247	-4.08606
H	-1.05018	-0.02508	-3.69117
Ni	-0.88505	-0.36303	-1.02277
O	0.74653	0.11212	-0.09238
C	-1.60215	0.41930	1.77547
N	-2.12235	0.09833	0.60472
C	2.22500	0.72104	1.66987
C	0.88944	0.45568	1.18988
C	-0.20771	0.57002	2.12415
C	0.06620	0.90972	3.48126
C	1.36205	1.14157	3.93519
C	2.43394	1.04801	3.01736
C	-4.32713	-1.01023	0.34613
C	-3.56099	0.18770	0.47448
C	-4.19678	1.46805	0.44253
C	-5.59608	1.51359	0.25627
C	-6.35532	0.34558	0.10783
C	-5.71882	-0.90506	0.15795
C	-3.43042	2.78596	0.61858
C	-3.75678	3.81937	-0.48988
C	-3.69891	3.40850	2.01510
C	-3.65458	-2.37471	0.49546
C	-4.32329	-3.48817	-0.34101
C	-3.58568	-2.79160	1.99018
C	2.74779	2.79835	-0.34910
C	3.61200	1.65608	-0.23471
C	3.38871	0.63040	0.72960
C	4.29225	-0.46993	0.81881
C	4.11143	-1.54212	1.76190
C	5.00623	-2.59618	1.83380
C	6.14151	-2.64963	0.96437
C	6.34820	-1.64764	0.03410
C	5.44199	-0.53750	-0.07607
C	5.64030	0.48046	-1.02841
C	4.75619	1.57247	-1.13183
C	4.96378	2.61565	-2.09824
C	4.10035	3.69257	-2.18057
C	2.98240	3.78428	-1.29201
H	-2.30085	0.62755	2.60600
H	-0.77990	0.99427	4.17307
H	1.55041	1.40413	4.97879
H	3.45748	1.24030	3.35449
H	-6.09720	2.48610	0.22980
H	-7.43777	0.40690	-0.03647
H	-6.31725	-1.81467	0.05962
H	-2.35121	2.56308	0.55412
H	-3.58331	3.40271	-1.49608
H	-3.11948	4.71329	-0.37220
H	-4.80802	4.15285	-0.43878
H	-4.76890	3.65626	2.13275
H	-3.11490	4.33695	2.14337
H	-3.42459	2.71355	2.82617
H	-2.61591	-2.24845	0.13228
H	-5.33549	-3.73002	0.02900
H	-3.72884	-4.41702	-0.27836
H	-4.40759	-3.19972	-1.40273
H	-4.60175	-2.90437	2.40866
H	-3.05004	-2.03884	2.59196
H	-3.06010	-3.75759	2.10063
H	1.89405	2.87649	0.32766
H	3.24781	-1.50838	2.43044
H	4.84711	-3.39791	2.56069
H	6.84098	-3.48712	1.03844
H	7.21125	-1.68138	-0.63882
H	6.50422	0.42457	-1.70013
H	5.82696	2.53972	-2.76748
H	4.27023	4.48104	-2.91922
H	2.31109	4.64510	-1.35993

Salicylaldiminato_2b

89

C	-0.98110	1.32454	-2.05433
C	-1.70676	0.38494	-2.91717
P	-0.06393	-2.49284	-1.10394
C	0.29104	-3.29106	0.54297
C	1.62913	-2.47867	-1.87913
C	-0.87860	-3.89185	-2.03870
C	-3.18078	0.68684	-3.25302
H	0.04921	1.59958	-2.30335
H	-1.55689	2.10153	-1.53848

H	-1.81839	-0.71023	-2.30478
H	0.84260	-4.23964	0.42432
H	-0.65352	-3.48070	1.07789
H	0.89538	-2.59134	1.14103
H	1.53743	-2.22734	-2.94876
H	2.14023	-3.45187	-1.77558
H	2.21922	-1.69072	-1.38678
H	-1.02735	-3.58677	-3.08797
H	-1.86536	-4.11260	-1.60119
H	-0.26063	-4.80603	-2.01648
H	-3.74526	0.95160	-2.34504
H	-3.67700	-0.17829	-3.72452
H	-3.22988	1.53590	-3.95583
H	-1.13263	0.06571	-3.80236
Ni	-0.84200	-0.38436	-1.06439
O	0.77636	0.09903	-0.13117
C	-1.59302	0.40734	1.74469
N	-2.13392	0.07464	0.58713
C	2.24052	0.71149	1.63661
C	0.90638	0.44038	1.15325
C	-0.19396	0.54315	2.08629
C	0.08027	0.87500	3.44625
C	1.37415	1.10681	3.90421
C	2.44758	1.02643	2.98660
C	-4.37206	-0.94794	0.28183
C	-3.56574	0.21850	0.46164
C	-4.16205	1.52042	0.47301
C	-5.55756	1.61722	0.27740
C	-6.35298	0.48165	0.07858
C	-5.75729	-0.79014	0.08677
C	-3.36242	2.81247	0.69413
C	-3.63379	3.87398	-0.40290
C	-3.64881	3.41640	2.09523
C	-3.74749	-2.33917	0.38598
C	-4.48250	-3.41249	-0.44688
C	-3.65135	-2.78548	1.87088
C	2.74912	2.80397	-0.37045
C	3.62114	1.66709	-0.26247
C	3.40480	0.63419	0.69555
C	4.31584	-0.46053	0.77835
C	4.14282	-1.53990	1.71465
C	5.04446	-2.58854	1.77965
C	6.17959	-2.62932	0.90940
C	6.37919	-1.62014	-0.01457
C	5.46586	-0.51510	-0.11718
C	5.65752	0.51016	-1.06288
C	4.76632	1.59698	-1.15939
C	4.96774	2.64791	-2.11862
C	4.09730	3.71962	-2.19447
C	2.97787	3.79770	-1.30651
H	-2.27962	0.64584	2.57819
H	-0.76665	0.95268	4.13792
H	1.55995	1.36087	4.95036
H	3.47004	1.22004	3.32616
H	-6.02689	2.60586	0.28347
H	-7.43142	0.58356	-0.07231
H	-6.38482	-1.67452	-0.05104
H	-2.28768	2.56423	0.65138
H	-3.43988	3.47146	-1.41111
H	-2.98014	4.75065	-0.25020
H	-4.67856	4.22971	-0.37553
H	-4.71385	3.69298	2.19140
H	-3.04214	4.32502	2.25608
H	-3.41563	2.69880	2.89959
H	-2.71467	-2.24552	-0.00457
H	-5.48829	-3.62725	-0.04437
H	-3.91952	-4.36240	-0.42208
H	-4.59379	-3.10262	-1.49994
H	-4.65902	-2.86304	2.31664
H	-3.06717	-2.06650	2.46844
H	-3.16492	-3.77491	1.94946
H	1.89361	2.87158	0.30516
H	3.27943	-1.51642	2.38388
H	4.89082	-3.39585	2.50154
H	6.88434	-3.46287	0.97757
H	7.24190	-1.64402	-0.68835
H	6.52175	0.46420	-1.73494
H	5.83185	2.58209	-2.78771
H	4.26257	4.51422	-2.92759
H	2.30047	4.65412	-1.36951

Salicylaldiminato_3a_4a_TS

89

Ni	0.85678	-0.28335	1.09302
O	-0.83954	-0.08533	0.08455
C	1.36669	-0.82527	-1.71109
N	1.92742	-0.42448	-0.57203
C	-2.43499	-0.57779	-1.62856
C	-1.07569	-0.55471	-1.13001
C	-0.02308	-1.03306	-2.00262
C	-0.35431	-1.57485	-3.28130
C	-1.67271	-1.64823	-3.71554
C	-2.70232	-1.13612	-2.88396
C	4.38304	-0.92963	-0.52082
C	3.32081	-0.00073	-0.69680
C	3.58115	1.36080	-1.03926
C	4.92447	1.77668	-1.15050
C	5.98438	0.88203	-0.93621
C	5.70994	-0.45804	-0.63384
C	2.44241	2.34493	-1.33391
C	2.72838	3.78147	-0.83281
C	2.12563	2.38430	-2.85473
C	4.13685	-2.42446	-0.30155
C	4.93414	-2.98982	0.89939
C	4.45720	-3.23016	-1.58965
C	-2.81074	2.31377	-1.25197
C	-3.69406	1.37353	-0.61945
C	-3.54837	-0.03476	-0.78525
C	-4.47688	-0.92336	-0.16635
C	-4.37986	-2.35381	-0.29135
C	-5.29530	-3.19409	0.31890
C	-6.36917	-2.65998	1.09881
C	-6.49561	-1.29209	1.25528
C	-5.56609	-0.38479	0.64039
C	-5.68557	1.00835	0.80335
C	-4.78117	1.89972	0.19410
C	-4.91481	3.32240	0.34616
C	-4.03672	4.19128	-0.27504
C	-2.97570	3.67802	-1.08626
H	2.04542	-0.96157	-2.56918
H	0.45928	-1.92694	-3.92617
H	-1.91679	-2.07160	-4.69266
H	-3.74020	-1.16569	-3.23095
H	5.14374	2.81523	-1.41289
H	7.01917	1.22572	-1.02231
H	6.53843	-1.15982	-0.49894
H	1.54199	1.97339	-0.80964
H	3.03258	3.79581	0.22734
H	1.82141	4.40139	-0.93926
H	3.52659	4.26885	-1.42015
H	3.00849	2.72837	-3.42278
H	1.29261	3.08084	-3.05478
H	1.83844	1.39232	-3.23875
H	3.06166	-2.55696	-0.09304
H	6.02156	-2.97060	0.70806
H	4.64852	-4.03916	1.08818
H	4.74557	-2.40968	1.81894
H	5.52177	-3.12568	-1.86438
H	3.85304	-2.87794	-2.44284
H	4.24516	-4.30278	-1.43552
H	-2.00046	1.92977	-1.87559
H	-3.56125	-2.77226	-0.88123
H	-5.19757	-4.27792	0.20881
H	-7.08427	-3.33863	1.57228
H	-7.31021	-0.87221	1.85443
H	-6.50378	1.40801	1.41292
H	-5.73520	3.70385	0.96284
H	-4.15211	5.27232	-0.15502
H	-2.29287	4.37451	-1.58146
P	1.79239	1.06594	2.52195
C	1.40021	-2.25702	2.12351
C	0.39388	-2.62321	1.25795
C	-1.03485	-2.84912	1.67931
C	1.00033	2.75265	2.59442
C	1.67019	0.55745	4.31404
C	3.61398	1.48721	2.45616
H	1.18299	-2.14042	3.19018
H	2.45469	-2.31421	1.85145
H	-0.01253	-0.09944	2.25954
H	0.64787	-2.89775	0.22575
H	-1.17769	-2.60665	2.74608
H	-1.32658	-3.90558	1.52492
H	-1.73278	-2.22347	1.09854
H	1.13236	3.26376	1.62825
H	1.43342	3.37225	3.39927
H	-0.08020	2.62217	2.76410
H	0.61386	0.39409	4.57944
H	2.09755	1.33639	4.96825
H	2.22070	-0.38356	4.47263
H	4.20262	0.56177	2.56116
H	3.87696	2.18191	3.27315
H	3.87060	1.93970	1.48754

Salicylaldiminato_3a

89

Ni	0.98955	-0.54349	-1.12543
O	-0.73140	0.02365	-0.21159
C	1.56067	0.10978	1.66174
N	2.09178	0.04725	0.44548
C	-2.25510	0.23494	1.62166
C	-0.91303	0.07574	1.09610
C	0.18075	-0.00076	2.04909
C	-0.10036	-0.00629	3.44938
C	-1.40242	0.07210	3.92976
C	-2.46959	0.20591	3.00452
C	3.67274	1.96923	0.42646
C	3.45071	0.56046	0.32083
C	4.53597	-0.33042	0.07575
C	5.83333	0.20468	-0.05789
C	6.06678	1.58336	0.04578
C	4.99345	2.44964	0.28750
C	4.32923	-1.84503	0.04596
C	5.18517	-2.55934	-1.02575
C	4.59875	-2.45374	1.44866
C	2.54837	2.97825	0.70210
C	2.58902	4.19161	-0.26288
C	2.59112	3.47755	2.17174
C	-4.23470	-1.91865	1.18089

C	-4.35402	-0.65261	0.50653
C	-3.40905	0.40208	0.68042
C	-3.57881	1.63010	-0.02380
C	-2.67775	2.73701	0.14103
C	-2.86410	3.92367	-0.54657
C	-3.96698	4.08118	-1.44422
C	-4.86472	3.04541	-1.62548
C	-4.70834	1.79937	-0.92687
C	-5.63091	0.74754	-1.08815
C	-5.48675	-0.46825	-0.39352
C	-6.43440	-1.53680	-0.55319
C	-6.28472	-2.73316	0.12352
C	-5.16820	-2.92473	0.99708
H	2.25260	0.34159	2.48839
H	0.74191	-0.06012	4.14918
H	-1.60443	0.06134	5.00335
H	-3.49538	0.30274	3.37472
H	6.67429	-0.47057	-0.23700
H	7.08100	1.97899	-0.05880
H	5.17858	3.52444	0.36942
H	3.26618	-2.01270	-0.20668
H	5.02499	-2.12220	-2.02545
H	4.92002	-3.63068	-1.07021
H	6.26382	-2.50453	-0.79629
H	5.64626	-2.27697	1.75109
H	4.42562	-3.54507	1.44190
H	3.94634	-2.00219	2.21513
H	1.58283	2.46655	0.54567
H	3.47955	4.82053	-0.08960
H	1.69985	4.82565	-0.10358
H	2.59975	3.87170	-1.31800
H	3.54134	4.00241	2.37633
H	2.50502	2.64414	2.88832
H	1.76207	4.18113	2.36291
H	-3.38668	-2.07389	1.85212
H	-1.83605	2.62627	0.82786
H	-2.16507	4.75265	-0.40379
H	-4.09766	5.02538	-1.98045
H	-5.71692	3.15707	-2.30372
H	-6.48232	0.87997	-1.76510
H	-7.28240	-1.38044	-1.22791
H	-7.01453	-3.53710	-0.00718
H	-5.05411	-3.87692	1.52332
P	0.61381	-2.75354	-0.73099
C	2.26897	-0.08597	-2.63909
C	1.44071	1.03241	-2.36260
C	0.29295	1.48166	-3.24158
C	0.87417	-3.50194	0.96447
C	-1.16156	-3.20697	-1.04527
C	1.49101	-3.98254	-1.82751
H	2.08785	-0.68531	-3.53882
H	3.28822	-0.13410	-2.24133
H	0.18686	-1.04730	-2.23121
H	1.84178	1.80433	-1.69475
H	-0.01535	0.68364	-3.93836
H	0.58519	2.36630	-3.84229
H	-0.58699	1.76217	-2.63898
H	1.92572	-3.39103	1.27175
H	0.60304	-4.57237	0.97156
H	0.24587	-2.96156	1.69034
H	-1.81704	-2.53917	-0.46644
H	-1.36363	-4.25745	-0.77608
H	-1.38756	-3.05082	-2.11228
H	1.29489	-3.71958	-2.87948
H	1.14054	-5.01225	-1.63971
H	2.57821	-3.93258	-1.65799

Salicylaldiminato_3b_4b_TS

89

C	-1.34614	-1.41063	-2.26592
C	-0.44791	-0.79076	-3.09045
P	-0.07201	2.33706	-1.47883
C	-0.00415	3.56206	-0.07381
C	-0.78901	3.36951	-2.85190
C	1.72385	2.24743	-1.95496
C	1.00741	-1.17348	-3.18736
H	-2.42144	-1.24777	-2.36580
H	-1.02534	-2.22320	-1.60640
H	-2.16033	1.07209	-1.60254
H	0.51041	4.49113	-0.37644
H	0.54470	3.09951	0.76179
H	-1.02538	3.80093	0.26311
H	-0.80630	2.77594	-3.78032
H	-0.19568	4.28502	-3.01697
H	-1.82526	3.64396	-2.59945
H	1.81706	1.83146	-2.97024
H	2.23844	1.57651	-1.25123
H	2.18916	3.24761	-1.92982
H	1.36804	-1.61724	-2.24646
H	1.65291	-0.31229	-3.42252
H	1.15701	-1.91377	-3.99825
H	-0.82408	-0.06187	-3.82049
Ni	-1.03567	0.45832	-0.89246
O	0.59685	-0.13821	-0.02154
C	-1.79655	-0.68182	1.64397
N	-2.23471	-0.21898	0.47972
C	2.02073	-0.82935	1.77084
C	0.70705	-0.58994	1.22990
C	-0.43500	-0.85436	2.07502
C	-0.23219	-1.33482	3.40192
C	1.04480	-1.55534	3.91052
C	2.16466	-1.29970	3.08389
C	-4.34680	-1.48523	0.05418
C	-3.68091	-0.24430	0.28267
C	-4.40795	0.97978	0.33249
C	-5.79962	0.94487	0.11494
C	-6.46748	-0.26225	-0.13992
C	-5.74322	-1.46058	-0.16110
C	-3.72682	2.30086	0.69335
C	-4.14461	3.46010	-0.24136
C	-3.99089	2.66767	2.17803
C	-3.62882	-2.84165	0.07623
C	-3.95396	-3.70967	-1.16539
C	-3.96706	-3.62817	1.37202
C	3.44265	1.73802	1.90627
C	3.90990	0.68850	1.04029
C	3.23763	-0.56300	0.93522
C	3.74265	-1.57074	0.06542
C	3.10768	-2.85390	-0.06584
C	3.61985	-3.82357	-0.91064
C	4.80123	-3.57133	-1.67814
C	5.44385	-2.35056	-1.58213
C	4.94581	-1.31714	-0.71675
C	5.59689	-0.07288	-0.60377
C	5.11291	0.93407	0.25403
C	5.77961	2.20123	0.37887
C	5.29696	3.18154	1.22674
C	4.11394	2.94545	1.99723
H	-2.56160	-0.97605	2.37951
H	-1.11290	-1.53243	4.02360
H	1.18476	-1.92263	4.92982
H	3.17508	-1.46945	3.46929
H	-6.37027	1.87724	0.15752
H	-7.54812	-0.26902	-0.30874
H	-6.26908	-2.40254	-0.34241
H	-2.64045	2.14406	0.56844
H	-3.96894	3.19540	-1.29793
H	-3.56372	4.37010	-0.00634
H	-5.21259	3.71709	-0.12746
H	-5.06987	2.82105	2.35887
H	-3.46166	3.59945	2.44710
H	-3.64441	1.86798	2.85428
H	-2.54220	-2.65163	0.07495
H	-5.01798	-4.00385	-1.18700
H	-3.35473	-4.63687	-1.14572
H	-3.72986	-3.17549	-2.10277
H	-5.04714	-3.85401	1.42117
H	-3.70297	-3.05470	2.27643
H	-3.41527	-4.58436	1.39705
H	2.54321	1.55800	2.50042
H	2.20789	-3.05070	0.52212
H	3.12121	-4.79330	-0.99463
H	5.19252	-4.34992	-2.33896
H	6.34921	-2.14981	-2.16410
H	6.50242	0.11330	-1.19201
H	6.68426	2.37232	-0.21368
H	5.81706	4.13960	1.31475
H	3.74343	3.72737	2.66637

Salicylaldiminato_3b

89

Ni	-1.00651	-0.21171	-1.04643
O	0.64910	0.21155	-0.07438
C	-1.71517	0.38990	1.72998
N	-2.18990	0.14146	0.52123
C	2.11021	0.55896	1.78131
C	0.78317	0.39570	1.23968
C	-0.33709	0.45795	2.15102
C	-0.10154	0.66427	3.54124
C	1.18689	0.80368	4.05081
C	2.28436	0.75206	3.15949
C	-4.44411	-0.89212	0.30526
C	-3.63242	0.27672	0.35116
C	-4.20457	1.57652	0.23160
C	-5.60266	1.67426	0.05884
C	-6.41432	0.53384	0.00452
C	-5.83414	-0.73741	0.12901
C	-3.36733	2.85833	0.31017
C	-3.70781	3.86168	-0.82031
C	-3.52402	3.54608	1.69321
C	-3.83553	-2.27994	0.50949
C	-4.51976	-3.37644	-0.33875
C	-3.84763	-2.67514	2.01130
C	2.82980	2.83260	0.05717
C	3.61939	1.63208	0.05129
C	3.30093	0.51152	0.87175
C	4.13201	-0.64701	0.84836
C	3.85766	-1.80977	1.65105
C	4.68137	-2.92177	1.61264
C	5.83591	-2.94513	0.76762
C	6.13490	-1.85263	-0.02564
C	5.30451	-0.67953	-0.01861
C	5.59901	0.43434	-0.82808
C	4.78923	1.58702	-0.81549
C	5.09631	2.72829	-1.63286
C	4.30420	3.86112	-1.60106
C	3.16016	3.91231	-0.74316
H	-2.45208	0.59387	2.52439

H	-0.96627	0.71605	4.21264
H	1.35154	0.96113	5.11920
H	3.30216	0.87183	3.54427
H	-6.05970	2.66375	-0.03428
H	-7.49512	0.63381	-0.13049
H	-6.47307	-1.62387	0.09463
H	-2.30848	2.57351	0.18926
H	-3.65019	3.38461	-1.81237
H	-2.99755	4.70665	-0.80122
H	-4.72269	4.28084	-0.70301
H	-4.57397	3.84502	1.86234
H	-2.89549	4.45249	1.74702
H	-3.22858	2.87411	2.51641
H	-2.78050	-2.20883	0.18609
H	-5.55220	-3.57304	0.00009
H	-3.96536	-4.32739	-0.24783
H	-4.55864	-3.09369	-1.40427
H	-4.88431	-2.73004	2.38857
H	-3.30074	-1.94059	2.62570
H	-3.37717	-3.66434	2.15774
H	1.95688	2.87928	0.71230
H	2.98091	-1.79765	2.30315
H	4.45252	-3.79175	2.23492
H	6.47830	-3.83009	0.75326
H	7.01497	-1.86103	-0.67694
H	6.48046	0.40576	-1.47837
H	5.97743	2.68138	-2.28098
H	4.54939	4.72346	-2.22734
H	2.54413	4.81571	-0.72240
P	-0.22931	-2.32116	-1.25559
C	-0.21609	0.65717	-2.78747
C	-0.98365	1.59025	-2.06278
C	0.06961	-3.25967	0.32866
C	-1.10851	-3.58916	-2.30085
C	1.47832	-2.33288	-1.99337
C	-0.65943	0.10069	-4.12611
H	0.86166	0.61987	-2.58324
H	-2.14324	-0.63004	-1.84875
H	-0.49749	2.27336	-1.36126
H	0.71068	-2.64587	0.98078
H	0.56851	-4.22508	0.13488
H	-0.88474	-3.44123	0.84844
H	-2.11020	-3.78153	-1.88521
H	-0.54565	-4.53716	-2.34982
H	-1.23291	-3.18812	-3.31977
H	1.43404	-1.98929	-3.03943
H	1.92554	-3.34114	-1.96035
H	2.10268	-1.63007	-1.42069
H	-0.22189	0.69709	-4.95132
H	-1.75699	0.13249	-4.22990
H	-0.33392	-0.94356	-4.27844
H	-1.97735	1.87942	-2.42059

Salicylaldiminato_4a

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O	0.86767	-0.01555	0.05110
C	-1.31488	0.23333	-1.87915
N	-1.84475	0.10167	-0.66041
C	2.48630	0.15791	-1.68740
C	1.11480	0.12432	-1.24997
C	0.06915	0.24441	-2.23387
C	0.41339	0.38993	-3.61289
C	1.74101	0.41775	-4.02108
C	2.77057	0.30166	-3.04954
C	-3.94326	1.39713	-0.39912
C	-3.30010	0.14671	-0.61857
C	-4.04082	-1.05175	-0.81370
C	-5.45027	-0.96924	-0.79844
C	-6.10438	0.25502	-0.59352
C	-5.35401	1.42468	-0.39355
C	-3.34295	-2.39326	-1.06283
C	-3.92444	-3.53982	-0.20037
C	-3.38736	-2.77398	-2.56681
C	-3.13172	2.68281	-0.20871
C	-3.69698	3.59840	0.90332
C	-3.01129	3.46951	-1.54151
C	3.49162	-2.46069	-0.80809
C	4.05641	-1.24710	-0.28421
C	3.59016	0.03864	-0.67866
C	4.17654	1.21229	-0.12621
C	3.73016	2.53263	-0.48010
C	4.31725	3.65932	0.06893
C	5.39128	3.53799	1.00686
C	5.84839	2.28718	1.37950
C	5.26367	1.09200	0.83699
C	5.71622	-0.18706	1.21470
C	5.14179	-1.35733	0.68153
C	5.60226	-2.66327	1.06516
C	5.03029	-3.80543	0.53541
C	3.96163	-3.70029	-0.41055
H	-2.02246	0.35012	-2.71454
H	-0.39480	0.47991	-4.34764
H	1.99697	0.52770	-5.07758
H	3.81809	0.32336	-3.36588
H	-6.04217	-1.87595	-0.95505
H	-7.19732	0.29863	-0.59150
H	-5.87200	2.37483	-0.23506
H	-2.28201	-2.26955	-0.77770
H	-3.89568	-3.28987	0.87435
H	-3.33625	-4.46141	-0.35232
H	-4.97130	-3.76703	-0.46812
H	-4.43021	-2.90286	-2.90793
H	-2.84828	-3.72169	-2.74094
H	-2.92095	-1.99424	-3.19190
H	-2.11216	2.37897	0.09546
H	-4.68272	4.01642	0.63308
H	-3.01360	4.44861	1.07108
H	-3.80827	3.05538	1.85781
H	-4.00790	3.78079	-1.90246
H	-2.54021	2.85780	-2.32861
H	-2.39657	4.37554	-1.39870
H	2.67356	-2.38638	-1.52860
H	2.90752	2.63102	-1.19243
H	3.95852	4.65361	-0.21222
H	5.84539	4.43932	1.42835
H	6.66733	2.18417	2.09896
H	6.53439	-0.27363	1.93855
H	6.42023	-2.73343	1.78966
H	5.39068	-4.79329	0.83633
H	3.51419	-4.61052	-0.81995
Ni	-0.79010	-0.12289	0.92669
P	-2.02165	-0.38022	2.66096
C	-1.67324	0.86972	3.99693
C	-3.89088	-0.35918	2.65478
C	-1.69712	-1.99663	3.52673
H	-0.62477	-2.07124	3.76283
H	-1.95966	-2.82954	2.85456
H	-2.29177	-2.07556	4.45294
H	-0.60117	0.84671	4.24447
H	-1.91847	1.87784	3.62583
H	-2.27157	0.65936	4.89983
H	-4.27869	-1.15155	1.99716
H	-4.25847	0.60391	2.26924
H	-4.26927	-0.51455	3.68025
H	0.04612	-0.29479	2.13895

Salicylaldiminato_4b

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O	0.53764	0.00017	-0.03845
C	-1.81016	0.29550	-1.77762
N	-2.23216	0.07589	-0.53390
C	2.00084	0.31648	-1.89832
C	0.67493	0.22134	-1.34753
C	-0.45475	0.37216	-2.23354
C	-0.22969	0.61324	-3.62273
C	1.05762	0.70506	-4.13905
C	2.16719	0.55513	-3.26782
C	-4.35923	1.28491	-0.09692
C	-3.67765	0.06098	-0.33241
C	-4.36296	-1.18382	-0.36227
C	-5.76173	-1.17428	-0.18349
C	-6.45937	0.02498	0.02926
C	-5.75924	1.23911	0.07774
C	-3.61530	-2.49956	-0.59166
C	-4.03240	-3.59790	0.41564
C	-3.78775	-2.99647	-2.05132
C	-3.62167	2.62439	-0.00729
C	-3.87569	3.32324	1.35249
C	-3.98946	3.55996	-1.18724
C	3.16463	-2.32325	-1.32975
C	3.74502	-1.13239	-0.77033
C	3.19609	0.16037	-1.00539
C	3.79676	1.30875	-0.41564
C	3.26530	2.63205	-0.60285
C	3.86524	3.73439	-0.01909
C	5.03910	3.58445	0.78604
C	5.58165	2.32970	0.99537
C	4.98600	1.15811	0.41395
C	5.52411	-0.12626	0.62671
C	4.93468	-1.27354	0.05989
C	5.48052	-2.58540	0.27626
C	4.89114	-3.70433	-0.28348
C	3.71829	-3.56961	-1.09266
H	-2.58665	0.43813	-2.54494
H	-1.09878	0.72650	-4.28032
H	1.21922	0.89040	-5.20357
H	3.18355	0.62514	-3.66779
H	-6.31136	-2.11993	-0.21107
H	-7.54519	0.01172	0.16114
H	-6.30557	2.17072	0.25470
H	-2.54098	-2.29523	-0.42736
H	-3.91615	-3.24388	1.45365
H	-3.40098	-4.49369	0.28103
H	-5.08277	-3.90854	0.27458
H	-4.85110	-3.19895	-2.27313
H	-3.21893	-3.92924	-2.21307
H	-3.42861	-2.24531	-2.77533
H	-2.53932	2.41406	-0.06597
H	-4.93802	3.59861	1.47646
H	-3.27721	4.24881	1.42208
H	-3.59335	2.66245	2.18905
H	-5.06646	3.80571	-1.17818
H	-3.75995	3.08910	-2.15827
H	-3.42359	4.50584	-1.12018
H	2.26887	-2.22563	-1.94774
H	2.36836	2.75064	-1.21547
H	3.44177	4.73104	-0.17208
H	5.50338	4.46749	1.23415

H	6.47861	2.20576	1.61095
H	6.42198	-0.23525	1.24541
H	6.37814	-2.67903	0.89618
H	5.31792	-4.69653	-0.11175
H	3.25910	-4.46215	-1.52695
Ni	-1.08250	-0.18196	0.93100
P	-0.07478	-0.45855	2.81073
C	-0.33689	-2.11965	3.60398
C	1.77101	-0.29048	2.78277
C	-0.58168	0.71504	4.16061
H	-1.66308	0.61432	4.34185
H	-0.37868	1.74796	3.83535
H	-0.02755	0.51075	5.09266
H	-1.41592	-2.28290	3.75008
H	0.04673	-2.90484	2.93309
H	0.18338	-2.18344	4.57493
H	2.03795	0.72820	2.46404
H	2.18406	-0.98501	2.03687
H	2.20209	-0.49817	3.77715
H	-2.23613	-0.36945	1.82979
C	2.75503	-3.63638	1.61773
H	2.13873	-2.60003	-0.18044
H	6.30168	1.36291	1.10617
C	4.32747	3.14367	0.19784
C	3.79058	2.52820	2.60809
H	2.59507	2.05619	0.86270
H	7.30457	-0.88591	0.74219
H	4.57153	-4.50910	-0.29150
H	2.93463	-4.79658	-0.92144
H	3.97151	-3.55138	-1.67579
H	3.67793	-3.99702	2.10620
H	2.25695	-2.93358	2.30604
H	2.08393	-4.50035	1.46665
H	4.24696	2.84559	-0.86024
H	3.82611	4.11986	0.31960
H	5.39628	3.28697	0.43599
H	4.85045	2.57662	2.91552
H	3.34589	3.52839	2.75398
H	3.27714	1.82305	3.28337

Salicylaldiminato_5a_7a_TS

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C	-0.24755	-0.41863	-2.66259
H	-0.46426	-2.27867	-1.57643
H	1.00296	-2.20702	-2.71538
C	0.18301	-1.67841	-2.22228
H	0.22452	0.06951	-3.51940
H	-1.22172	-0.03427	-2.35310
C	3.07462	-0.62134	-3.11794
H	3.18383	0.67607	-1.38340
H	1.95630	1.18750	-2.58730
C	2.42323	0.31153	-2.09255
C	4.24097	0.06780	-3.87023
H	2.33499	-0.97056	-3.86387
H	3.46479	-1.52352	-2.60886
H	5.02456	0.39183	-3.16349
H	3.88443	0.96130	-4.41328
H	4.70382	-0.61558	-4.60461
C	-0.68874	4.12482	0.62577
C	0.70599	4.96664	-1.72256
C	-1.54486	3.21510	-1.94874
P	0.03267	3.38723	-0.94627
H	-1.27046	3.34880	1.15032
H	0.13147	4.44401	1.29106
H	-1.34452	4.99041	0.42294
H	1.04215	4.75481	-2.75189
H	1.57992	5.31592	-1.14671
H	-0.04921	5.77269	-1.75201
H	-2.16579	2.41868	-1.50659
H	-1.29051	2.91834	-2.98049
H	-2.12931	4.15192	-1.97788
Ni	0.92500	-0.26051	-0.95712
C	-1.01480	-0.33862	1.29945
O	-0.76713	-0.37324	-0.00363
C	-2.37722	-0.41470	1.76881
C	0.04665	-0.23954	2.27037
C	-2.63411	-0.33718	3.14323
C	-3.49979	-0.58321	0.79062
C	1.42843	-0.27124	1.90037
C	-0.27186	-0.17392	3.66064
C	-1.59111	-0.20948	4.09674
H	-3.67298	-0.39146	3.48357
C	-4.36796	0.50888	0.49697
C	-3.71300	-1.84901	0.17083
N	1.97226	-0.31022	0.68283
H	2.13321	-0.29605	2.74579
H	0.54813	-0.09886	4.38351
H	-1.82776	-0.15777	5.16201
C	-4.20356	1.80850	1.09224
C	-5.46597	0.32613	-0.44521
C	-2.89162	-2.99228	0.46159
C	-4.80598	-2.01707	-0.77673
C	3.42863	-0.44889	0.68183
C	-5.06534	2.85059	0.79519
H	-3.37844	1.96068	1.79207
C	-5.65074	-0.92643	-1.06095
C	-6.33748	1.43396	-0.72535
C	-3.11927	-4.21375	-0.14894
H	-2.08043	-2.88264	1.18503
C	-5.00536	-3.29989	-1.39285
C	3.98529	-1.74055	0.45816
C	4.25045	0.68926	0.90861
C	-6.14793	2.66306	-0.12109
H	-4.91941	3.82855	1.26255
H	-6.47498	-1.05753	-1.77089
H	-7.16043	1.28082	-1.43097
C	-4.18493	-4.37106	-1.09078
H	-2.48369	-5.07075	0.09175
H	-5.82894	-3.41110	-2.10554
C	5.38917	-1.87026	0.48552
C	3.08777	-2.96599	0.25674
C	5.65034	0.50164	0.93007
C	3.66819	2.09125	1.12426
H	-6.82053	3.49655	-0.34194
H	-4.34927	-5.34299	-1.56426
C	6.21794	-0.76241	0.72280
H	5.84044	-2.85247	0.32227
C	3.68196	-4.01071	-0.71583

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C	0.04554	0.86874	-2.59852
H	-0.02572	2.34783	-1.01578
H	-1.54548	2.27606	-2.07552
C	-0.60169	1.81515	-1.77764
H	-0.38436	0.57533	-3.56206
H	1.11711	0.68840	-2.47504
C	-3.28770	0.50171	-2.79238
H	-2.97245	-1.26722	-1.55785
H	-1.94890	-1.18069	-3.03083
C	-2.38533	-0.58892	-2.20405
C	-4.48067	-0.11080	-3.56904
H	-2.71395	1.14832	-3.48314
H	-3.68104	1.15118	-1.99128
H	-5.10906	-0.72435	-2.90006
H	-4.12696	-0.75775	-4.39224
H	-5.11864	0.67816	-4.00593
C	0.37898	-3.11409	0.42993
C	-0.91074	-3.63685	-2.09275
C	1.62083	-2.26365	-2.01829
P	-0.03688	-2.25980	-1.17646
H	1.00425	-2.44298	1.03735
H	-0.54262	-3.33676	0.99137
H	0.92856	-4.05383	0.24826
H	-1.07153	-3.34269	-3.14251
H	-1.89514	-3.83013	-1.63685
H	-0.31331	-4.56416	-2.06988
H	2.26257	-1.52890	-1.50890
H	1.50066	-1.95961	-3.07093
H	2.09339	-3.25988	-1.97869
Ni	-0.85923	-0.09360	-1.02727
C	1.07276	0.34418	1.26631
O	0.86366	0.16222	-0.03537
C	2.42775	0.49616	1.74108
C	0.00199	0.39823	2.23178
C	2.67207	0.65911	3.11210
C	3.56817	0.47941	0.76781
C	-1.39455	0.33695	1.88189
C	0.30806	0.57219	3.61308
C	1.62118	0.69386	4.05958
H	3.70839	0.76995	3.44700
C	4.39215	-0.67803	0.65004
C	3.84371	1.63194	-0.02392
N	-1.95724	0.15409	0.69659
H	-2.07751	0.48642	2.73493
H	-0.52147	0.61276	4.32836
H	1.84082	0.82621	5.12143
C	4.16806	-1.86742	1.42864
C	5.50692	-0.68090	-0.29084
C	3.06699	2.83621	0.08302
C	4.95653	1.61711	-0.96385
C	-3.41263	0.25446	0.69566
C	4.98343	-2.97842	1.29696
H	3.33758	-1.87701	2.13862
C	5.75540	0.46222	-1.07456
C	6.32940	-1.85477	-0.39568
C	3.35578	3.94723	-0.69015
H	2.24039	2.86108	0.79692
C	5.22042	2.78986	-1.75118
C	-4.02472	1.54098	0.64978
C	-4.19604	-0.93235	0.76070
C	6.07836	-2.97465	0.37568
H	4.79391	-3.86886	1.90333
H	6.59300	0.45605	-1.78099
H	7.16486	-1.84058	-1.10316
C	4.44201	3.92518	-1.62126
H	2.75143	4.85327	-0.59094
H	6.05819	2.76535	-2.45556
C	-5.43459	1.60759	0.65191
C	-3.20268	2.83547	0.64663
C	-5.60134	-0.80981	0.75431
C	-3.53738	-2.30505	0.91798
H	6.71422	-3.85999	0.28699
H	4.65413	4.81173	-2.22533
C	-6.22046	0.44751	0.69644
H	-5.92272	2.58603	0.61981
C	-3.70106	3.86217	-0.39992
C	-3.18459	3.48410	2.05751

H	-2.16530	2.56808	0.38209
H	-6.21903	-1.71058	0.80475
C	-4.26303	-3.42570	0.13723
C	-3.41908	-2.69214	2.41771
H	-2.51170	-2.21192	0.51382
H	-7.31163	0.52256	0.69375
H	-4.70746	4.24372	-0.15279
H	-3.01832	4.72916	-0.43138
H	-3.74344	3.42090	-1.40937
H	-4.20737	3.75616	2.37405
H	-2.76858	2.79838	2.81441
H	-2.57053	4.40192	2.05181
H	-4.39918	-3.15619	-0.92383
H	-3.67939	-4.36190	0.18752
H	-5.25803	-3.64213	0.56427
H	-4.42074	-2.76596	2.87703
H	-2.91798	-3.67070	2.52800
H	-2.84003	-1.94399	2.98393

Salicylaldiminato_6a

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Ni	-0.99087	0.26207	-1.05371
O	0.65565	0.03665	-0.19091
C	-1.63107	-0.54699	1.52775
N	-2.10158	-0.19931	0.32559
C	2.18315	-0.43865	1.58586
C	0.84262	-0.33047	1.07626
C	-0.26762	-0.62474	1.95304
C	-0.00567	-1.01720	3.30227
C	1.29467	-1.11779	3.78109
C	2.38198	-0.82766	2.91554
C	-4.17728	-1.38933	-0.33282
C	-3.55153	-0.21145	0.15937
C	-4.29622	0.95403	0.48551
C	-5.69933	0.90238	0.34241
C	-6.34078	-0.25690	-0.11841
C	-5.58243	-1.38771	-0.45792
C	-3.61657	2.23090	0.99002
C	-4.10023	3.49248	0.23357
C	-3.80936	2.40626	2.51956
C	-3.36454	-2.63591	-0.69480
C	-3.79682	-3.25754	-2.04473
C	-3.42815	-3.69410	0.43845
C	3.02298	2.32093	1.01242
C	3.72571	1.20742	0.43624
C	3.34653	-0.14203	0.68747
C	4.07618	-1.21239	0.09493
C	3.71904	-2.59151	0.29478
C	4.44593	-3.61309	-0.29147
C	5.57881	-3.32240	-1.11597
C	5.95163	-2.01043	-1.34341
C	5.22116	-0.91973	-0.75891
C	5.58398	0.42007	-0.99637
C	4.86665	1.48904	-0.42467
C	5.23631	2.85646	-0.66641
C	4.52859	3.89814	-0.09526
C	3.40954	3.62453	0.75375
C	-2.20774	0.68858	-2.45718
C	-0.89274	0.96083	-3.13928
C	-0.62080	2.41928	-3.55715
H	-2.38777	-0.80570	2.28231
H	-0.85493	-1.23906	3.95783
H	1.48486	-1.41668	4.81458
H	3.40734	-0.90497	3.29006
H	-6.29584	1.78394	0.59472
H	-7.42982	-0.27769	-0.21772
H	-6.08805	-2.28492	-0.82642
H	-2.53362	2.12523	0.79574
H	-3.97578	3.37614	-0.85630
H	-3.51781	4.37317	0.55578
H	-5.16488	3.70698	0.43333
H	-4.88047	2.50506	2.77089
H	-3.28840	3.31363	2.87232
H	-3.40981	1.54280	3.07770
H	-2.31018	-2.31914	-0.79994
H	-4.81690	-3.67777	-1.99668
H	-3.11282	-4.07991	-2.31740
H	-3.77526	-2.50868	-2.85467
H	-4.46662	-4.03636	0.59609
H	-3.05847	-3.28292	1.39293
H	-2.81074	-4.57266	0.18125
H	2.16867	2.11897	1.66287
H	2.85198	-2.82109	0.91859
H	4.15290	-4.65406	-0.12802
H	6.14346	-4.14275	-1.56785
H	6.81280	-1.77722	-1.97801
H	6.44427	0.63585	-1.63987
H	6.09608	3.05530	-1.31449
H	4.82125	4.93440	-0.28672
H	2.85822	4.45615	1.20171
H	-2.84168	1.56454	-2.25166
H	-2.79064	-0.17111	-2.81746
H	-0.00632	0.68565	-2.41332
H	-0.69393	0.25174	-3.96260
H	-1.28962	2.69812	-4.38843
H	-0.81207	3.10639	-2.71631
H	0.42158	2.56309	-3.88596

Salicylaldiminato_6a_7a_TS

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Ni	-0.97338	0.10683	-1.04066
O	0.68416	-0.03370	-0.14317
C	-1.59992	-0.52787	1.60515
N	-2.08746	-0.23250	0.39424
C	2.21276	-0.35167	1.67251
C	0.87541	-0.31629	1.14344
C	-0.23329	-0.60020	2.02621
C	0.02818	-0.93680	3.38967
C	1.32721	-0.98710	3.88229
C	2.41144	-0.69034	3.01709
C	-4.28485	-1.31593	-0.05083
C	-3.54475	-0.15604	0.30173
C	-4.18625	1.08409	0.57935
C	-5.59460	1.13109	0.50973
C	-6.34480	-0.00548	0.17232
C	-5.69163	-1.21427	-0.10636
C	-3.38890	2.33277	0.96973
C	-3.89718	3.61299	0.26328
C	-3.38142	2.53568	2.50885
C	-3.60561	-2.65844	-0.33137
C	-4.05601	-3.26921	-1.68110
C	-3.84415	-3.65954	0.82985
C	2.89681	2.41349	0.94224
C	3.68290	1.31256	0.45667
C	3.37838	-0.04032	0.78277
C	4.19339	-1.09666	0.28202
C	3.91537	-2.48139	0.55709
C	4.72545	-3.48854	0.06165
C	5.86763	-3.17705	-0.74200
C	6.16646	-1.86034	-1.04028
C	5.34840	-0.78463	-0.55160
C	5.63649	0.55826	-0.86242
C	4.83378	1.61256	-0.38443
C	5.12884	2.98308	-0.70013
C	4.34057	4.01148	-0.21727
C	3.21307	3.72052	0.61441
C	-2.25332	0.67920	-2.34259
C	-1.11102	1.46301	-2.96945
C	-1.26043	2.99611	-2.93456
H	-2.34916	-0.72474	2.38532
H	-0.82062	-1.15352	4.04769
H	1.51646	-1.24550	4.92680
H	3.43532	-0.71982	3.40251
H	-6.11033	2.07148	0.72324
H	-7.43611	0.05176	0.12732
H	-6.28129	-2.09811	-0.36789
H	-2.34371	2.16738	0.64791
H	-3.94620	3.47713	-0.83007
H	-3.21666	4.45554	0.47678
H	-4.90197	3.90568	0.61560
H	-4.40816	2.68917	2.88640
H	-2.77917	3.42131	2.77771
H	-2.95545	1.66202	3.02966
H	-2.51994	-2.47106	-0.39561
H	-5.12679	-3.53871	-1.66881
H	-3.48437	-4.18969	-1.89356
H	-3.89627	-2.56032	-2.51126
H	-4.92036	-3.88075	0.94405
H	-3.47896	-3.25463	1.78887
H	-3.31764	-4.61026	0.63446
H	2.03628	2.19991	1.58053
H	3.04258	-2.72734	1.16663
H	4.49164	-4.53406	0.28159
H	6.49830	-3.98568	-1.12191
H	7.03456	-1.61224	-1.65963
H	6.50549	0.78805	-1.48913
H	5.99698	3.19501	-1.33269
H	4.57641	5.05037	-0.46464
H	2.59947	4.54202	0.99509
H	-3.06656	1.29212	-1.92648
H	-2.65277	-0.15878	-2.93556
H	-0.14040	1.21246	-2.40876
H	-0.88278	1.10591	-3.99100
H	-2.10162	3.31238	-3.57465
H	-1.46262	3.34412	-1.90748
H	-0.34635	3.50033	-3.29087
C	0.60150	-1.39956	-2.97251
C	-0.33457	-2.09404	-2.28131
H	1.56367	-1.14116	-2.52425
H	0.42734	-1.06953	-4.00165
H	-0.12686	-2.48607	-1.28241
H	-1.28605	-2.38700	-2.73475

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C	1.00082	-1.78208	-1.87137
C	-0.32013	-2.49239	-1.59506
C	-0.27986	-3.95256	-2.12283
C	0.47955	0.71622	-3.03436
C	1.90252	0.71020	-2.85429

H	1.84719	-2.17586	-1.28381
H	1.25582	-1.78922	-2.94430
H	-0.53679	-2.49837	-0.51408
H	-1.15395	-1.95078	-2.07259
H	0.52635	-4.53264	-1.64003
H	-0.10976	-3.97871	-3.21364
H	-1.23815	-4.45903	-1.91452
H	2.52577	-0.03701	-3.35742
H	2.43700	1.63440	-2.60191
H	-0.10253	1.63550	-2.88866
H	-0.00733	-0.02602	-3.67563
Ni	0.96725	0.06964	-1.23978
O	-0.64615	0.17446	-0.18113
C	1.68962	-0.10514	1.60024
N	2.14838	0.04029	0.36162
C	-2.13397	-0.02975	1.67841
C	-0.80108	-0.01585	1.12583
C	0.32089	-0.19663	2.02276
C	0.07915	-0.40819	3.41422
C	-1.21283	-0.44530	3.92462
C	-2.31197	-0.24984	3.04897
C	4.08318	1.51993	-0.05185
C	3.58292	0.20553	0.19358
C	4.45668	-0.91644	0.26142
C	5.83653	-0.69799	0.05312
C	6.34213	0.58159	-0.20933
C	5.46825	1.67940	-0.25443
C	3.96494	-2.33335	0.57847
C	4.42057	-3.36364	-0.48542
C	4.41848	-2.78015	1.99394
C	3.15756	2.73999	-0.00983
C	3.55839	3.85765	-1.00025
C	3.06945	3.31078	1.43255
C	-3.82154	-2.27207	0.77577
C	-4.11596	-0.92105	0.37832
C	-3.31407	0.18613	0.77973
C	-3.64248	1.50194	0.34449
C	-2.87429	2.65267	0.73362
C	-3.21697	3.92284	0.30388
C	-4.35286	4.12492	-0.54245
C	-5.12264	3.04629	-0.93740
C	-4.80126	1.71185	-0.51246
C	-5.58559	0.60781	-0.89958
C	-5.27585	-0.69889	-0.47649
C	-6.07772	-1.82447	-0.87024
C	-5.76216	-3.10589	-0.45767
C	-4.61807	-3.32985	0.37180
H	2.43482	-0.13651	2.41349
H	0.93988	-0.53830	4.07992
H	-1.38579	-0.60986	4.99073
H	-3.33068	-0.26382	3.44862
H	6.52370	-1.54816	0.10113
H	7.41396	0.72660	-0.37119
H	5.87095	2.67783	-0.44427
H	2.86061	-2.31889	0.57504
H	4.10944	-3.05707	-1.49806
H	5.51839	-3.48084	-0.48967
H	5.52024	-2.81631	2.06057
H	4.02839	-3.78705	2.22445
H	4.05844	-2.08366	2.77029
H	2.14254	2.39428	-0.28582
H	4.50399	4.34586	-0.70543
H	2.77942	4.63918	-1.01952
H	3.68221	3.46973	-2.02561
H	4.06139	3.66043	1.76957
H	2.71624	2.54931	2.14772
H	2.37057	4.16497	1.46738
H	-2.94753	-2.45231	1.40597
H	-2.00626	2.50839	1.38110
H	-2.61719	4.78371	0.61289
H	-4.60876	5.13579	-0.87205
H	-5.99599	3.18985	-1.58183
H	-6.45826	0.76946	-1.54220
H	-6.94832	-1.64326	-1.50891
H	-6.38196	-3.95297	-0.76469
H	-4.37344	-4.34818	0.68722
H	3.98052	-4.35332	-0.27118

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82

Ni	0.76230	0.01501	-1.04577
O	-0.87197	-0.00651	-0.13121
C	1.32132	-0.38292	1.77863
N	1.85207	-0.19056	0.57081
C	-2.47640	-0.14212	1.62153
C	-1.10910	-0.16264	1.17250
C	-0.06274	-0.36273	2.13993
C	-0.40231	-0.54951	3.51427
C	-1.72658	-0.53066	3.93599
C	-2.75600	-0.32486	2.98117
C	4.03749	0.96336	0.83255
C	3.30781	-0.22174	0.53037
C	3.96464	-1.43919	0.19529
C	5.37524	-1.44885	0.17600
C	6.11334	-0.29041	0.46526
C	5.44766	0.90100	0.78898
C	3.17161	-2.71957	-0.08532
C	3.71698	-3.51434	-1.29568
C	3.11662	-3.62290	1.17581
C	3.33297	2.25946	1.25460
C	3.89217	3.51532	0.54364
C	3.39884	2.44613	2.79487
C	-4.00139	-2.41164	0.53977
C	-4.31150	-1.06382	0.14401
C	-3.58388	0.05953	0.63101
C	-3.91485	1.37189	0.18909
C	-3.21011	2.53621	0.65107
C	-3.54966	3.80260	0.20784
C	-4.62024	3.98610	-0.72390
C	-5.32755	2.89359	-1.19124
C	-5.00514	1.56192	-0.75826
C	-5.72156	0.44212	-1.22427
C	-5.40493	-0.86247	-0.79897
C	-6.13423	-2.00570	-1.27458
C	-5.80767	-3.28387	-0.86011
C	-4.72532	-3.48671	0.05381
C	-0.28077	-0.31843	-2.66998
C	1.07599	-0.60465	-3.06201
C	2.27284	0.86563	-2.35035
C	3.63443	0.43005	-2.90975
C	4.57601	1.63173	-3.15231
H	2.02338	-0.57272	2.60541
H	0.40710	-0.70417	4.23664
H	-1.97811	-0.67119	4.98982
H	-3.80093	-0.30819	3.30607
H	5.90210	-2.37583	-0.06785
H	7.20651	-0.31807	0.44319
H	6.03095	1.79680	1.02167
H	2.13485	-2.41395	-0.32257
H	3.78585	-2.88053	-2.19603
H	3.04859	-4.36357	-1.52080
H	4.72028	-3.93011	-1.09548
H	4.13268	-3.93809	1.47326
H	2.51823	-4.52895	0.97540
H	2.66153	-3.09360	2.02962
H	2.26749	2.16557	0.97465
H	4.94295	3.71045	0.82085
H	3.30374	4.40329	0.83266
H	3.84053	3.41395	-0.55316
H	4.44731	2.53279	3.13131
H	2.94257	1.59423	3.32565
H	2.86319	3.36389	3.09427
H	-3.17286	-2.57403	1.23329
H	-2.39189	2.40290	1.36276
H	-2.99760	4.67416	0.57100
H	-4.87596	4.99442	-1.06163
H	-6.15025	3.02408	-1.90181
H	-6.54448	0.58972	-1.93262
H	-6.95719	-1.84046	-1.97757
H	-6.37097	-4.14490	-1.23078
H	-4.46907	-4.50293	0.36676
H	-0.95023	-1.11455	-2.33289
H	1.48714	-1.59983	-2.84365
H	1.43096	-0.23741	-4.03188
H	2.40376	1.30271	-1.34053
H	1.79166	1.63111	-2.98125
H	4.11531	-0.27866	-2.21420
H	3.49933	-0.10706	-3.86878
H	4.12637	2.35327	-3.85765
H	4.79657	2.16390	-2.21198
H	5.53604	1.29322	-3.57913
H	-0.78481	0.55284	-3.10425

Salicylaldiminato_7a

82

Ni	0.84297	0.16087	-1.15576
O	-0.79904	0.07234	-0.13783
C	1.45941	0.15951	1.67791
N	1.96705	0.14980	0.44065
C	-2.34314	-0.04726	1.68296
C	-0.99887	0.03606	1.17254
C	0.09821	0.08923	2.10361
C	-0.16889	0.07774	3.50768
C	-1.47029	0.00108	3.98709
C	-2.55010	-0.06424	3.06603
C	4.03038	1.48485	0.10377
C	3.42872	0.23057	0.41032
C	4.21293	-0.91939	0.70864
C	5.61927	-0.78002	0.69600
C	6.22907	0.44600	0.39971
C	5.43738	1.56693	0.10667
C	3.59387	-2.27548	1.07394
C	4.26921	-3.45915	0.33628
C	3.64639	-2.52367	2.60650
C	3.17730	2.72500	-0.17598
C	3.74673	3.61244	-1.30733
C	2.97036	3.55537	1.11900
C	-3.28786	-2.60169	0.57872
C	-3.92969	-1.36674	0.21784
C	-3.49676	-0.10962	0.72681
C	-4.15858	1.08811	0.33374
C	-3.74940	2.38282	0.80792
C	-4.40901	3.53308	0.41031
C	-5.52176	3.46247	-0.48669
C	-5.94686	2.23824	-0.96921
C	-5.28767	1.02050	-0.58528
C	-5.70796	-0.23107	-1.07594
C	-5.05931	-1.42388	-0.70076

C	-5.48587	-2.70160	-1.20098
C	-4.83944	-3.86557	-0.82720
C	-3.72738	-3.81228	0.07186
H	2.19276	0.23375	2.49480
H	0.67587	0.12627	4.20377
H	-1.66819	-0.01054	5.06138
H	-3.57653	-0.12739	3.44045
H	6.24361	-1.64879	0.92305
H	7.31962	0.52935	0.39715
H	5.91965	2.52088	-0.12260
H	2.53150	-2.25284	0.76997
H	4.30503	-3.29312	-0.75251
H	5.30276	-3.62048	0.68966
H	4.69304	-2.54364	2.95853
H	3.18132	-3.49382	2.85451
H	3.11705	-1.73755	3.16978
H	2.18338	2.36584	-0.50537
H	4.69748	4.09346	-1.01675
H	3.03180	4.41906	-1.54543
H	3.92452	3.02629	-2.22461
H	3.93750	3.92564	1.50334
H	2.49721	2.95244	1.91239
H	2.32188	4.42637	0.91816
H	-2.43759	-2.56683	1.26417
H	-2.90044	2.44298	1.49340
H	-4.07974	4.50730	0.78275
H	-6.03220	4.38150	-0.78793
H	-6.79643	2.17431	-1.65678
H	-6.55870	-0.27789	-1.76490
H	-6.33767	-2.73248	-1.88807
H	-5.17387	-4.83139	-1.21614
H	-3.22236	-4.73927	0.35772
H	3.70690	-4.38977	0.52637
C	-0.13003	1.42259	-2.44357
C	-0.44196	0.09997	-2.78486
H	-0.79756	1.99264	-1.79138
H	-1.34427	-0.37043	-2.38876
H	0.03595	-0.38944	-3.63771
H	0.59989	2.00178	-3.01700
C	2.32115	-0.10368	-2.40741
C	2.48143	-1.61562	-2.62992
C	3.66928	-1.95002	-3.56892
H	3.23284	0.33737	-1.97205
H	2.10701	0.41221	-3.36254
H	3.76535	-3.04035	-3.71943
H	3.53120	-1.48093	-4.55914
H	4.61823	-1.57508	-3.14711
H	2.63711	-2.12544	-1.66118
H	1.55299	-2.04297	-3.05531

Salicylaldiminato_7b_TS

82

Ni	1.08756	-0.20007	-1.09253
O	-0.53060	-0.00440	-0.07232
C	1.83089	0.17281	1.63358
N	2.25023	-0.00710	0.37990
C	-1.96926	0.40581	1.79539
C	-0.65553	0.23768	1.22993
C	0.48921	0.32236	2.10559
C	0.29435	0.55301	3.50128
C	-0.98030	0.70784	4.03306
C	-2.10407	0.63409	3.17055
C	4.47641	1.09277	0.19386
C	3.69767	-0.09672	0.20932
C	4.29154	-1.38058	0.05637
C	5.69300	-1.45052	-0.08006
C	6.48334	-0.29008	-0.07732
C	5.87607	0.96629	0.05255
C	3.44129	-2.65328	0.08032
C	3.90404	-3.71016	-0.94891
C	3.39227	-3.26359	1.50665
C	3.84691	2.48515	0.32447
C	4.30188	3.44227	-0.80626
C	4.14484	3.11110	1.71252
C	-3.60579	-2.03526	1.62190
C	-3.96836	-0.85370	0.88544
C	-3.18447	0.33546	0.91955
C	-3.57338	1.46894	0.14936
C	-2.81590	2.69065	0.14962
C	-3.21467	3.78147	-0.60323
C	-4.40125	3.72208	-1.40101
C	-5.16246	2.56787	-1.42708
C	-4.78175	1.41206	-0.66268
C	-5.55284	0.23311	-0.67612
C	-5.17941	-0.89828	0.07481
C	-5.96460	-2.10182	0.06019
C	-5.58292	-3.21195	0.79093
C	-4.38651	-3.17740	1.57536
C	2.41105	0.07135	-2.50040
C	1.11593	0.35324	-3.08936
C	-0.14478	-1.18116	-2.51551
C	-1.51343	-0.67709	-2.96070
C	-2.52028	-1.83893	-3.13270
H	2.61422	0.21817	2.40525
H	1.17530	0.61014	4.15030
H	-1.12120	0.88716	5.10143
H	-3.11068	0.75914	3.58161
H	6.17256	-2.42717	-0.18898
H	7.56946	-0.36652	-0.18096
H	6.49554	1.86814	0.04254
H	2.40996	-2.35447	-0.19150
H	3.96932	-3.27989	-1.96263
H	3.18615	-4.54830	-0.97510
H	4.89183	-4.13201	-0.69170
H	4.40309	-3.56140	1.83826
H	2.74604	-4.15892	1.52074
H	2.99302	-2.54165	2.23887
H	2.75205	2.36782	0.23521
H	5.38327	3.65736	-0.74794
H	3.76560	4.40392	-0.72679
H	4.09545	3.01458	-1.80205
H	5.23162	3.24800	1.85517
H	3.77576	2.47133	2.53175
H	3.65992	4.09891	1.80287
H	-2.69229	-2.01639	2.22094
H	-1.91102	2.74239	0.75942
H	-2.62180	4.70044	-0.58913
H	-4.70271	4.59494	-1.98693
H	-6.07348	2.51383	-2.03195
H	-6.46467	0.19630	-1.28273
H	-6.87478	-2.12033	-0.54800
H	-6.18958	-4.12162	0.77002
H	-4.08858	-4.06487	2.14087
H	3.05159	0.89768	-2.17498
H	0.68172	1.35237	-2.93563
H	0.87540	-0.02832	-4.08718
H	-0.22320	-1.71814	-1.54634
H	0.34118	-1.85761	-3.23599
H	-1.89214	0.02708	-2.20137
H	-1.42858	-0.12463	-3.91682
H	-2.17138	-2.56616	-3.88804
H	-2.66685	-2.37624	-2.18051
H	-3.50311	-1.45555	-3.45585
H	2.96512	-0.80397	-2.86359

Salicylaldiminato_7b

82

Ni	-0.93878	-0.13229	-1.22159
O	0.57763	0.07317	-0.10562
C	-1.79339	0.20567	1.60135
N	-2.20106	0.03755	0.34667
C	2.00320	0.40713	1.77639
C	0.68803	0.26454	1.21041
C	-0.45183	0.33191	2.08349
C	-0.26060	0.53104	3.48351
C	1.01479	0.66627	4.01947
C	2.13853	0.60329	3.15682
C	-4.28242	-1.31142	0.18382
C	-3.65104	-0.03409	0.19111
C	-4.40014	1.16929	0.05421
C	-5.80065	1.06465	-0.09193
C	-6.43988	-0.18326	-0.10239
C	-5.68447	-1.35770	0.03565
C	-3.73354	2.54982	0.11395
C	-4.26770	3.52490	-0.96404
C	-3.88998	3.18248	1.52374
C	-3.47532	-2.59922	0.38576
C	-3.96320	-3.77121	-0.49900
C	-3.47453	-3.02260	1.87989
C	2.90695	2.73694	0.22490
C	3.62753	1.49452	0.16778
C	3.21495	0.34271	0.89593
C	3.96653	-0.86430	0.81333
C	3.58332	-2.05975	1.51596
C	4.33309	-3.21934	1.42081
C	5.51618	-3.25890	0.61689
C	5.91668	-2.13524	-0.08245
C	5.16501	-0.91241	-0.01518
C	5.55963	0.23502	-0.73005
C	4.82401	1.43442	-0.66108
C	5.22987	2.60738	-1.38504
C	4.50516	3.78222	-1.30303
C	3.33060	3.84492	-0.48820
C	-2.20413	0.57061	-2.62974
C	-2.30118	-0.83149	-2.56496
C	0.43651	-0.41757	-2.60576
C	1.03488	-1.81739	-2.44525
C	2.19682	-2.06743	-3.44274
H	-2.57484	0.26105	2.37569
H	-1.14289	0.57793	4.13148
H	1.15598	0.82129	5.09158
H	3.14538	0.71240	3.57149
H	-6.39744	1.97523	-0.19560
H	-7.52616	-0.24130	-0.21540
H	-6.19167	-2.32638	0.03108
H	-2.65285	2.40516	-0.06931
H	-4.20914	3.08803	-1.97520
H	-5.31936	3.80421	-0.77689
H	-4.95696	3.33612	1.76429
H	-3.38294	4.16241	1.56300
H	-3.45558	2.54052	2.30804
H	-2.42963	-2.37717	0.10060
H	-4.96172	-4.12902	-0.19205
H	-3.26739	-4.62295	-0.40863

H	-4.01653	-3.48407	-1.56273
H	-4.50201	-3.24136	2.22110
H	-3.06375	-2.22885	2.52587
H	-2.86207	-3.93024	2.02145
H	2.00907	2.79287	0.84490
H	2.67979	-2.03815	2.12996
H	4.02016	-4.11688	1.96177
H	6.09771	-4.18302	0.55578
H	6.81721	-2.15753	-0.70470
H	6.46109	0.19464	-1.35162
H	6.13088	2.54976	-2.00426
H	4.82558	4.66795	-1.85869
H	2.76522	4.77939	-0.43098
H	-3.67344	4.45483	-0.95706
H	-2.94929	1.19289	-2.12652
H	-3.12824	-1.29737	-2.02226
H	-1.79824	-1.46940	-3.29689
H	-1.62454	1.06942	-3.41178
H	1.15885	0.37716	-2.35604
H	0.03570	-0.26278	-3.62511
H	2.61806	-3.07992	-3.31125
H	1.85207	-1.97214	-4.48818
H	3.00831	-1.33697	-3.28333
H	1.41071	-1.93792	-1.41479
H	0.25758	-2.59237	-2.60188

Pyrazolonato-phosphane catalyst (IV)

Pyrazolonato-phosphane_1a_2a_TS

68

P	1.19303	-0.44074	0.01366
O	-1.60171	0.56991	0.67235
C	-0.33879	-1.13897	-0.57880
C	-1.52109	-0.47606	-0.12553
C	2.17634	-1.86634	0.70468
C	1.50250	-2.74463	1.58890
C	2.17857	-3.82914	2.17206
C	3.53955	-4.05031	1.88589
C	4.21574	-3.18470	1.00886
C	3.54040	-2.09849	0.42035
C	2.23980	0.15030	-1.40503
C	1.88178	-0.11339	-2.74598
C	2.67579	0.37001	-3.80328
C	3.83425	1.12055	-3.53343
C	4.19181	1.39987	-2.20019
C	3.39566	0.92536	-1.14268
Ni	0.39834	1.16111	1.21429
C	1.46410	0.71022	2.77502
C	0.40232	1.55636	3.41475
P	0.13940	3.09307	-0.04174
C	-0.44132	2.85079	-1.79652
C	1.54419	4.30370	-0.29454
C	-1.19852	4.23086	0.60035
C	-0.58303	0.82639	4.34483
H	0.44129	-2.58270	1.80113
H	1.64206	-4.50262	2.84620
H	4.06591	-4.89449	2.33955
H	5.27000	-3.35610	0.77349
H	4.07599	-1.44557	-0.27271
H	0.97147	-0.67976	-2.95759
H	2.38602	0.16058	-4.83674
H	4.45063	1.49382	-4.35571
H	5.08581	1.99209	-1.98462
H	3.65917	1.16938	-0.10902
H	2.48144	1.12553	2.72817
H	1.46106	-0.35359	3.04977
H	-0.25403	2.05641	2.56901
H	-0.66568	3.81668	-2.28177
H	-1.34862	2.22673	-1.78406
H	0.33597	2.32493	-2.37345
H	1.91455	4.64627	0.68603
H	1.22942	5.18001	-0.88837
H	2.36891	3.79137	-0.81666
H	-0.91756	4.61079	1.59723
H	-2.12790	3.64694	0.69845
H	-1.37299	5.08765	-0.07389
H	-1.01553	-0.04901	3.83397
H	-1.41450	1.48365	4.64927
H	-0.06412	0.48185	5.25530
H	0.82561	2.46448	3.88289
N	-2.59283	-1.19778	-0.67364
N	-2.12766	-2.31895	-1.42638
C	-0.78166	-2.27244	-1.34658
C	0.02136	-3.36267	-1.98876
C	-4.87742	-1.82078	-1.26798
C	-3.99033	-0.97140	-0.56682
C	-4.49849	0.08448	0.22572
C	-5.88793	0.28129	0.30174
C	-6.77773	-0.55679	-0.39396
C	-6.26079	-1.60771	-1.17591
H	0.58058	-3.94435	-1.23465
H	0.76091	-2.97041	-2.70854
H	-0.65874	-4.04469	-2.52183
H	-3.80098	0.72411	0.76754
H	-6.27477	1.09935	0.91685
H	-7.85723	-0.39583	-0.32722
H	-6.93996	-2.26961	-1.72137
H	-4.45939	-2.63032	-1.86696

Pyrazolonato-phosphane_1a

68

Ni	0.27165	1.43076	0.15421
P	-0.84024	3.32861	0.35769
P	1.14677	-0.61838	0.08859
O	-1.54717	0.59833	0.00068
C	-0.36545	-1.55761	-0.07134
C	-1.51925	-0.73220	-0.07926
C	2.06643	-1.18996	1.59555
C	1.93793	-0.43247	2.78253
C	2.54976	-0.86299	3.97311
C	3.30091	-2.05217	3.98931
C	3.44089	-2.80870	2.81068
C	2.82911	-2.38145	1.61885
C	2.26558	-1.06831	-1.31801
C	1.70849	-1.53330	-2.53285
C	2.53404	-1.78946	-3.64173
C	3.92290	-1.58006	-3.55465
C	4.48459	-1.11240	-2.35233
C	3.66342	-0.85631	-1.23985
C	-1.93434	3.68343	-1.10340
C	-2.04343	3.25010	1.77140
C	-0.00348	4.96699	0.64147
C	2.03001	2.29202	0.18177
C	2.39930	2.79128	-1.22994
C	3.79056	3.46958	-1.28076
H	1.35601	0.49466	2.76120
H	2.44263	-0.26860	4.88474
H	3.77785	-2.38689	4.91458
H	4.02638	-3.73239	2.81852
H	2.94996	-2.97132	0.70656
H	0.62893	-1.69480	-2.60099
H	2.09123	-2.15448	-4.57260
H	4.56358	-1.78074	-4.41767
H	5.56324	-0.94809	-2.27798
H	4.11108	-0.50089	-0.30799
H	2.80032	1.58140	0.54321
H	2.01630	3.13243	0.90481
H	2.38616	1.94541	-1.94297
H	1.63572	3.50652	-1.59686
H	4.57936	2.76353	-0.96650
H	3.83224	4.34147	-0.60311
H	4.03287	3.81731	-2.30105
H	0.69804	5.18085	-0.18049
H	0.56607	4.93665	1.58407
H	-0.74981	5.77700	0.69889
H	-1.31082	3.90830	-1.98378
H	-2.52220	2.77808	-1.31705
H	-2.60994	4.53395	-0.90808
H	-1.48751	3.20797	2.72212
H	-2.62574	2.32232	1.66832
H	-2.71800	4.12348	1.78285
N	-2.61697	-1.58722	-0.17853
N	-2.19020	-2.95363	-0.22360
C	-0.84298	-2.90867	-0.15236
C	-0.06530	-4.18785	-0.15781
H	0.49915	-4.31650	0.78274
H	0.66141	-4.21772	-0.98882
H	-0.75840	-5.03592	-0.26682
C	-4.92452	-2.37737	-0.26949
C	-4.00746	-1.30219	-0.22931
C	-4.47920	0.03012	-0.24286
C	-5.86226	0.27353	-0.29380
C	-6.78167	-0.78970	-0.33321
C	-6.30114	-2.11321	-0.32141
H	-3.75918	0.84775	-0.21356
H	-6.22057	1.30726	-0.30413
H	-7.85611	-0.59141	-0.37329
H	-7.00388	-2.95089	-0.35222
H	-4.53376	-3.39508	-0.26106

Pyrazolonato-phosphane_3b_TS$_{BHE}$

68

P	1.21192	-0.37764	0.03429
O	-1.55903	0.55075	-0.68511
C	-0.30295	-1.17789	0.54318
C	-1.48236	-0.53705	0.06150
C	2.28914	-0.26063	1.55383
C	1.66976	-0.12890	2.81979
C	2.44348	0.00801	3.98596
C	3.84811	0.01902	3.90693
C	4.47352	-0.11264	2.65392
C	3.70184	-0.25239	1.48637

C	2.17659	-1.53367	-1.06819
C	1.77987	-2.87899	-1.23658
C	2.49245	-3.73178	-2.09969
C	3.60968	-3.25268	-2.80668
C	4.00257	-1.90901	-2.66130
C	3.28608	-1.05367	-1.80559
N	-2.55783	-1.28310	0.55954
N	-2.09768	-2.37959	1.35089
C	-0.75035	-2.29801	1.32962
C	0.04278	-3.30683	2.10480
C	-4.84885	-1.96783	1.05237
C	-3.95559	-1.08975	0.39621
C	-4.45706	-0.03946	-0.40737
C	-5.84667	0.12127	-0.54265
C	-6.74277	-0.74633	0.10709
C	-6.23218	-1.78992	0.90277
H	0.57847	-0.14635	2.88590
H	1.94698	0.09896	4.95625
H	4.44966	0.12180	4.81414
H	5.56492	-0.11581	2.58292
H	4.20732	-0.37789	0.52619
H	0.89464	-3.24757	-0.71332
H	2.16828	-4.76886	-2.22325
H	4.16183	-3.91632	-3.47757
H	4.85837	-1.52343	-3.22287
H	3.57509	-0.00011	-1.73250
H	0.62194	-2.83232	2.91646
H	0.76538	-3.84706	1.46876
H	-0.64767	-4.03956	2.55004
H	-3.75531	0.62746	-0.90882
H	-6.22809	0.93516	-1.16652
H	-7.82226	-0.61329	-0.00522
H	-6.91626	-2.47414	1.41333
H	-4.43569	-2.77124	1.66280
Ni	0.33901	1.38332	-1.03490
C	-0.39445	2.35987	-2.62643
C	0.49961	1.34499	-3.13410
C	-0.02032	0.01798	-3.66796
P	0.18566	3.19328	0.29783
C	0.41078	3.09491	2.14771
C	-1.48681	4.01463	0.21599
C	1.32551	4.61715	-0.10996
H	-0.11148	3.41406	-2.72856
H	-1.46890	2.15371	-2.58971
H	1.53774	1.26009	-1.92028
H	0.73984	-0.77598	-3.59272
H	-0.29131	0.12466	-4.73687
H	-0.91462	-0.30315	-3.11215
H	1.37963	1.72298	-3.68042
H	0.24727	4.07901	2.62074
H	1.42420	2.73784	2.38804
H	-0.31369	2.37331	2.55834
H	-1.70618	4.30195	-0.82453
H	-1.53819	4.90947	0.86022
H	-2.24837	3.28457	0.53336
H	1.21137	4.88523	-1.17314
H	2.36866	4.30060	0.05435
H	1.11277	5.50501	0.51072

Pyrazolonato-phosphane_2a_3b_TS

68

P	1.29631	-0.35446	0.09408
O	-1.59005	0.59867	0.52423
C	-0.18543	-1.16765	-0.49883
C	-1.41412	-0.52343	-0.15582
C	2.28338	-1.68822	0.94902
C	1.58620	-2.60475	1.77552
C	2.27981	-3.58883	2.50106
C	3.68209	-3.67397	2.41876
C	4.38343	-2.77057	1.60037
C	3.69232	-1.78525	0.87173
C	2.37550	0.08862	-1.35835
C	2.09251	-0.34265	-2.67443
C	2.90722	0.05748	-3.75009
C	4.01757	0.89235	-3.52725
C	4.30229	1.33956	-2.22335
C	3.48145	0.94993	-1.14912
Ni	0.26877	1.35808	1.22264
C	0.17149	0.32077	2.94183
C	0.03806	1.70740	3.29295
P	0.03086	2.96166	-0.25063
C	-0.38228	2.44846	-1.98638
C	1.40106	4.19123	-0.51448
C	-1.41479	4.05342	0.17195
C	-1.31980	2.32511	3.59464
H	0.49512	-2.55569	1.82957
H	1.72190	-4.29165	3.12647
H	4.22144	-4.44032	2.98208
H	5.47252	-2.83496	1.52033
H	4.25518	-1.10561	0.22751
H	1.22056	-0.97563	-2.85532
H	2.67297	-0.28458	-4.76222
H	4.65155	1.19881	-4.36368
H	5.15781	1.99720	-2.04340
H	3.68787	1.32794	-0.14241
H	1.09204	-0.21293	3.19636
H	-0.73162	-0.29339	2.85654
H	0.82506	2.46522	2.06080
H	-0.64226	3.32963	-2.59810
H	-1.23627	1.75550	-1.95244
H	0.47630	1.92871	-2.43829
H	1.65112	4.67360	0.44415
H	1.10765	4.96213	-1.24724
H	2.29381	3.66204	-0.88416
H	-1.23098	4.55672	1.13428
H	-2.30724	3.41649	0.27149
H	-1.58621	4.81152	-0.61162
H	-2.10526	1.87557	2.96765
H	-1.32174	3.41543	3.42993
H	-1.58123	2.14963	4.65651
H	0.86167	2.12868	3.88990
N	-2.43391	-1.34443	-0.65860
N	-1.89434	-2.50780	-1.28341
C	-0.55535	-2.38709	-1.16934
C	0.31422	-3.49706	-1.67804
C	-4.66285	-2.13723	-1.25857
C	-3.84410	-1.17833	-0.61779
C	-4.43267	-0.07820	0.04827
C	-5.83207	0.05181	0.06229
C	-6.65357	-0.89587	-0.57371
C	-6.05734	-1.98916	-1.23122
H	0.93161	-3.92217	-0.86767
H	1.00710	-3.16187	-2.46957
H	-0.32427	-4.29338	-2.09046
H	-3.78794	0.64816	0.54333
H	-6.28071	0.90460	0.58064
H	-7.74139	-0.78647	-0.55660
H	-6.68276	-2.73596	-1.72912
H	-4.18365	-2.97829	-1.76028

Pyrazolonato-phosphane_2a

68

P	1.24897	-0.37843	0.08388
O	-1.65779	0.68019	0.54639
C	-0.27307	-1.08292	-0.52411
C	-1.49213	-0.41125	-0.16483
C	2.20350	-1.78336	0.85621
C	1.48317	-2.74693	1.60390
C	2.15355	-3.79897	2.25146
C	3.55395	-3.90649	2.16486
C	4.27777	-2.95743	1.42143
C	3.60975	-1.90351	0.77150
C	2.34246	0.12488	-1.33909
C	2.04591	-0.24330	-2.67049
C	2.88074	0.16632	-3.72717
C	4.02097	0.94827	-3.46738
C	4.31669	1.33448	-2.14628
C	3.47756	0.93440	-1.09028
Ni	0.44343	1.25923	1.25548
C	0.39068	0.18434	2.86961
C	-0.01719	1.52046	3.40386
P	0.25879	2.99713	-0.12475
C	-0.18159	2.65306	-1.89555
C	1.64215	4.23564	-0.30015
C	-1.16719	4.07695	0.39880
C	-1.46376	1.63365	3.91951
H	0.39354	-2.67812	1.65920
H	1.57937	-4.53702	2.81857
H	4.07511	-4.72602	2.66713
H	5.36541	-3.03855	1.33887
H	4.18851	-1.18689	0.18441
H	1.14762	-0.82945	-2.87793
H	2.63717	-0.12496	-4.75274
H	4.66989	1.26310	-4.28911
H	5.19500	1.95273	-1.93906
H	3.68996	1.26494	-0.06834
H	1.36367	-0.21168	3.18514
H	-0.39949	-0.57704	2.82042
H	0.05948	2.33704	2.53008
H	-0.44103	3.58852	-2.42012
H	-1.04273	1.96802	-1.91172
H	0.66424	2.16986	-2.40735
H	1.92841	4.61078	0.69599
H	1.33986	5.08530	-0.93650
H	2.51640	3.73984	-0.75183
H	-0.95814	4.52295	1.38527
H	-2.05914	3.43654	0.48105
H	-1.35492	4.88443	-0.32965
H	-2.16253	1.25153	3.15849
H	-1.73411	2.67722	4.15474
H	-1.58087	1.03257	4.83688
H	0.72293	1.93158	4.11256
N	-2.52286	-1.19707	-0.71828
N	-2.00340	-2.34485	-1.38457
C	-0.66506	-2.26465	-1.24987
C	0.17929	-3.37661	-1.79686
H	0.72403	-3.90017	-0.99150
H	0.93627	-3.01877	-2.51619
H	-0.47267	-4.10181	-2.30779
C	-4.76324	-1.93735	-1.34500
C	-3.92920	-1.00344	-0.68619
C	-4.50209	0.09948	-0.01013
C	-5.89878	0.25529	-0.00246
C	-6.73481	-0.66813	-0.65508
C	-6.15481	-1.76306	-1.32438
H	-3.84581	0.80729	0.49604

H	-6.33388	1.11046	0.52365
H	-7.82054	-0.53865	-0.64229
H	-6.79093	-2.49122	-1.83639
H	-4.29769	-2.78010	-1.85663

Pyrazolonato-phosphane_3b

68

P	1.34252	-0.37600	0.09009
O	-1.52059	0.47530	0.54770
C	-0.10108	-1.23871	-0.52493
C	2.37851	-1.65493	0.96202
C	1.71581	-2.52718	1.86103
C	2.43926	-3.47607	2.60267
C	3.83687	-3.56857	2.46309
C	4.50318	-2.71077	1.57052
C	3.78156	-1.76063	0.82420
C	2.40656	0.15219	-1.33922
C	2.11161	-0.21665	-2.67134
C	2.90520	0.25161	-3.73517
C	4.00377	1.09354	-3.48353
C	4.29791	1.48023	-2.16210
C	3.49965	1.02202	-1.09871
Ni	0.21213	1.27152	1.18897
C	0.10883	0.44713	3.08440
C	-0.47317	1.72623	3.16248
P	-0.07344	3.06335	-0.10068
C	-0.39567	2.69745	-1.89600
C	1.29000	4.32524	-0.19961
C	-1.54969	4.11843	0.32045
C	-1.96827	1.94100	3.27390
H	0.62875	-2.47101	1.96301
H	1.90992	-4.14464	3.28743
H	4.39960	-4.30659	3.04114
H	5.58753	-2.78293	1.44643
H	4.31495	-1.11483	0.12285
H	1.24731	-0.85413	-2.87301
H	2.66356	-0.04292	-4.76033
H	4.62139	1.45340	-4.31084
H	5.14337	2.14428	-1.96012
H	3.71441	1.35201	-0.07719
H	1.13381	0.27006	3.42179
H	-0.53513	-0.43738	3.02451
H	1.48182	1.88231	1.54591
H	-0.63996	3.61967	-2.45115
H	-1.23797	1.99193	-1.96719
H	0.49385	2.22658	-2.34255
H	1.49322	4.72289	0.80789
H	1.02404	5.15656	-0.87443
H	2.20385	3.83415	-0.57065
H	-1.41838	4.55813	1.32186
H	-2.44488	3.47743	0.33243
H	-1.68795	4.92838	-0.41687
H	-2.52102	1.15404	2.73872
H	-2.28109	2.91829	2.87118
H	-2.27434	1.91641	4.33937
H	0.15569	2.55379	3.51649
C	-1.33593	-0.62543	-0.17825
N	-2.34195	-1.43460	-0.71244
N	-1.78128	-2.57465	-1.36664
C	-0.44434	-2.44196	-1.23402
C	0.45068	-3.52063	-1.76352
C	-4.55782	-2.26152	-1.31519
C	-3.75490	-1.28493	-0.68238
C	-4.35853	-0.18139	-0.03700
C	-5.75927	-0.06705	-0.03215
C	-6.56603	-1.03318	-0.65905
C	-5.95398	-2.12829	-1.29866
H	1.02101	-3.99887	-0.94786
H	1.18742	-3.13439	-2.48917
H	-0.16165	-4.28844	-2.26055
H	-3.72652	0.56127	0.45014
H	-6.22028	0.78831	0.47060
H	-7.65500	-0.93607	-0.64916
H	-6.56800	-2.88857	-1.79012
H	-4.06609	-3.10268	-1.80436

Pyrazolonato-phosphane_7a_7b_TS

61

Ni	0.15045	1.46240	-1.33432
C	2.20869	0.17996	1.33513
C	1.62960	0.28233	2.62075
C	2.38227	0.77450	3.70316
C	3.71904	1.16916	3.51575
C	4.30288	1.07390	2.23759
C	3.55315	0.58936	1.15255
C	2.16559	-1.71811	-0.90041
C	3.13991	-2.47593	-0.21051
C	3.81187	-3.52801	-0.85957
C	3.51770	-3.83876	-2.19964
C	2.54768	-3.09189	-2.89354
C	1.88052	-2.03566	-2.25025
C	-0.32737	3.09893	-0.35918
C	0.79917	4.10656	-0.18007
C	0.37706	5.22411	0.81466
C	1.57484	2.08524	-2.60074
C	0.28774	2.53958	-3.00453
H	0.58922	-0.02231	2.76518
H	1.92246	0.84577	4.69283
H	4.30285	1.54995	4.35808
H	5.34129	1.38122	2.08473
H	4.01428	0.52405	0.16249
H	3.37438	-2.24493	0.83157
H	4.56218	-4.10774	-0.31454
H	4.04147	-4.65728	-2.70061
H	2.31377	-3.32792	-3.93529
H	1.12563	-1.45861	-2.79443
H	-0.60634	2.59757	0.58409
H	-1.22555	3.50844	-0.84897
H	1.70470	3.60636	0.20894
H	1.07433	4.57366	-1.14334
H	0.13428	4.80151	1.80450
H	-0.51185	5.76542	0.44798
H	1.19558	5.95321	0.94480
H	-0.00078	3.58919	-2.90047
H	-0.29806	1.97728	-3.74435
H	2.02452	1.20105	-3.06770
H	2.29551	2.77418	-2.15141
P	1.19167	-0.33942	-0.12389
O	-1.56469	0.74121	-0.74900
C	-0.34593	-1.03207	0.47635
C	-1.50663	-0.34770	0.02475
N	-2.60256	-1.04594	0.52226
N	-2.17617	-2.18103	1.27902
C	-0.82736	-2.15354	1.23508
C	-0.04610	-3.22901	1.92378
C	-4.91120	-1.65655	1.02471
C	-3.99676	-0.80097	0.37008
C	-4.46675	0.27294	-0.41939
C	-5.85120	0.48131	-0.54105
C	-6.76984	-0.36367	0.10690
C	-6.28911	-1.43204	0.88766
H	0.62486	-2.81402	2.69653
H	0.58195	-3.78691	1.20748
H	-0.74071	-3.93390	2.40538
H	-3.74942	0.92247	-0.92159
H	-6.21020	1.31372	-1.15317
H	-7.84504	-0.19396	0.00415
H	-6.99151	-2.09874	1.39610
H	-4.51985	-2.47947	1.62324

Pyrazolonato-phosphane_7a

61

Ni	0.29296	1.81472	0.41538
P	0.98503	-0.31339	0.07542
O	-1.57300	1.17082	0.14774
C	-0.61332	-1.07561	-0.13817
C	-1.68025	-0.14158	-0.05556
N	-2.56806	-2.25770	-0.41249
C	1.88388	-1.09167	1.49759
C	1.88945	-0.42335	2.74300
C	2.49597	-1.01447	3.86554
C	3.10645	-2.27653	3.75330
C	3.11002	-2.94680	2.51551
C	2.50308	-2.35981	1.39152
C	2.03106	-0.71415	-1.39824
C	1.40760	-0.98999	-2.63827
C	2.18402	-1.21072	-3.78944
C	3.58822	-1.15325	-3.71862
C	4.21560	-0.87370	-2.49056
C	3.44436	-0.65302	-1.33574
C	2.11389	2.51092	0.38553
C	2.37050	3.00631	-1.05011
C	3.76578	3.66665	-1.20109
C	-0.52293	3.70801	0.75557
C	-0.35725	3.02839	1.96229
C	-1.22374	-2.35806	-0.35084
N	-2.85480	-0.86726	-0.22767
C	-0.58025	-3.70239	-0.49053
H	1.41696	0.56029	2.82243
H	2.49428	-0.48827	4.82396
H	3.57947	-2.73583	4.62544
H	3.58459	-3.92775	2.42467
H	2.51454	-2.88459	0.43289
H	0.31622	-1.03472	-2.69279
H	1.69058	-1.42921	-4.74035
H	4.19017	-1.32611	-4.61474
H	5.30644	-0.82900	-2.42931
H	3.94246	-0.44484	-0.38525
H	2.85873	1.74917	0.68438
H	2.17703	3.34426	1.11214
H	2.29560	2.16623	-1.76553
H	1.59559	3.73903	-1.34822
H	4.56715	2.94933	-0.95213
H	3.86690	4.53515	-0.52665
H	3.92840	4.01541	-2.23612
H	0.48102	3.25251	2.62925
H	-1.17909	2.44655	2.38990
H	-1.47418	3.66670	0.21874
H	0.18939	4.47552	0.43842
H	-0.06068	-3.99691	0.43861
H	0.16355	-3.71367	-1.30664
H	-1.35269	-4.45540	-0.70882

C	-5.23270	-1.40804	-0.32734
C	-4.21086	-0.43670	-0.23400
C	-4.53846	0.93556	-0.15317
C	-5.88970	1.32125	-0.16313
C	-6.91443	0.36250	-0.25522
C	-6.57521	-1.00147	-0.33782
H	-3.73868	1.67282	-0.08205
H	-6.13881	2.38450	-0.10015
H	-7.96273	0.67295	-0.26341
H	-7.36160	-1.75824	-0.41019
H	-4.94972	-2.45883	-0.39306

Pyrazolonato-phosphane_7b_TS

61

Ni	0.23137	1.69752	-0.66314
P	1.29978	-0.11745	-0.02520
O	-1.48092	0.71226	-0.43188
C	-0.09457	-1.19797	0.23518
C	-1.32773	-0.54727	-0.02585
C	2.29426	-0.01573	1.53740
C	2.01434	1.03728	2.43891
C	2.67999	1.11430	3.67460
C	3.63639	0.14254	4.02127
C	3.92239	-0.90815	3.12994
C	3.25616	-0.98986	1.89390
C	2.43755	-0.90363	-1.25792
C	1.91627	-1.83715	-2.18379
C	2.73935	-2.37594	-3.18848
C	4.08814	-1.98705	-3.28371
C	4.61339	-1.05490	-2.36946
C	3.79458	-0.51264	-1.36316
C	-1.08595	3.35354	-1.06009
C	-1.49528	3.77581	0.35464
C	-2.92390	4.37308	0.37855
C	0.93718	3.56756	-1.42785
C	1.91813	2.60711	-0.96928
H	1.26622	1.78935	2.16829
H	2.45324	1.93237	4.36374
H	4.15634	0.20306	4.98113
H	4.66373	-1.66662	3.39638
H	3.48650	-1.80821	1.20694
H	0.86654	-2.13507	-2.11138
H	2.32526	-3.09947	-3.89598
H	4.72654	-2.40747	-4.06539
H	5.66116	-0.74935	-2.43816
H	4.21522	0.20532	-0.65361
H	-1.70496	2.53733	-1.46998
H	-1.15500	4.20231	-1.75773
H	-1.45821	2.90900	1.03818
H	-0.78102	4.52780	0.74493
H	-3.66469	3.62771	0.04339
H	-2.99967	5.25306	-0.28494
H	-3.19948	4.69006	1.39931
H	2.50664	2.06586	-1.72107
H	2.46197	2.81733	-0.03919
H	0.88005	4.51636	-0.88219
H	0.83100	3.68491	-2.51218
N	-2.32940	-1.47768	0.23310
N	-1.76363	-2.71898	0.67084
C	-0.42800	-2.52491	0.66956
C	0.47865	-3.63605	1.09871
H	1.06101	-3.35462	1.99393
H	1.19788	-3.90291	0.30430
H	-0.12296	-4.52557	1.33980
C	-4.54429	-2.47113	0.48914
C	-3.74309	-1.36443	0.12819
C	-4.34459	-0.17099	-0.33094
C	-5.74492	-0.09745	-0.42281
C	-6.55135	-1.19281	-0.06564
C	-5.94035	-2.37684	0.38944
H	-3.71302	0.67390	-0.60603
H	-6.20583	0.82825	-0.77955
H	-7.64005	-1.12601	-0.14091
H	-6.55461	-3.23717	0.67047
H	-4.05279	-3.37951	0.83815